AB INITIO STUDIES OF A PENTACYCLO-UNDECANE CAGE LACTAM

by

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DECLARATION

I, Thishana Singh, declare that unless indicated, this dissertation is my own work and it has not been submitted for a degree at another Technikon or University.

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T. Singh

_____day of_____2003

APPROVED FOR FINAL SUBMISSION

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Date

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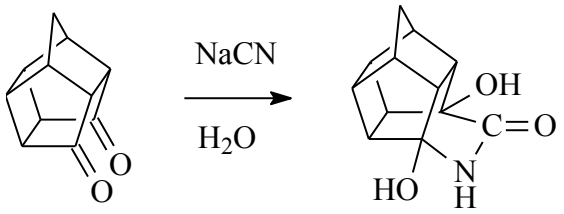
"Jai Shree Krishna"

ABSTRACT

The purpose of this study is to utilize computational techniques in the determination of the mechanistic pathways for the one-pot conversion of a pentacyclo-undecane (PCU) dione **1.1** to a pentacyclo-undecane cage lactam **1.2**.



1.1 **1.2**

In pursuance of this objective, the *ab initio* quantum mechanical level of theory was employed. The primary goal of this study was to compute the relative difference in energies for the reactants, products and transition-states of the proposed mechanistic pathways. The energy values obtained were used to predict the thermodynamic and kinetic pathways of the mechanism. All calculations were performed using the GAUSSIAN 98 series of programs, and GAUSSVIEW was used to visualize the transition-state structures.

Full geometry optimizations were performed at the Hartree-Fock (HF) level of theory using the 3-21+G* basis set. In addition, the transition-states were established using a SCAN technique to obtain a starting structure. Transitions states were verified by using second-derivative analytical vibrational frequency calculations and the visual inspection of the movement of atoms associated with the transition.

Hess's Law was applied to compute the heats of formation. It was found that two transition structures in the gas phase had abnormally high energies. However, these energies were found to be considerably lower in the presence of a solvent molecule. Furthermore, it was observed that the one-step conversion of the dione **1.1** to the lactam **1.2** proceeded via a single transition-state.

Previous experimental work found that the reaction proceeds through a cyanohydrin intermediate which in all likelihood represents the rate determining step. Sound

arguments exist to demonstrate that the computationally determined rate-determining step agrees with the experimentally observed rate-determining step.

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SUPPLEMENTARY MATERIAL:

A CD accompanying this thesis includes the following:

- Text containing Chapters 1-6 (including References).
- Cartesian coordinates of all the 3-D structures from Chapter 5.
- Frequency calculations of the TS's.

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LIST OF ABBREVIATIONS

CPU	Central Processing Unit
DEC	Digital Equipment Corporation
DFT	Density Functional Theory
G98W	Gaussian 98 Windows
GTOs	Gaussian-Type Orbitals
GUI	Gaussian User Interface
HF	Hartree Fock
IR	Infra Red
LCAO	Linear Combination Atomic Orbitals
MM	Molecular Mechanics
NMR	Nuclear Magnetic Resonance
PCU	Pentacyclo-Undecane
PES	Potential Energy Surface
RFO	Rational Functional Optimization
RHF	Restricted Hartree Fock
SCF	Self Consistent Field
SE	Semi-Empirical
SP	Single Point
STOs	Slater-Type Orbitals
STQN	Synchronous Transit-Guided Quasi Newton
TS	Transition-State/Structure
UV	Ultra Violet

CHAPTER 1

1. INTRODUCTION

1.1 Computational Chemistry and Molecular Modeling

The terms "theoretical chemistry", "computational chemistry" and "molecular modeling" are used interchangeably and indeed most molecular modelers use all three concepts to describe various aspects of their research.

"Theoretical chemistry" is often considered synonymous with quantum mechanics, whereas computational chemistry encompasses not only quantum mechanics but also molecular mechanics, minimizations, simulations, conformational analysis and other computer-based methods for the understanding and the prediction of the behaviour of molecular systems. However theoretical chemistry is a subfield of chemistry where mathematical methods are used in combination with the fundamental laws of physics to study chemical processes.[1] In particular, this involves the breaking of new ground that ultimately leads to the writing of new mathematical codes or software that can model certain aspects of a chemical structure.

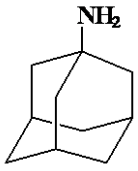
Computational chemistry has therefore become one of the mainstays of modern industrial and academic chemistry that makes use of the established codes or software to study chemical systems. The ever-increasing power of modern computers coupled with the development of new theoretical approaches can be used for accurate and precise prediction of molecular properties.[2] It is interesting to note that computational chemistry accounts for roughly a third of the super computer usage worldwide. Computer methods are used extensively to solve chemical problems that would be intractable or even impossible experimentally.[3]

Computer-aided molecular design became a subject worthy of discussion in the media around 1981, with the advancement of sophisticated computer graphics hardware.[3] The general aims of computational chemistry is the characterization and the prediction of chemical structures and their stability; the prediction of NMR, IR and UV spectra, the prediction of thermodynamic data, and the simulation and modulation of reaction

courses.[4] To achieve this computational chemists are using advanced computer software that enables them to gain insight into chemical processes and to avoid time-consuming and expensive experiments.[3] This approach does not replace the traditional wet chemistry experiments but it is a powerful aid in the understanding of experimental observations and the prediction of new reaction pathways. Some methods can be used to model not only stable molecules, but also short-lived, unstable intermediates and even transition-states which are required for kinetic information. In this way, they can provide information about molecules and reactions that may be impossible to obtain experimentally. Computational chemistry is therefore both an independent research area and a vital adjunct to experimental studies.

1.2 Pentacyclo-undecane (PCU) Cage Compounds

During the past half-century,[5,6,7,8] many research groups focused on the synthesis and chemistry of novel polycyclic cage molecules. Davis and co-workers[9] were responsible for discovering that 1-amino-adamantane **1.3**, commonly known as amantadine, exhibits antiviral activity thus realizing that polycyclic cage molecules also have the potential as biologically active agents.



1.3

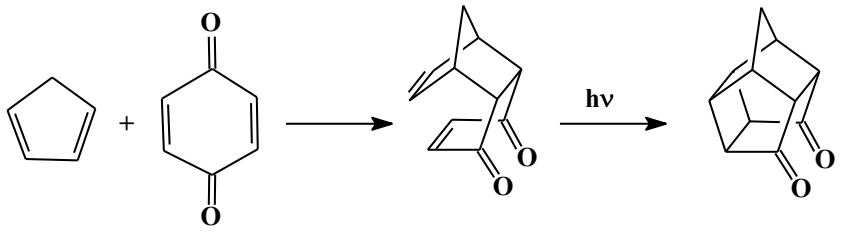
An unexpected observation[10] of the biological activity profile of amantadine revealed that it could be beneficial to patients with Parkinson's disease. The hydrocarbon cage of amantadine has the ability to cross the blood-brain barrier and to enter the central nervous system[10] due to the hydrophobicity of the "cage" despite the fact that the amino group is protonated at physiological pH. Drugs containing hydrocarbon cage moieties promote their transport across cell membranes and increase their affinity for lipophilic regions in receptor molecules.[11]

While the hydrophobicity of the cage facilitates transport of the drug across membranes, the size and stability of the cage inculcate the drug with a structural property which

results in controlled release of the active ingredients of the drug, namely, stability towards degradation. In practice this translates into slow metabolism of the drug. The important implications of this is that the intervals between drug administration is increased.[12] Another factor that was found to influence the rate of release of the active ingredient and the potency of the drug was the presence of the amantadine substituent in the drug. It has been shown that the inclusion of amantadine has given rise to longer time over which the drug is effective, greater potency of the drug and faster drug action. Furthermore the nature of the substituent influences the specificity of the drug to antibacterial[13], anabolic[14] and analgesic action.[15]

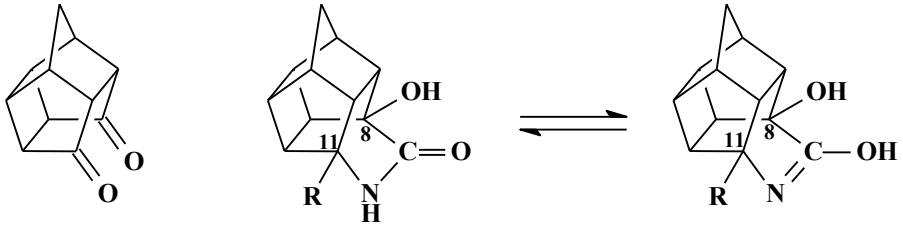
A number of cases[16,17,18] have recently demonstrated the potential therapeutic value of novel pentacyclic cage compounds. These compounds have promising potential as an important new class of medicinal and pharmaceutical agents and might extend the existing range[19,20,21] of bio-active pentacyclo-undecane compounds. Further investigation is required into the influence of the unique steric distribution of important functional groups around a rigid cage structure on the pharmacological activity.

The Diels-Alder **1.6** adduct of cyclopentadiene **1.4** and p-benzoquinone **1.5** produces the PCU dione **1.1**. The reaction in which the dione **1.1** is synthesized is carried out by intramolecular photocyclisation.[22]



1.4 **1.5** **1.6** **1.1**

Treatment of the dione **1.1** with Strecker reagents (HCN, NH_4OH) unexpectedly produced[23] the δ-lactam compounds **1.2a-1.2c**. Strecker reactions normally produce cyanohydrins or amino nitriles.[24]

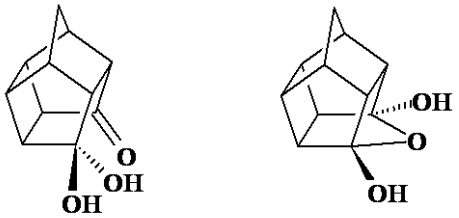


1.1 **Lactam** **1.2 a, R=OH** **Lactim**
1.2 b, R=CN
1.2 c, R=NH_2

The mechanism of this unique one pot conversion[23,25,26,27] is not well understood. The mechanism proposed by the authors[23,25,26] was based on basic chemical principles and is discussed below.

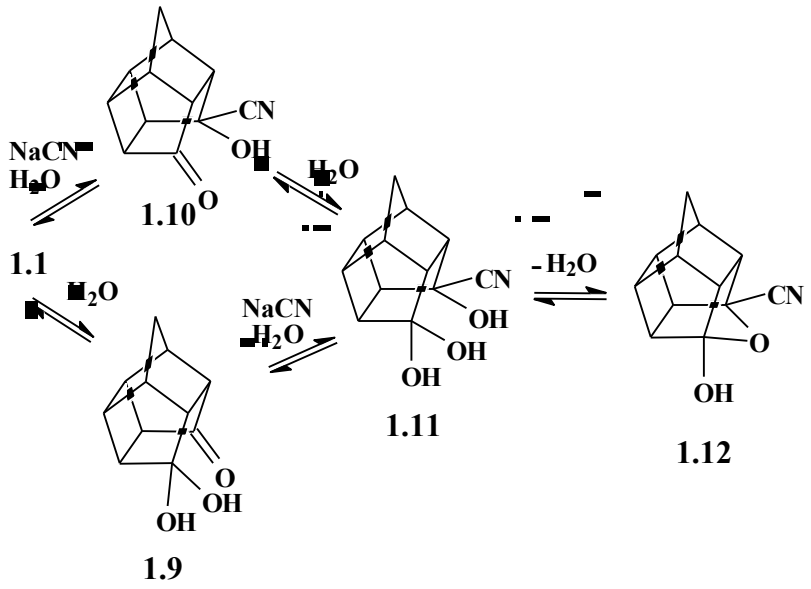
1.3 Lactam formation

In a previous study[28] it was shown that the dione **1.1** is easily hydrated to form the hydrates **1.7** and **1.8** in a 4:1 ratio. Thus it can be expected that this phenomenon should also play a significant role in the nucleophilic addition reactions on the carbonyl groups of the dione **1.1** in aqueous media.



1.7 **1.8**

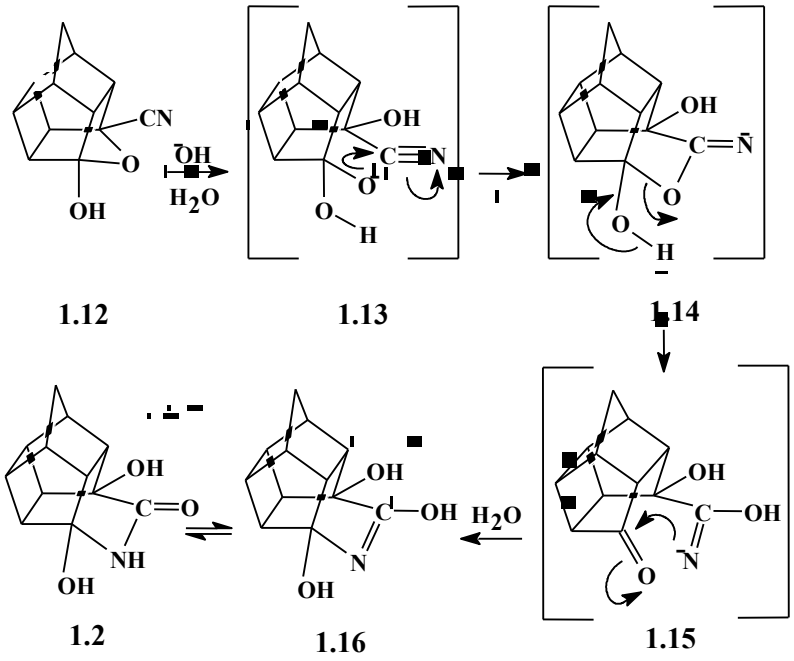
It can subsequently be assumed that both **1.1** and **1.9** (in Scheme I shown below) can participate in the formation of the dihydroxylactam **1.2**. Nucleophilic attack is expected to take place on the *exo* face of the carbonyl groups[27] in the dione **1.1** or the hydrate **1.9** as a result of the proximity of the groups and could lead to the formation of **1.11**. Transannular cyclisation of **1.11** is expected to form the cyclic ether **1.12**. Scheme I shown below was one of the two proposed mechanistic pathways, based on basic chemical principles and intuition.[23,25,26,27]



Scheme I: Conversion of the dione to the cyclic ether

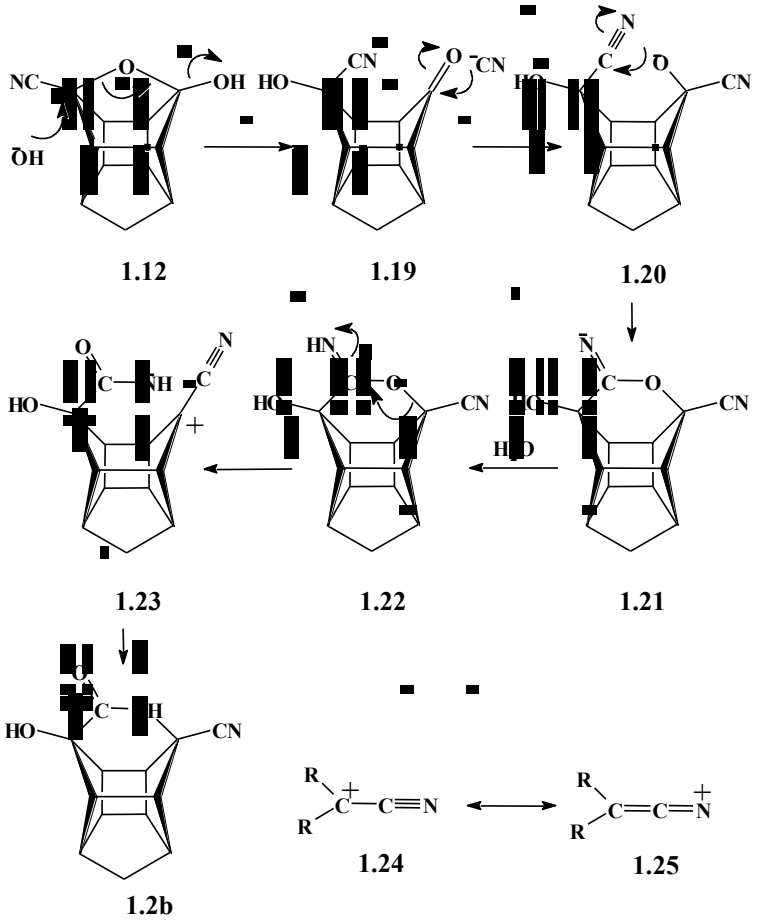
It was assumed that the cyclic ether **1.12** plays an intermediate role in the conversion of the dione **1.1** to the dihydroxylactam[27] **1.2**, since the "inversion" of a nitrile group can be explained as in Scheme II shown below.[27] The authors later showed[27] that the cyanohydrin **1.11** and **1.12** can be converted to the corresponding hydroxyl lactam **1.17** upon treatment with aqueous NaOH, providing experimental proof for their assumption above.

The explanation[27] for the conversion of **1.12** to **1.2** is discussed in Scheme II below. Under basic reaction conditions, ring cleavage of the cyclic ether **1.12** forms the intermediate **1.13** which is converted to intermediate **1.14**. The electron deficient nitrile carbon atom of the *endo*-orientated cyano group in **1.13** is in an extremely favourable position to suffer attack from the nearby negatively charged oxygen atom. Intermediate **1.14** rearranges to form intermediate **1.15**. Cyclisation of the intermediate **1.15** results in the formation of lactim **1.16** and by implication the lactam **1.2**.[27]



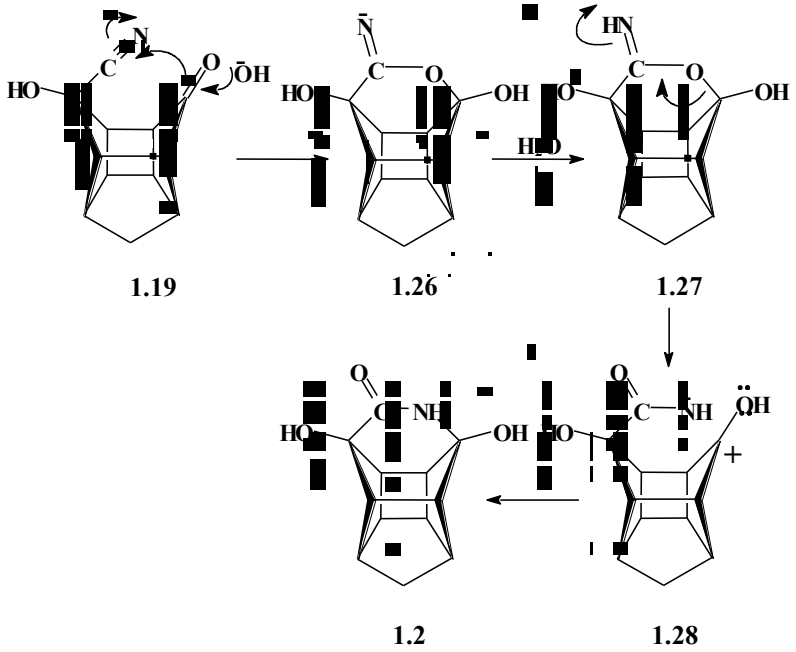
Scheme II: Conversion of the cyclic ether

The above explanation does not account for the formation of a compound such as the cyano hydroxylactam **1.2b** (Scheme III).[23,26] The nucleophilic attack of the hydroxide on the cyclic cyanohydrin **1.12** is shown is Scheme III. This is necessary to "invert" the cyanide group and is expected to be combined with the loss of the hydroxide group in the cyclic cyanohydrin **1.12**, whereby the cyanohydrin **1.19** should be formed. The *endo* cyano group in **1.20** has an electron deficient carbon atom which is in an extremely favourable position to suffer attack from the nearby negatively charged oxygen atom thus producing the intermediate **1.21** and subsequently **1.22**. The rearrangement of **1.22** to the α-cyano cation **1.23** is a postulated rearrangement and is not a controversial one. This is so since α-cyano cations of the general formula shown in **1.24** are significantly stabilized by charge delocalisation through resonance structures such as **1.25**, even though this requires a portion of the charge to reside on a divalent nitrogen.[29,30] When attached to very unstable cations[30] then only is the β-donor effect of cyano substituents manifested. The rearrangement proposed in Scheme III is promoted since the negative charge on the nitrogen atom of **1.23** is sufficiently stabilized by the adjacent carbonyl group to facilitate the rearrangement.



Scheme III: Nucleophilic attack of hydroxide to form the cyano hydroxy lactam[23,27]

The formation of **1.2** shown in Scheme IV below is also based on the explanation of the cyano group stabilization as postulated in Scheme III. The hydroxy group in **1.26** should similarly stabilize the cation and result in the formation of **1.2**. Attack of hydroxy anions instead of cyanide ions on the carbonyl carbon atom of the cyanohydrin **1.19** also results in the conversion of dione **1.1** to the dihydroxylactam.[27]



Scheme IV: Nucleophilic attack of hydroxide to form the dihydroxylactam[23,25,26,27]

CHAPTER 2

2. THEORETICAL TOOLS FOR MOLECULAR ORBITAL CALCULATIONS

2.1 Molecular Orbital Theory

Molecular orbital theory is an approach to molecular quantum mechanics which uses one-electron functions or *orbitals* to approximate the full wavefunction. A molecular orbital, $\psi(x, y, z)$, is a function of the cartesian coordinates of a single electron. Its square, ψ^2(or square modulus $|\psi|^2$ if ψ is complex) is interpreted as the probability distribution of the electron in space. To describe the distribution of an electron completely, the dependence on the spin coordinates ξ, also has to be included. This coordinate takes on one of two possible values ($\pm$½) and measures the spin angular momentum component along the z-axis in units of $h/2\pi$.[31]

2.2 Molecular Mechanics

Molecular mechanics (MM) simulations use the laws of classical physics to predict the structures and properties of molecules. There are many different molecular mechanics methods. Each one is characterized by its particular *force-field.* A force-field comprises a set of equations defining how the potential energy of a molecule varies with the locations of its component atoms and a series of *atom types*, defining the characteristics of an element within a specific chemical context.[32,33] The atom types describe different characteristics and behaviour for an element depending upon its environment. For example, a carbon atom in a carbonyl is treated differently than one bonded to three hydrogens. The atom type depends on hybridization, charge and the types of the other atoms to which it is bonded. Molecular mechanics calculations don't explicitly treat the electrons in a molecular system. Instead, they perform computations based upon the interactions among the nuclei. Electronic effects are implicitly included in force-fields through parameterization. This approximation makes molecular mechanics computations quite inexpensive computationally, and allows them to be used for very large systems containing many thousands of atoms. However, it also carries several limitations as well. The most important is that each force-field achieves only good results for a limited class of molecules, related to those for which it was

parameterized. No force-field can generally be used for all molecular systems of interest. Neglect of electrons means that molecular mechanics methods cannot treat chemical problems where electronic effects predominate. For example, they cannot describe processes which involve bond formation or bond breaking. Molecular properties which depend on subtle electronic details are also not reproducible by molecular mechanics methods.[34]

2.3 Electronic Structure Methods

These methods use the laws of quantum mechanics rather than classical physics as the basis for their computations. According to quantum mechanics, the energy and other related properties of a molecule may be obtained by solving the Schrödinger equation:

$$H\Psi = E\Psi \qquad (2.1)$$

where, H = Hamiltonian, a differential operator which like the energy in classical mechanics, is representative of the kinetic and potential energy of the molecule,

E = numerical energy of the state, and

Ψ = corresponding wavefunction for molecular state.

The Hamiltonian used in the Schrödinger equation is that for nuclear motions, describing the vibrational, rotational and translational states of the nuclei.[35]

Schrödinger's equation for molecular systems can only be solved approximately. Exact solutions of the Schrödinger equation may only be obtained for the very simplest molecules (e.g., H_2) because of the inter-electronic repulsion terms in the equation, where the motion of each electron depends on the motion of the other electrons, so approximate methods have to be used for larger molecules, for example the variation method.[36] The two main classes of electronic structure methods are semi-empirical methods and *ab initio* methods.[33] Semi-empirical methods use parameters derived from experimental data or high level *ab initio* calculations to simplify the computation. An approximate form of the Schrödinger equation is solved which depends on having appropriate parameters available for the type of chemical system in question.

2.3.1 The *Ab Initio* Method

The term a*b initio* is given to computations which are derived directly from theoretical principles with no inclusion of experimental data. The approximations are usually mathematical approximations, such as using a simpler functional form for a function or getting an approximate solution to a differential equation. The square of the wavefunction Ψ^2 is interpreted as the probability density for the electrons within the system. The first step in simplifying the general molecular problem in quantum mechanics is in the separation of the nuclear and electronic motions. This is possible because the nuclear masses are much greater than those of the electrons and, therefore, nuclei move much more slowly. This separation of the general problem into two parts is called the adiabatic or Born-Oppenheimer Approximation.[37] Thus, the electron distribution within a molecular system depends on the positions of the nuclei, and not on their velocities.

The advantage of *ab initio* methods is that they eventually converge to the exact solution, once all of the approximations are made sufficiently small in magnitude. However, this convergence is not monotonic. Sometimes, the smallest calculation gives the best result for a given property.

The disadvantage of *ab initio* methods is that they are expensive. These methods often take enormous amounts of computer CPU time, memory and disk space. In practice, extremely accurate solutions are only obtainable when the molecule contains about half a dozen electrons or less.

Restricted Hartree Fock (RHF) or Unrestricted Hartree Fock are the two forms of the wave function that are used in quantum mechanic calculations. The RHF wave function is used for singlet electronic states, for example, the ground states of stable organic molecules. The UHF wave function is most often used for multiplicities greater than singlets.[38] The Møller-Plesset second order perturbation theory (MP2) specifies the calculation of electron correlation energy. The MP2 option can only be applied to Single Point calculations.[39]

In general, *ab initio* calculations give very good qualitative results and can give increasingly accurate quantitative results as the molecules in question become smaller.[31]

2.3.2 Semi-Empirical

Semi-empirical (SE) calculations are set up with the same general structure as a Hartree Fock (HF) calculation. Within this framework, certain pieces of information such as two electron integrals are approximated or completely omitted. In order to correct for the errors introduced by omitting part of the calculation, the method is parameterized, by curve fitting a few parameters or numbers in order to give the best possible agreement with experimental data.[40]

The advantage of semi-empirical calculations is that they are much faster than the *ab initio* calculations. The disadvantage is that the results can be erratic. If the molecule being computed is similar to molecules in the database used to parameterize the method, then the results may be very good. If the molecule being computed is significantly different from anything in the parameterization set, the answers may be very poor.[40]

Semi-empirical calculations have been very successful in the description of organic chemistry where there are only a few elements used extensively and the molecules are of moderate size. However, semi-empirical methods have been devised specifically for the description of inorganic chemistry as well.[40]

2.3.3 Density Functional Theory (DFT) Methods[40]

Density Functional Theory (DFT) is the third class of electronic structure methods that have recently come into wide use. These methods are similar to the *ab initio* methods in many ways. DFT calculations require approximately the same amount of resources as the Hartree-Fock theory, but they produce results approaching the quality of the MP2 level of theory.

DFT methods include the effects of electron correlation, where electrons in a molecular system react with each other's motion and attempt to keep out of each other's way. This is what makes DFT methods more attractive than the expensive *ab initio* methods.[40]

DFT methods are based on the theory developed by Hohenberg and Kohn[41] in which they demonstrated that the ground state energy of any molecule can be described in terms of the total electron density, in other words, each molecule has a unique functional form which exactly determines the ground state energy and electron density

(i.e. geometry) of the molecule.[40,42] This system is different to the wave function approach of *ab initio* techniques, where the complexity of the wave function increases by a factor of 3*N* for an *N*-electron system (no spin included). For the DFT system, the complexity of the function is less dependent to the system size since the electron density has the same number of variables. The aim of DFT methods, therefore, is to design functions which connect the electron density with energy.[43] Kohn and Sham[44] were responsible for the introduction of orbitals which formed the basis for the use of DFT calculations in computational chemistry.

The advantage of DFT is that only the total density is to be considered and to calculate the kinetic energy with accuracy, orbitals need to be re-introduced. The disadvantage of DFT is the derivation of suitable formulae for the exchange-correlation term. DFT methods, however, have the ability to produce accurate results.[42]

2.3.4 Basis Sets[45]

A basis set is a mathematical description of the orbitals within a system used to perform the theoretical calculation. The wavefunction Ψ, can be expanded in terms of a set of atomic orbitals, χ_μ in the linear combination of atomic orbitals (LCAO) method, to give[45]:

$$\Psi = \Sigma c_\mu \chi_\mu \qquad (2.4)$$

where c_μ = molecular orbital expansion coefficient, and

χ_μ = basis function of atomic orbital.

The coefficient c_μ is varied to obtain the wavefunction Ψ, which will give the lowest energy in the Schrödinger equation. The more vibrational parameters used to describe an individual orbital, the lower the energy. However, a situation is reached when the energy is no longer decreased when the number of vibrational parameters is increased and then the best single determinant wavefunction is obtained. When this occurs, changing the wavefunction Ψ, by an infinitesimal amount will not alter the energy. The number and quality of the atomic orbitals χ_μ determine the quality of the molecular orbital Ψ. If there are many electrons in a molecule then the number of atomic integrals

required increases rapidly and can be as many as several million for quite small molecules. For this reason a fast computer which has a large storage capacity is essential. The two types of atomic basis functions are Slater-type atomic orbitals (STOs) and Gaussian-type atomic orbitals (GTOs). The former is not well suited to numerical work, and their use in practical molecular orbital calculations has been limited. Almost all modern *ab initio* calculations employ GTO basis sets. These basis sets, in which each orbital is made up of a number of Gaussian probability functions, has considerable advantages over STOs. The Gaussian series of programs deals, as the name implies, almost exclusively with Gaussian-type orbitals.

2.3.4.1 Minimal Basis Sets[45]

These contain the minimum number of basis functions needed for each atom. Minimal basis sets are characterized by fixed-size atomic-type orbitals. Each orbital is characterized by its coefficient and its exponent. They therefore do not have the capability to expand or contract because the exponent is fixed.

(i) The STO-3G Basis Set[45]

The series of minimal basis sets consists of expansions of Slater-type orbitals (STOs). The STO-3G basis set yields properties that are reasonably close to limiting values and in view of the relative computational times of the various expansions, it is this level that has been selected as an optimum compromise for widespread application. Another possible exception to the use of the three-gaussian expansion as the standard minimal basis level occurs in the consideration of the properties of weakly-bound complexes where long-range forces are important.

2.3.4.2 Split Valence Basis Sets[45]

The way that a basis set can be made larger is to increase the number of basis functions per atom. Inclusion of two sets of isotropic p-functions in the representation, one tightly held to the nucleus and the other relatively diffuse, will allow independent variation of the radial parts of the two sets of p-functions, thus producing more contracted or more diffuse functions that would be suitable for the descriptions of say, s- and p-systems, respectively. A basis set formed by doubling all functions in a minimal representation

is known as a double-zeta basis, while one in which only the basis functions for the outer valence shells are doubled, is known as a split-valence basis set.

(i) The 3-21G Basis Set[45]

The 3-21G basis set defined through the fourth row of periodic table of elements, typify representations in which two basis functions, instead of one have been allocated to describe each valence atomic orbital. Except for hydrogen, the 3-21G basis sets are employed as is, that is, without rescaling of the valence functions to account better for changes that might occur as a result of molecule formation.

2.3.4.3 Polarised Basis Sets[45]

While split valence basis sets allow orbitals to change their size, but not their shape, polarised basis sets remove this limitation by adding orbitals with angular momentum beyond that which is required for the ground state description of each atom. For example, polarised basis sets add p-functions to hydrogen atoms, d-functions to the main groups and f-functions to transition metals.

(i) The 6-31G* Basis Set[45]

The 6-31G* basis set was originally proposed for first-row atoms and later extended to second-row elements. The 6-31G* basis set is constructed by the addition of a set of six second order (d-type) gaussian primitives to the split valence 6-31G basis set description of each heavy (non-hydrogen) atom.

(ii) The 6-31G Basis Set[45]**

The basis set described above does not allow for any polarisation of the s orbitals of either hydrogen or helium atoms. The 6-31G** basis set is identical to 6-31G* except for the addition of a single set of gaussian p-type functions to each hydrogen and helium atom.

(iii) The 3-21G* Basis Set[45]

The 3-21G* basis set for second-row elements are constructed directly from the corresponding 3-21G representations by the addition of a complete set of six second-order gaussian primitives. Although the resulting representations contain the same number of atomic basis functions per second-row atom as the 6-31G* polarisation basis

set previously described, these are made up of significantly fewer gaussians (three instead of six for each inner-shell atomic orbital, and two gaussians instead of three for the inner part of the valence description).

2.3.4.4 Basis Sets Incorporating Diffuse Functions[45]

The basis sets that have been discussed thus far are more suitable for molecules in which electrons are tightly held to the nuclear centers than they are for species with significant electron density far removed from those centers. Calculations involving anions pose special problems. Since the electron affinities of the corresponding neutral molecules are typically quite low, the extra electron in the anion is only weakly bound. One way to overcome problems associated with anion calculations is to include in the basis representation one or more sets of highly diffuse functions. These are then able to describe properly the long-range behavior of molecular orbitals with energies close to the ionization limit.

(i) The 3-21+G and 3-21+G* Basis Set[45]

The 3-21+G basis set for the first-row elements and the 3-21+G* basis set for the second-row are constructed from the underlying 3-21G and 3-21G* representations by the addition of a single set of diffuse gaussian s- and p-type functions. For first-row elements with lone pairs, the effects of diffuse and polarisation functions are complementary to some extent. Hence, the energies of processes involving changes in the number of lone pairs, for example, protonation, hydrogen bonding, or other interactions, are improved at diffuse-orbital-augmented levels even when large basis sets are used.

This basis set produces entry level results and is relatively inexpensive in terms of computer resources and time. If the system under study involves only C, H, N and O atoms, the system (with RHF) is ideal for student training. Upgrading to a better basis set is trivial and one does not loose too much valuable time during your learning curve.

2.3.5 Hartree-Fock Theory[46]

The most common type of *ab initio* calculation is the Hartree Fock (HF) calculation in which the primary approximation is the central field approximation. This means that the Coulombic electron-electron repulsion is not specifically taken into account.

However, its net effect is included in the calculation. This is a variational calculation, meaning that the approximate energies calculated are all equal to or greater than the exact energy. Because of the central field approximation, the energies from HF calculations are always greater than the exact energy and tend to a limiting value called the Hartree Fock limit. This variational principle leads to the following equations describing the molecular orbital expansion coefficients, derived by Roothaan and Hall[46]:

$$\sum_{v=}^{N} F_{\mu} - \varepsilon S_{\mu} \widetilde{c}_{vi} =) \qquad (2.2)$$

where, $\mu = 1, 2, \ldots, N$ and c_{vi} = molecular orbital expansion coefficient.
Equation (2.2) can be re-written in matrix form:

$$FC = SC\varepsilon \qquad (2.3)$$

where F = the Fock matrix,
S = the overlap matrix,
ε = the diagonal matrix, and
N = one-electron function or basis function.

Equation (2.3) is not linear and therefore must be solved *iteratively*. The procedure by which this is carried out is called the self-consistent field (SCF) method.[46] Slater and Gaussian type orbitals are used in these equations. The Hartree Fock equations are applicable no matter how many electrons there are in the molecule. However, this theory does not include a full treatment of the effects of *electron correlation*, that is, the energy contributions arising from electrons interacting with one another. It is reasonably good at computing the structures and vibrational frequencies of stable molecules and some transition-states. As such, it is a good base-level theory.[46]

The second approximation in HF calculations is that the wave function must be described by some functional form, which is only known exactly for a few one electron systems. The functions used most often are linear combinations of Slater-type orbitals

(STOs) or Gaussian-type orbitals (GTOs). The wave function is formed from linear combinations of atomic orbitals or more often from linear combinations of basis functions. Because of this approximation, most HF calculations give computed energy greater than the Hartree Fock limit. The exact set of basis functions[46] used is often specified by an abbreviation, such as STO-3G or 6-31g**.

CHAPTER 3

3. TRANSITION STRUCTURE MODELING[47]

A transition structure (TS) is the molecular species that is represented by the top of the potential energy graph in a simple one dimensional reaction coordinate shown in Figure 3.1. In order to determine the energy barrier to reaction rate, the energy of this transition-state species is needed. The geometry and energy of a transition structure include important pieces of information for describing reaction mechanisms.

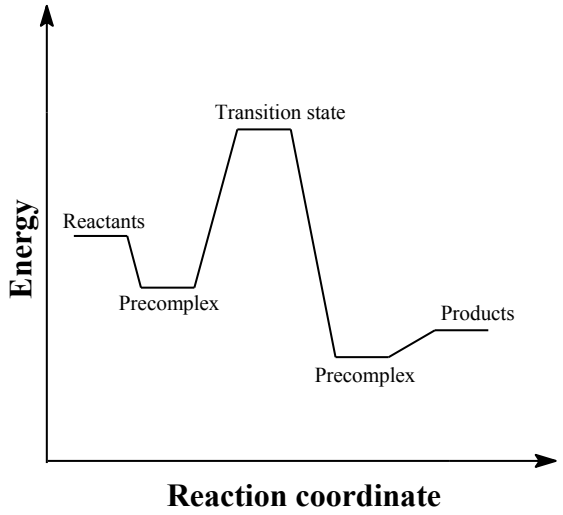


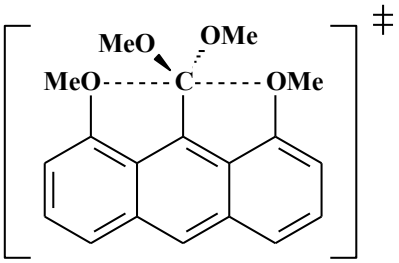
Figure 3.1 Points on a simple reaction coordinate[48]

A transition structure is defined mathematically as the geometry which has a zero derivative of energy with respect to moving every one of the nuclear coordinates and has a positive second derivative of energy of all but one geometric movement which has a negative curvature.[47] This description however, describes many structures other than a reaction transition, for example an eclipsed conformation or the intermediate point in a ring flip, a simple rotation of a methyl group or any structure with a higher symmetry than the ground state of the compound.

It is difficult to predict what a transition structure will look like without the aid of computer simulation. Such a prediction might be made based on a proposed mechanism, which may be incorrect. The potential energy surface (PES) around the transition structure is often much more flat than the surface around a stable geometry, thus there may be large differences in the transition structure geometry between two

seemingly very similar reactions and with very small differences in energy.[47] It has however been possible computationally, to determine transition structures, although it is not always easy. Experimentally, it has only become possible to examine reaction mechanisms directly using femtosecond pulsed laser spectroscopy. It will be some time before these techniques can be applied to all of the compounds that are accessible computationally. Furthermore, these techniques yield indirect information such as vibrational information rather than a likely geometry for the transition structure.[47]

Synthetic approaches to obtain information about transition-states are also limited to very special cases, such as the static S_N2 transition-state **3.1** shown below.[49]



3.1

An X-ray structure of the above mentioned molecule was reported.[49]

3.1 Transition-state modeling with empirical force-fields[50]

The transition-states (TS) involved in a conformational equilibrium can be studied using the ground-state parameters developed from geometries and heats of formation of stable molecules. One of the earliest applications of empirical force-fields to organic chemistry was Westheimer's study of rotational barriers in biphenyls, which begun in the 1940's and was reviewed in the 1950's.[51,52] In the subsequent half-century, there have been many studies of conformational rate processes in organic systems. Ground-state parameters are fully appropriate to such studies; transition-states have more torsion and non-bonded strains than energy minima, but have the same type of bonds. However, when bonds are being formed or broken, the parameters suitable for ground states are no longer appropriate.[50] Consequently, parameters must be developed to model partial bonds in a quantitative way when using semi-empirical methods. Theoretical studies on transition structures of several class of reactions have shown that

bond lengths and other geometrical parameters in transition structures have a relatively narrow range of values. For example, in pericyclic reactions, forming C-C single bonds generally have bond lengths from 1.95 to 2.28 Å, even though some of these reactions are very exothermic and others are thermoneutral.[53] Radical additions to alkenes have been studied for a variety of carbon- and oxygen- centred radicals, with constant angles and bond lengths around 105 ± 3° and 2.25 ± 0.01 Å, respectively.[54]

Hydroborations of alkenes and alkynes have been studied for a variety of alkylboranes and substituted ethylenes. Even in the presence of high steric hindrance, the formation and the breaking up of bond lengths are relatively constant.[55] These examples support one critical procedure often used in simple force-field transition-state modeling, namely the breaking and forming bonds are either fixed at some lengths, or these values are treated as energy minima. The energy is actually a maximum for the reaction coordinate, but the simple expedient of calculating transition-states as minima has been used in many cases. The TS is a saddle point along the free-energy surface. This saddle point has a negative curvature in only one direction. The negative force constant corresponds to motion along the reaction coordinate. All other vibrational motions have positive force constants exactly like energy minima on potential energy surfaces. However the negative force constant causes the transition structures to have unique properties different from force minima.

As mentioned at the beginning of this chapter the energy surface at the TS is often very flat. This normally causes problems for using SE methods to determine transition-states.

Due to the structural features and characteristics in the highly strained moieties, the outer limits of what can be prepared and studied regarding thermodynamic stability and kinetic reactivity is investigated. Studies of such systems provide an excellent test for existing chemical theory and thus perhaps furnish the best opportunity for advancing the frontiers of our chemical knowledge.[7] It is therefore likely that SE methods will give poor results for transition-states involving the cage structure.

3.2 Locating minima on the seams of intersecting semi-empirical PES[56]

Although the word "minima" is used above, it actually implies the lowest maximum on the energy surface between the product and the reactant.

In recent years, the location of TS's has become relatively routine due to improvements in the optimization algorithms. The TS can be refined to any desired accuracy, if the energy-generating function is of the *ab initio* type. However, the practical consideration usually limits both the size and the level of sophistication. Semi-empirical methods can be used for somewhat larger systems, but in this case only comparison with experiments or accurate *ab initio* calculations can be used to assess the quality of results.

The primary concern in many applications is not in the prediction of absolute values of activation parameters, but rather on how they vary for closely related systems. There are two or more reaction pathways that have activation energies which differ by only a few kcal mol^{-1} and synthetic sequences are often dependent on these pathways. In such cases, the desired reaction can often be favoured by a careful selection of substituents at specific sites in the molecule being studied. According to the influence they have on a reaction, substituents can be divided into two limiting cases; those of a "structural" or "steric" nature and those which mainly exert an "electronic" influence. While the latter requires an explicit description of the electrons in the system, the former can be modeled by less rigorous theoretical methods, i.e. SE or MM. However, the above classification of substituents will depend on the given reaction.[56]

The treatment of a TS as a minimum on the PES is a more fundamental problem with Houk's approach.[56] These directions can in general be written as a linear combination of internal or cartesian coordinates. Three different strategies can be employed in transferring the *ab initio* structure to the force-field model:

(i) The "fixed atom" procedure, where the atoms directly involved in the reaction are frozen by fixing their cartesian coordinates;

(ii) The "fixed parameter" procedure, where certain internal coordinates are constrained by assigning large force constraints to these variables; and

(iii) The "flexible parameter" procedure, where all atoms are allowed to move.

As an alternative, the *equivalent* of a TS in a force-field environment can be defined as the lowest energy structure linking the reactant and product. When different sets of parameters are needed for describing the two end points, the TS equivalent is thus the lowest energy structure on the seam of the intersecting PES's. The advantage of the current strategy over Houk's TS modeling, is that only information regarding the two minima (reactant and product) on the PES is needed, and such data are in principle accessible by experiments. The disadvantage is that the functional form of the energy must be reasonably accurate over a wider range of geometries than just near the "minima".

SE methods were initially employed in this study for the determination of transition structures. It was found that the method indeed produced poor quality results, and in many cases the correct transition structures could not be found. It was therefore decided to use *ab initio* techniques for the determination of the required transition-states.

3.3 Transition-structure modeling of a PCU Cage Lactam using *ab initio* methods

The TS algorithm uses a combination of Rational Functional Optimization (RFO) and linear search step to search for the lowest maximum on the energy surface between the reactant and the product. A mathematical algorithm by default uses a crude semi-empirical (SE) guess (INDO guess is used for the first-row systems, CNDO for the second-row, and Hückel for the third-row and beyond)[57] for the initial start structure to the solution of the transition-state wave function. If the starting structure is too far from the real maximum on the energy surface, the search algorithm would not find the correct transition structure within the multitude of local maxima.

In order to obtain a better guess for the solution to the wave function, one could use either of two methods:

(i) carry out a Single Point (SP) calculation of the starting structure at the same level of theory using the same basis set, followed by an additional

step in the calculation, with the option to read the guess (guess = read) from the calculation done (obtained from the checkpoint file) at the required level and basis set or

(ii) use the option "CALCFC" where the force constant is calculated at the required level/basis set and used to start the solution to the wave function. The second option is considerably more expensive in terms of resources and time, since the "CALCFC" option does the same calculation as required for a frequency calculation. (see Chapter 4 for a discussion on CALCFC).[57]

A third method is the QST2 and QST3 methods in Gaussian which has the facility for automatically generating a starting structure for a transition-state optimization based upon the reactants and products that the transition-state connects,[58] known as the Synchronous Transit-Guided Quasi Newton (STQN) method. This method uses a quadratic synchronous transit approach to get closer to the quadratic region of the transition-state, and uses a quasi-Newton or eigenvector-following algorithm to complete the optimization.[57] QST2 requires two molecule specifications, i.e., the reactants and products. QST3 requires three molecule specifications, that is, the reactants, the products and an initial structure for the transition-state, respectively. The QST2 and QST3 methods were utilized in this study, but it did not yield favourable results.

A fourth option is to use the "CALCALL" option in combination with the transition-state optimization. During this calculation, the force constant will be calculated for each optimization step. This option is very expensive and is only used as a last resort when the methods above do not show positive results.

In this study, the TS for a PCU cage lactam were found by locating maxima on the potential energy surfaces using Restricted Hartree-Fock theory and the 3-21+G* basis set. For each TS (see Chapter 5 for the mechanistic pathway) a SCAN calculation (see Chapter 4 for computational details) was performed to establish the maxima. The final structure corresponds to a minimum on the potential energy surface, or saddle point. In order to determine the nature of the stationary point found, a frequency calculation was

performed. The frequency output file has information that is critical in characterizing the stationary point, namely, the number of imaginary frequencies and the normal mode corresponding to the imaginary frequencies. Imaginary frequencies are listed in the output file as negative numbers. By definition, a structure which has *n* imaginary frequencies is an n^{th} order saddle point. Thus transition structures are usually characterized by one imaginary frequency since they are first-order saddle points.[59] The movement of atoms associated with the imaginary frequency should follow the atoms on the reaction coordinate between the reactant and product. Any reaction profile will have only one transition-state. Although many intermediate transition structures on the reaction profile might exist, only one of them will be the rate-determining step. That transition structure is defined as the transition-state for the reaction.

CHAPTER 4

4. COMPUTATIONAL DETAILS EMPLOYED

This study was carried out on a series of related molecules using the GAUSSIAN 98[60] program implemented on a DEC Alpha DS20 workstation with two CPU's and a Pentium II desktop computer. A true 64 bit operating system was implemented on the DEC Alpha workstation with a parallelized version of GAUSSIAN 98 program.

4.1 The GAUSSIAN 98 Program

GAUSSIAN 98 (G98) is one of the series of electronic structure computer programs which began with GAUSSIAN 70, GAUSSIAN 92 and GAUSSIAN 94. GAUSSIAN 03 is the latest program which was released in April 2003.

The GAUSSIAN programs are general-purpose programs capable of performing *ab-initio* Hartree-Fock (HF) molecular orbital calculations based on the linear combination of atomic orbitals (LCAO) approach. As the name implies, the program deals mainly with Gaussian-type orbitals, which has been described in Chapter 2. However new methods have been added to G98 so as to improve optimization procedures for transition-state calculations.

In addition, G98 can compute energies, molecular structures, vibrational frequencies and numerous other molecular properties for systems in the gas phase and in solution, including the ground state and excited states.

The input section to the GAUSSIAN programs consists of the molecular charge and the multiplicity, the symbols of the constituent atoms and a definition of the molecular structure, either in the form of cartesian coordinates or the Z-matrix notation, which defines the molecular geometry in terms of bond lengths, bond angles and dihedral angles. The task to be performed, i.e. whether a single-point calculation, geometry optimization or frequency calculation, must also be specified, together with the appropriate basis set and the level of theory.

The 3-D structures on the CD accompanying this thesis are written in the Gaussian input file format (gjf). The geometries of the structures can be viewed by using the Gausview

program or the freeware (Molekel) program. The installation files for Molekel can be downloaded from the site: www.cscs.ch/molekel

4.2 The GaussView Program[61]

GaussView is a Graphical User Interface (GUI) program designed to simplify and extend the use of the Gaussian 98 program. In this study, Gaussview was used to build and edit molecules, set up and submit Gaussian jobs, and to display and use the results from the Gaussian jobs. However, GaussView is not directly integrated into the Gaussian program system, but acts as a front-end/back-end processor to facilitate its use on a desktop computer workstation. GaussView was also used to verify the animation of atoms associated with the negative eigenvalue of the different transition-states.

4.3 The SCAN Calculation

The scan option was exclusively used as an aid to finding an approximate starting structure for a normal transition-state optimization. A relaxed SCAN calculation involved changing of bond length from reactants to products, in a step-wise manner. The only constraint in this calculation is the required reaction coordinate (i.e. bond length, angle or the dihedral angles). The rest of the molecule is then optimized to find the lowest possible structure and energy, subject to the imposed constraints, after which the reaction coordinate is modified by a prescribed value and in the next step the procedure is repeated. In this study only relaxed SCAN calculations were used. The energy of each step was plotted against the reaction coordinate. By inspecting the different structures at each step of the scan job, one could follow the course of the reaction. The approximate starting structure for a full (non-restrained) transition-state optimization was obtained by manually extracting the coordinates of the structure closest to the maxima on the energy vs. reaction coordinate plot. The TS was verified by performing a frequency (FREQ) calculation. A frequency calculation produces only one negative eigenvalue, which is usually associated with the movement of atoms involved in either bond breaking or bond formation.

4.3.1 Commands used during a SCAN or a TS Search[60]

(i) GDIIS

Specified the use of the modified GDIIS algorithm, recommended for use with larger systems, tight optimizations and molecules with flat potential energy surfaces. It is the default for semi-empirical calculations. This command makes use of a smaller step-size down the potential energy valley.[60]

(ii) MODREDUNDANT or ModRed

Used in geometry optimization, e.g. the bond length to be scanned. The specific coordinates that are to be constraint (Modified Redundant coordinates = ModRed) is specified below the Cartesian coordinates.[60]

(iii) TS

Used in a search to request the optimization to use a mathematical search algorithm which aims to find a local maxima on the potential energy surface (i.e. a transition-state) rather than a local minimum.[60]

(iv) NOEIGENTEST

The default transition-state search in G98 makes use of the EigenTest. If only one imaginary frequency is found, the calculation continues to find the transition-state associated with this negative eigenvalue. If more than one imaginary frequency exists, the default routine is to terminate the calculations. Since it is practically almost impossible to find a starting structure for a TS with one and only one negative eigenvalue, the default TS calculation terminates very often. In order to overcome this oversensitive search criterion, one uses the "NoEigenTest" option which overrides the default search criteria in G98.[60]

(v) CALCFC

Specified the force constants be computed at the first point using the current method (available for the HF, MP2, CASSCF, DFT, and semi-empirical methods only). By default Gaussian uses a MNDO (semi-empirical) guess for the solution to the wave function of the specified system. The optimization uses this guess as starting point

where, after the *ab initio* calculation is "built" on this starting point. Since the MNDO guess is based on a rather crude or inaccurate method, the calculation could sometimes follow a wrong solution for the wave function. One observes this by inspecting the geometry of the structure produced by the optimization, there are basically two choices: (a) start with a better structure, i.e., a structure that was optimized at a lower level of theory or (b) if a better starting structure was already used, use the CalcFc option.[3,60]

4.4 Calculation Details

In this study the procedure for all structures was the structures in HyperChem Version 5.[62] In order to remove any van der Waals contacts or overlap, an energy minimization was performed with ChemOffice,[63] using a molecular mechanics force-field. The final structures were saved as input files for GAUSSIAN 98[60] (G98W). A low level (STO-3G) *ab initio* (full geometry optimization) calculation was carried out on the unconstrained molecule. The (OPT) keyword requests that a geometry optimization be performed. The geometry is adjusted according to a mathematical algorithm to follow the energy surface "down hill" until a stationary point on the potential energy surface is found. Note that the algorithm by nature would not overcome local minima and special techniques such as automatic or manual conformational searches or molecular dynamics[64,65,66] should be employed to overcome, mainly, rotational energy barriers. This is more problematic in flexible molecules such as peptides.

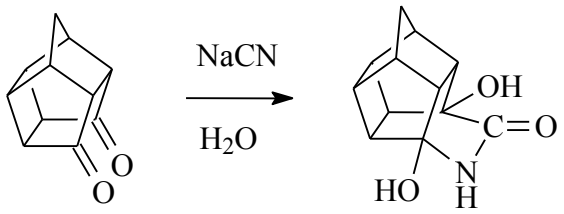
For the Hartree-Fock, DFT and semi-empirical methods, the Berny algorithm is the default algorithm for minimizations to a local minimum and optimizations to transition-states and higher order saddle points.[57] The purpose of a geometry optimization is to locate the lowest energy of the molecular structure that is in close proximity to the specified starting structure. The output structure of the optimization was submitted on a DEC Alpha workstation using the RHF/3-21+G* level of theory. A SCAN calculation was performed to locate the maxima on the PES. The starting structure for the transition-state (TS) calculation was obtained by manually extracting the coordinates of the structure that correspond to the maxima. Once a TS was obtained a frequency calculation was carried out to verify that there is only one negative eigenvalue.

CHAPTER 5

5. RESULTS AND DISCUSSION

5.1 Introduction

The purpose of this study is to utilize computational techniques in the determination of the proposed mechanistic pathways, for the one-pot conversion of pentacyclo-undecane (PCU) dione **5.1** to pentacyclo-undecane cage lactam **5.2**.[23,25]



5.1 **5.2**

This chapter focuses on the calculation results obtained for the proposed mechanistic pathway as illustrated in Figure 5. 1 (see Page 31). The basis set incorporating diffuse functions, that is, 3-21+G* was used in this study as discussed in Chapter 2. The mechanism, which was one of two possible pathways that was proposed[23,25,26,27] is based on basic chemical principles and intuition and was discussed in Chapter 1. In this study, the pathway proposed above was used as basis for the calculation of the reaction profile. Based on the observations made during this investigation (i.e., a starting structure optimized to a different intermediate or transition structure) the proposed pathway was also modified. The energies for the calculated mechanism proposed in this study are depicted in the form of a reaction profile (Figure 5.2 Page 32).

The reaction profile was investigated by first calculating the geometries and energies of the minima on the energy surface (Figure 5.2). Since the cage is very rigid, very few problems with conformational isomers of higher energies, were experienced.

The structures and energies of the corresponding TS's were then calculated. The procedure for locating the TS's is described in Chapter 3, Section 3.3.

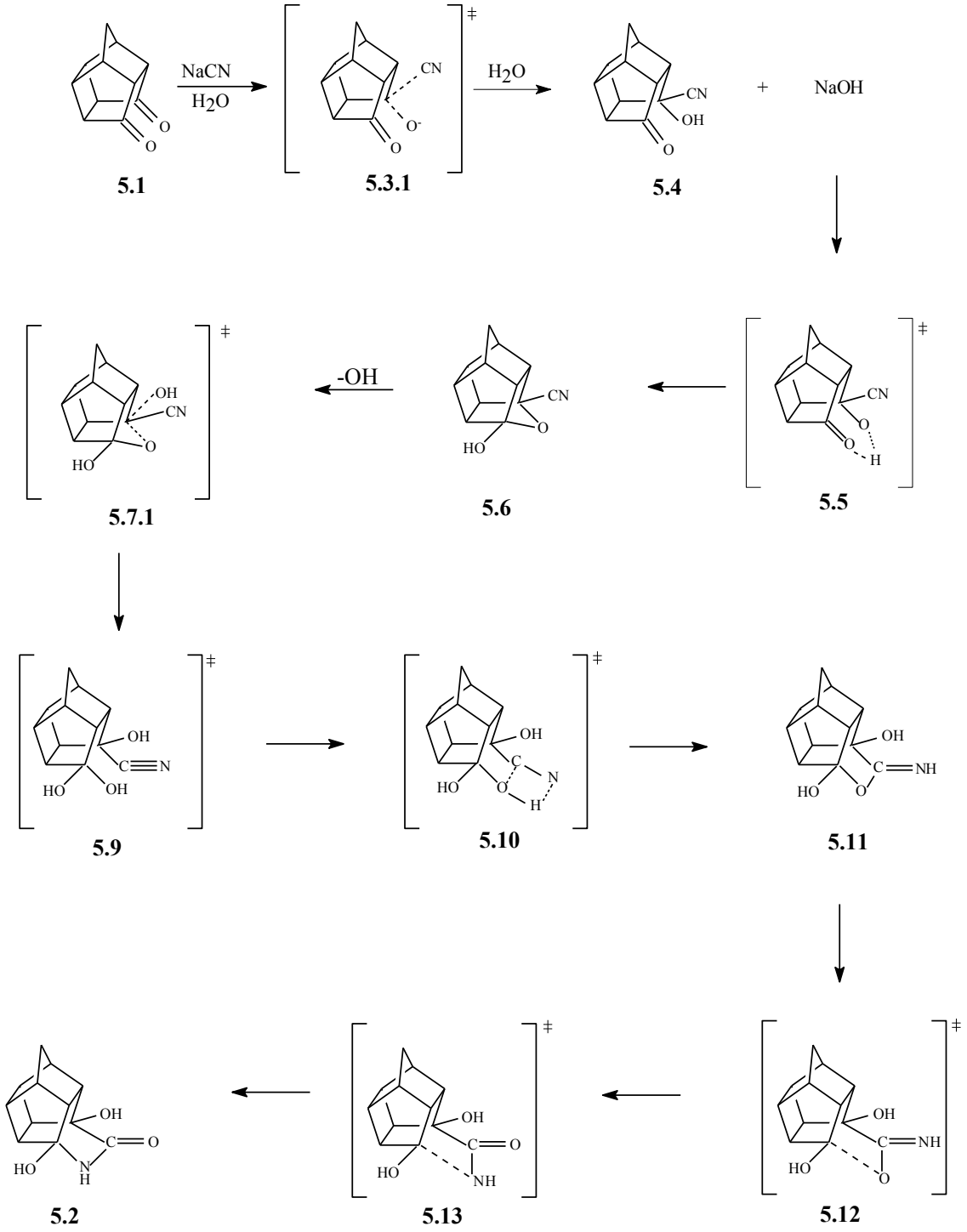


Figure 5. 1 Modified[23,25,26,27] mechanism for the conversion of the dione 5.1 to the lactam 5.2.

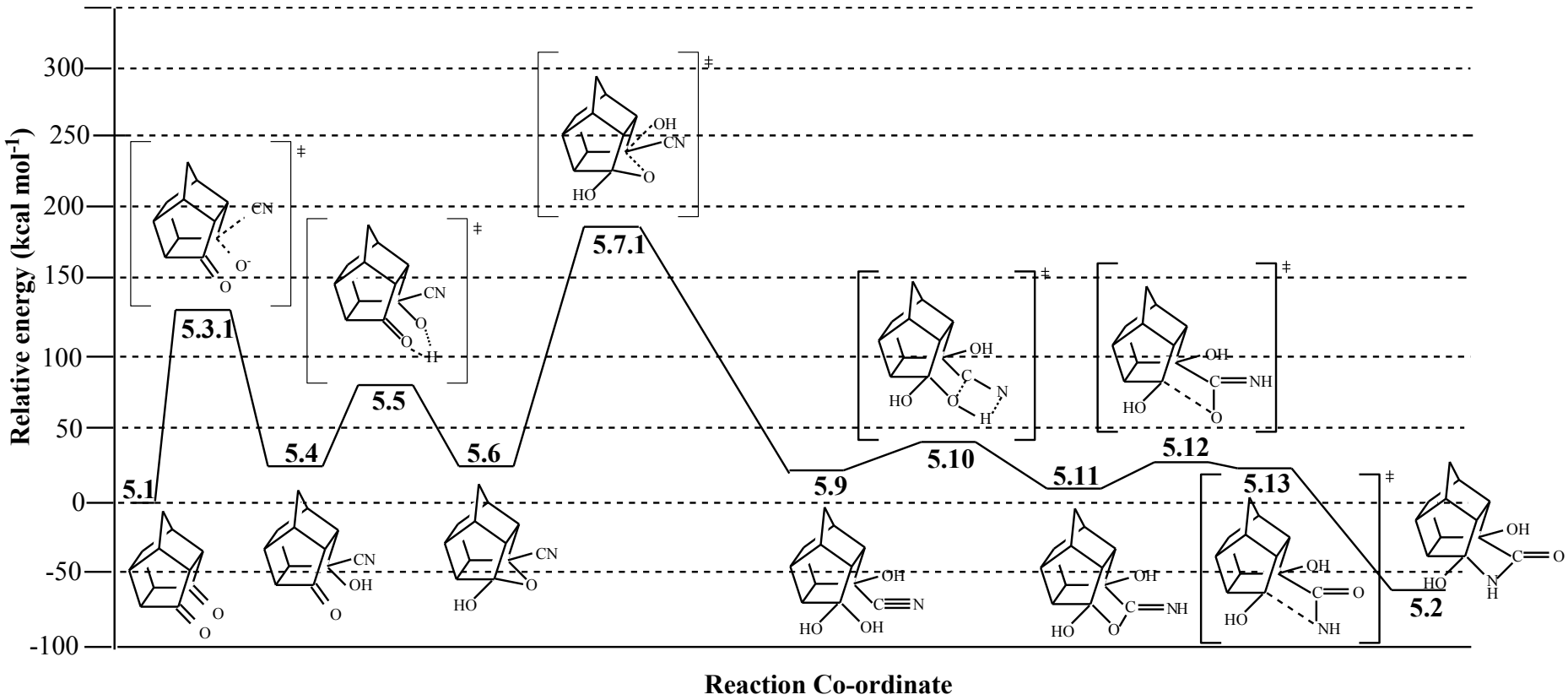
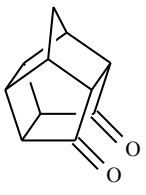


Figure 5.2 Calculated reaction profile for the proposed mechanism.

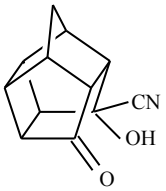
The cartesian coordinates of all the 3D structures presented in this Chapter are included on the CD accompanying this Thesis.

5.2 Local minima on the energy profile

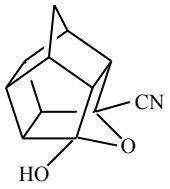
Structures **5.1**, **5.4**, **5.6**, **5.9**, **5.11**, and **5.2** shown below are stationary points classified as local minima on the energy profile of the reaction.



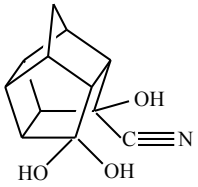
5.1



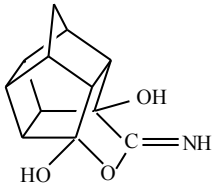
5.4



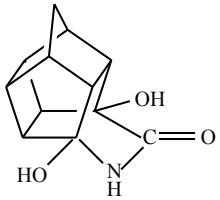
5.6



5.9



5.11



5.2

An energy minimization was performed for each of the above structures to remove any Van der Waals contacts or bond overlap. The calculated energies for the above structures are presented in the Table 5.1. Note that the only rotational flexibility in these structures are the C-OH bonds illustrated above. The corresponding bonds were rotated at angles of 30º intervals and re-optimized to ensure the lowest possible isomer was obtained.

Table 5.1 Calculated energies of the local minima.

	Relative energies[a]		
Structure number[b]	**STO-3G/Hartrees**	**3-21+G*/Hartrees**	**3-21+G*/kcal mol^{-1}**
5.1	-565.0296	-568.9543	0
5.4	-656.7586	-661.3513	27.66
5.6	-656.8147	-661.3657	18.66
5.9	-731.7744	-731.9821	19.79
5.11	-731.8214	-737.0049	6.19
5.2	-771.8263	-737.0314	-10.46

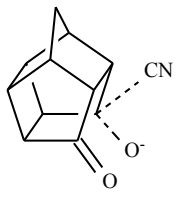
[a]Relative energies are expressed in Hartrees and kcal mol^{-1}, performed at the HF level using the STO-3G basis set, followed by a higher 3-21+G* level of theory.

[b]Structure number as per proposed reaction mechanism shown in Figure 5.1.

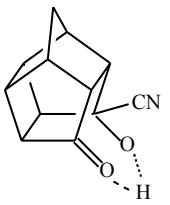
From the results presented in Table 5.1, it is evident that the higher level basis set produces a significantly lower energy value. (Note that energies obtained with different basis sets cannot be directly compared). In addition, when the reaction profile as shown in Figure 5.2, was plotted, it was also evident that the energy values (heats of formation) confirm that structures **5.1**, **5.4**, **5.6**, **5.9**, **5.11**, and **5.2** are indeed minima.

5.3 The Transition Structures (TS)

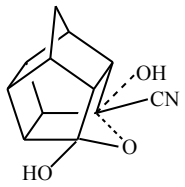
Structures **5.3.1, 5.5, 5.7.1, 5.10, 5.12** and **5.13** shown in Figure 5.1 are characterized as the following transition-state structures.



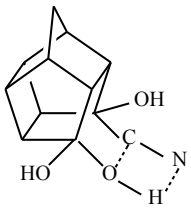
5.3.1



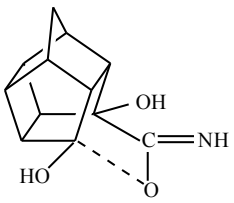
5.5



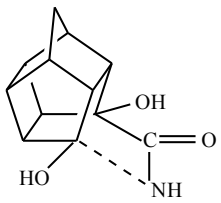
5.7.1



5.10



5.12



5.13

The cartesian coordinates of all the 3-D structures presented in this Chapter are contained on the CD accompanying this Thesis. Please refer to Chapter 3 for a discussion on the techniques used to determine the transition-states below.

An explanation of the different types of SCAN calculations used in the route section for the location of the various transition structures is given in Chapter 4. The calculated energies for the above structures are presented in the Table 5.2.

Table 5.2 Calculated energies of the transition structures.

	Relative energies[a]	
Structure number[b]	**3-21+G*/Hartrees**	**3-21+G*/kcal mol^{-1}**
5.3.1	-660.7663	127.39
5.3.2	-736.9142	63.11
5.5	-661.2569	86.90
5.7.1	-736.3609	188.43
5.7.2	-812.5102	77.74
5.10	-736.8741	88.27
5.12	-736.8873	79.95
5.13	-736.8880	79.55

[a]Relative energies are expressed in Hartrees and kcal mol^{-1}, performed at the HF level using the 3-21+G* level of theory.

[b]Structure number as per proposed reaction mechanism shown in Figure 5.1.

In the discussion of the results for each of the transition-states, the three dimensional (3-D) structures have been referred to as **Scan start** or **Scan end**. Scan start implies the starting structure that was submitted for the calculation. Scan end refers to the corresponding structure that was obtained at the end of the scan calculation. By inspecting the different structures at each step of the scan job, one could follow the reaction profile and by plotting the corresponding energies vs. the reaction coordinate, one can obtain an approximate indication of the transition structure involved. This approximate starting structure for a full (non-restrained) transition-state search was obtained from the SCAN calculation by manual isolation of the coordinates of the structure closest to the maxima on the reaction profile (see Figure 5.3).

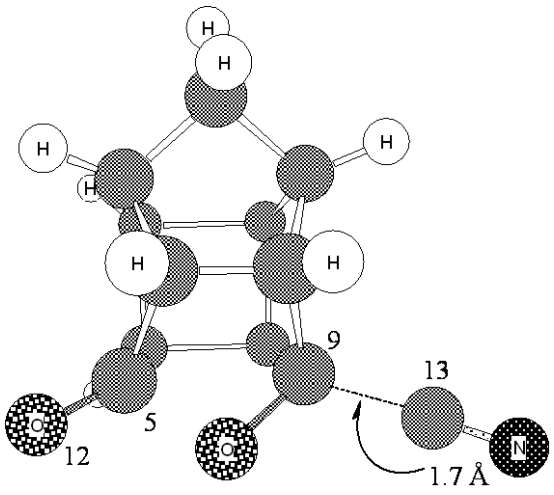
The same basic computational methods used for the calculation of the local minima energies were utilized in locating the geometries of the transition-state structures. The only difference is that the last part of the procedure made use of a transition-state optimization during a scan close to the maxima associated with the corresponding TS. The transition structure that was obtained is referred to **TS end**. A summary of the results obtained for each of the transition-state structures follows.

Note that the Gaussian 98 frequency output files of the different transition-states are available on the CD attached to this thesis. Molekel (freeware) at the site:

www.cscs.ch/molekel can also be used to view the frequency output files, in particular the vibrations associated with the negative eigenvalue.

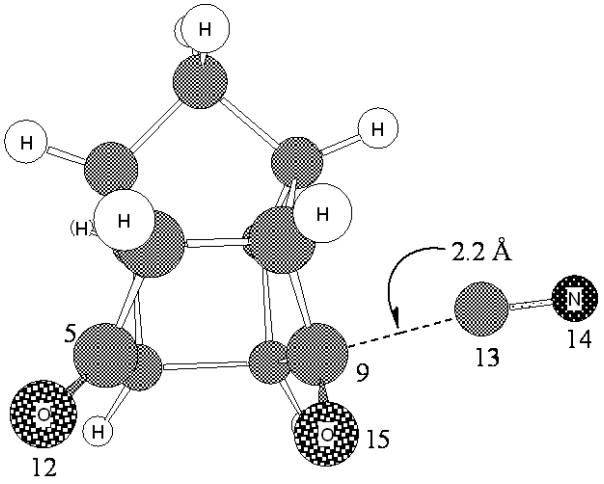
5.3.1 Transition Structure 5.3.1

A constrained optimized structure (C9-C13, fixed at 1.7 Å) was used as input for a relaxed SCAN calculation. The three dimensional (3-D) input structure for the relaxed SCAN calculation is represented below.



5.3.1 (Scan start)

It is clear from the geometry of the structure above that the structure would be close to the maxima on the energy profile or perhaps closer to the formation of the intermediates **5.4** or **5.6** (see Figure 5.2). Note the carbonyl carbon (C5) is bending out of plane, starting to become sp^3 hybridised. The reaction coordinate C9 and C13 was scanned from 1.7 Å to 2.2 Å since the TS involved the formation of the bond between atoms C9 and C13. The output of the Scan optimization is shown below as **5.3.1 (Scan end)**.



5.3.1 (Scan end)

On closer inspection of the Scan end file, it is clear that, as the reaction coordinate between atoms C9 and C13 increased, the CN group moved away from the cage, and the distance between atoms C5 and O15 increased accordingly. The carbonyl carbon (C5) is again sp^2 hybridised. The reaction profile of the step-wise increase in bond length between atoms C9 and C13 is graphically presented in Figure 5.3.

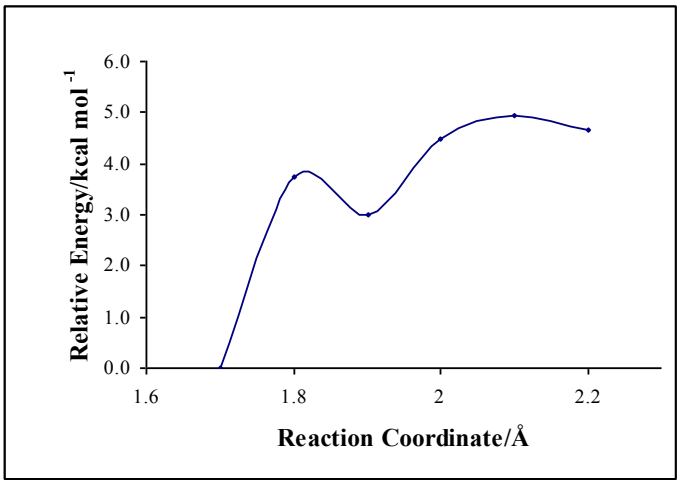
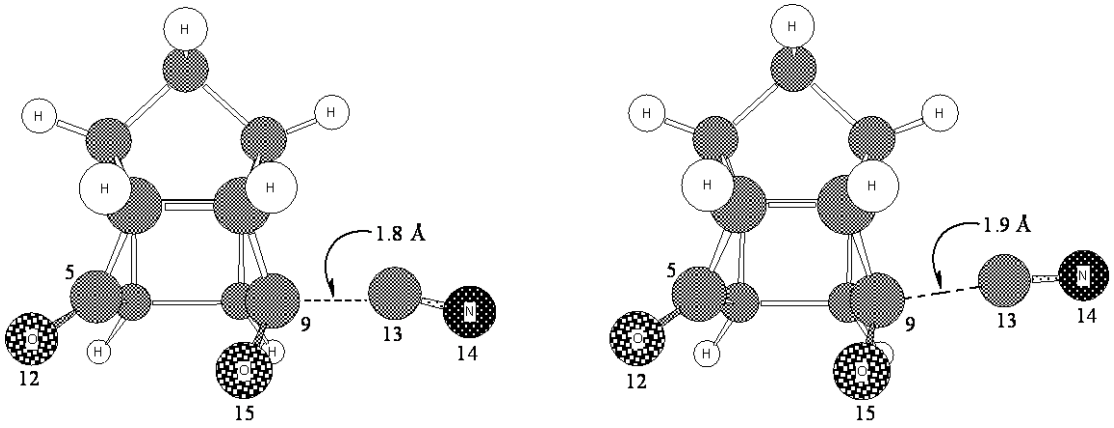


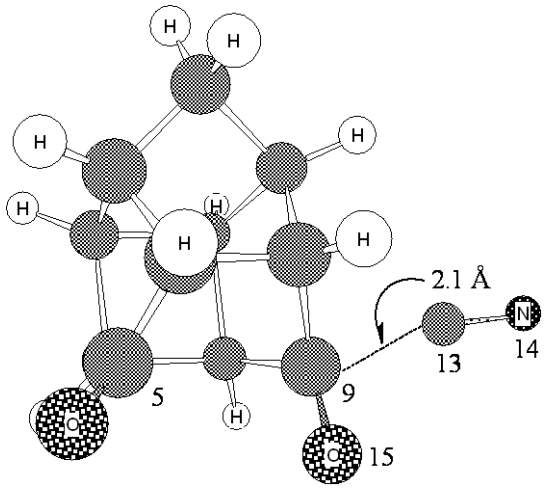
Figure 5.3 Graphical representation of energy vs reaction coordinate for structure 5.3.1.

Figure 5.3 shows that a minimum energy value occurs at 1.9 Å and a maximum energy at 2.1 Å. Closer examination of the structure at the maxima of 1.8 Å and the structure at the minima of 1.9 Å suggests that it is due to the rotation of the cyano CN group (C13-N14), that is, the cyano group moving from the front of the cage to the

back, as shown in the 3-D structures below. This phenomenon is therefore not likely to be associated with the required transition structure - one would rather expect bond formation/dissociation between C9 and C13.



The coordinates of the structure closest to the second maxima (2.1 Å) was manually extracted from the Scan output file. This geometry of the structure was found to be close to the expected TS. Thus a TS search was carried out using the structure at 2.1 Å as approximate starting structure for a full transition-state optimization. The 3-D TS optimization is shown below.



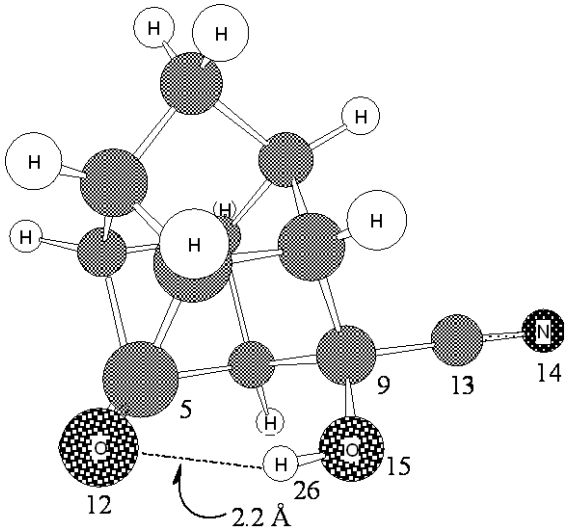
5.3.1 TS end

The TS calculation was verified by performing a frequency (FREQ) calculation resulting in ONE negative eigenvalue only. The FREQ calculation was viewed using the GaussView[61] program, enabling the vibration mode, associated with the negative eigenvalue, so that the bond formation between the cyano group (C13-N14) and C9 is clearly visualized. The vibration associated with the imaginary frequency shows the

cyano group (C13) moving towards the cage to form a bond with C9. It is also clear that the carbonyl carbon (C9) is converted to a sp^3 carbon while O15 is moving towards C5 as the nucleophile C13 is approaching the carbonyl carbon C9.

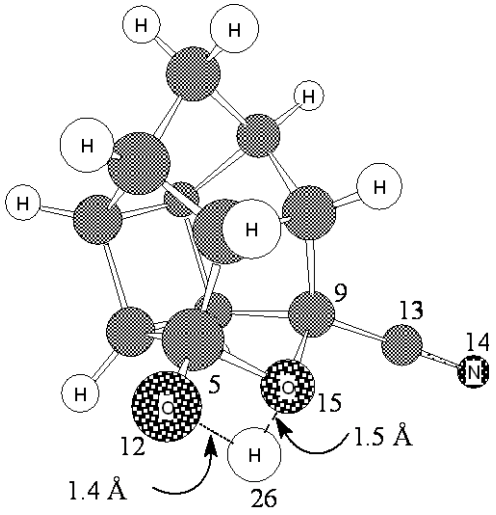
5.3.2 Transition Structure 5.5

Finding transition structure **5.5**, (see Figure 5.2), involved monitoring the intramolecular transfer of the hydrogen atom (H26) between the two oxygen atoms (O12 and O15). Shown below is the 3-D structure (**5.5-Scan start**) which was used as the starting structure for the relaxed scan.



5.5 (Scan start)

The bond was scanned from 2.2 Å to 1.4 Å. The output 3-D structure **5.5 (Scan end)** is shown below.



5.5 (Scan end)

It is clear that the hydrogen (H26) is transferred during the Scan calculation. The structure **5.5 (Scan end)**, above, when compared to the **5.5 (Scan start)** shows that the atoms C9-C13-N14 keep a linear bond as expected. Atoms C5 and O15 forms a bond as the distance between atoms O12 and H26 decreases as a result of the H-transfer. Atom H26 orientates itself between atoms O12 and O15. The scan is graphically depicted below.

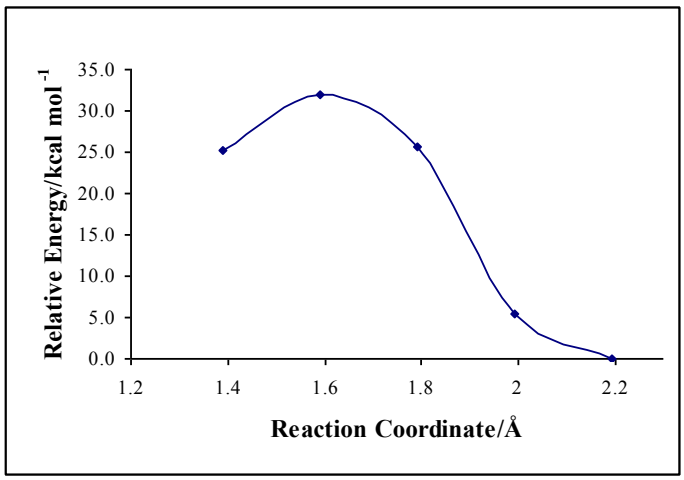
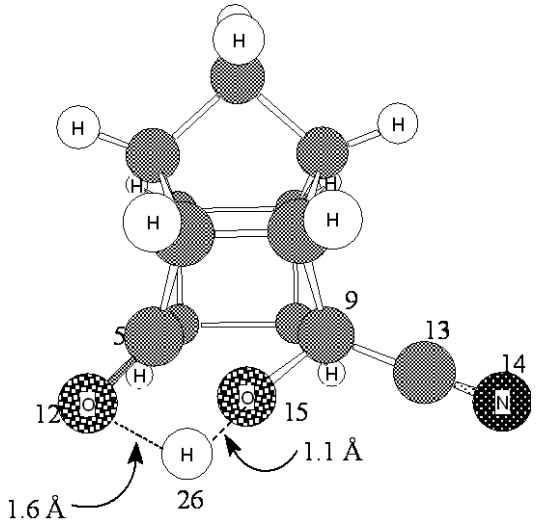


Figure 5.4 Graphical representation of energy vs. reaction coordinate for structure 5.5.

The corresponding structure closest to the maximum in Figure 5.4 is at 1.6 Å. The structure at this bond length was manually extracted from the scan output file and

submitted as input structure for a TS optimization. The resultant TS structure that was obtained at the end of the TS optimization is represented below.



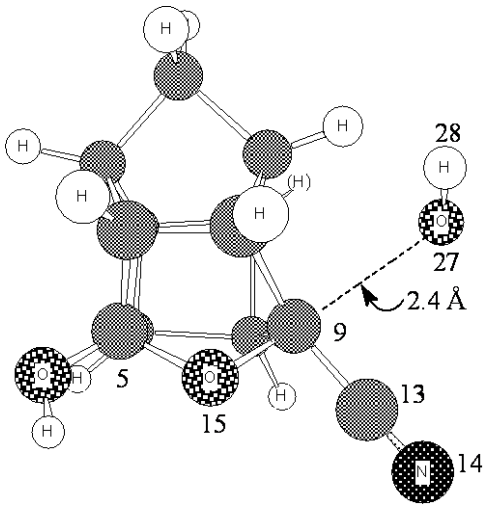
5.5 TS end

The TS structure was verified to be correct since the FREQ calculation produced only one negative eigenvalue and the movement of atoms associated with the negative eigenvalue correspond to the expected movement of atoms on the reaction profile. This movement includes transfer of atom H26 between atoms O15 and O12 and bond formation/dissociation between C5-O15 as discussed above.

5.3.3 Transition Structure 5.7.1

The transition structure depicted as structure **5.7.1** was complex and difficult to find as will be described next.

In structure **5.7.1** the calculations involved monitoring the progress of the hydroxyl group (O27-H28) attaching to the cage and the breaking of the C9-O15 (ether/acetal) bond.



5.7.1 (Scan start)

The graphical presentation of the relaxed scan, that is, the decrease of the reaction coordinate as the hydroxyl group (O27-H28) attaches to C9 from 2.4 Å to 1.3 Å is shown below.

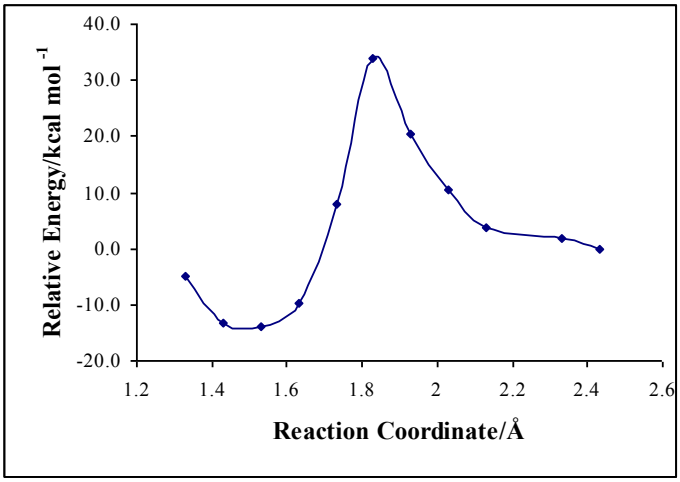
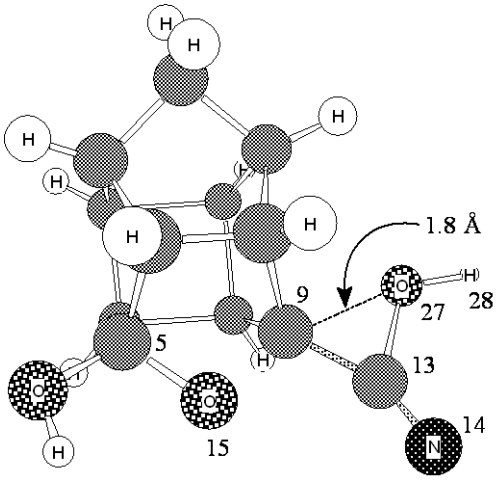


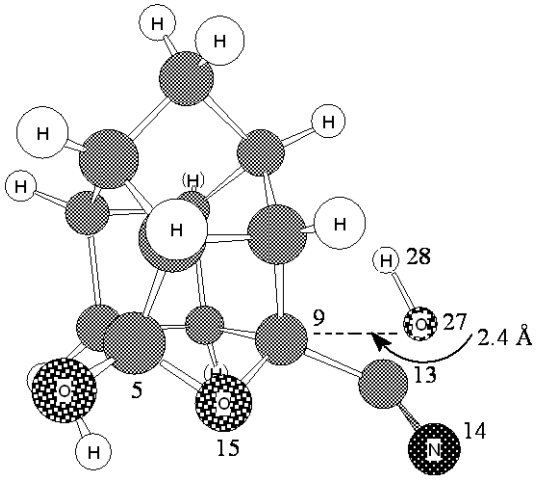
Figure 5.5 Graphical representation of energy vs. reaction coordinate for structure 5.7.1.

This transition structure is also an example of a case for which the graph exhibits a maximum, but is not necessarily indicative of the required transition-state. The explanation of how the "transition-state" was found follows. The maximum in Figure 5.5 is at 1.8 Å. Thus the transition-state optimization for structure **5.7.1** was carried out using the structure closest to this maximum bond length (1.8 Å). The 3-D input structure (**5.7.1 TS1 start)** which was used for the transition structure optimization

and the corresponding 3-D non-restricted output structure (**5.7.1 TS1 end)** that was obtained are shown below.



5.7.1 TS1 start



5.7.1 TS1 end

The input structure, **5.7.1 TS1 start**, had the hydroxyl group (O27-H28) at bond length 1.8 Å coming in to attach to the atom C9 thereby forming a bond. In the output structure, **5.7.1 TS1 end**, the hydroxyl group (O27-H28) has moved away from atom C9 and a bond has formed between atoms C9 and O15. The distance between C9 and O27 is 2.4 Å suggesting that the structure has gone all the way back to reactant, i.e., structure **5.7.1 (Scan start)**. The frequency calculation for **5.7.1 TS1 end** at 1.8 Å was then calculated and although having a negative eigenvalue, shows the incorrect vibration, i.e. the "waving" of the O27-H28 group away from the cage, confirming that this is not the required transition structure.

A second attempt to locate the transition structure **5.7.1** was carried out. A narrow-range relaxed scan (using a smaller step size of 0.05 Å) from 2.0 Å to 1.7 Å was performed. The graphical representation of the narrow-range relaxed scan is shown below.

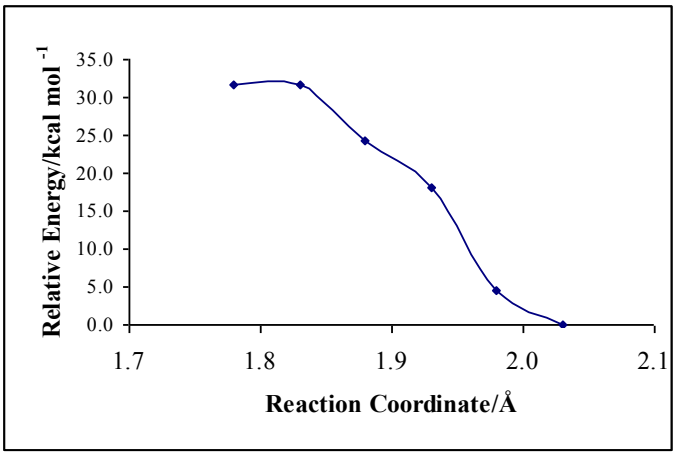
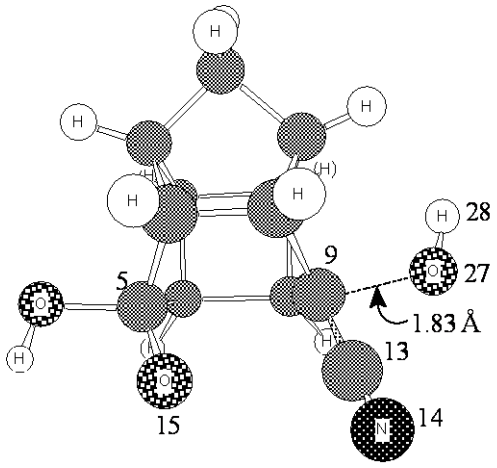
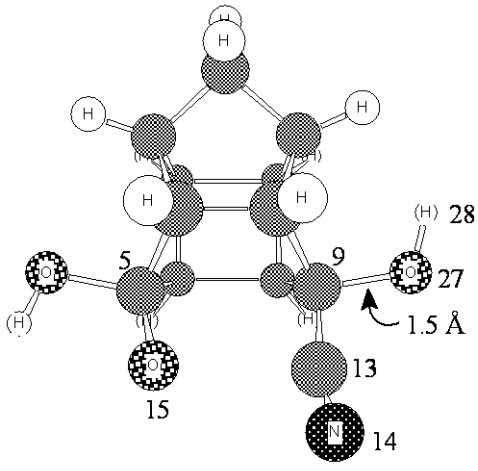


Figure 5.6 Graphical representation of energy vs. reaction coordinate of the zoomed in (2.03 Å to 1.78 Å) relaxed scan for structure 5.7.1.

The maximum in Figure 5.6 is at 1.83 Å. The structure closest to this maximum bond length was extracted from the scan output file and used in the transition structure optimization. This second transition structure optimization was performed using CALCFC (refer to Chapter 4 for a discussion on the CALCFC option) in the route section of the Gaussian input file. The 3-D input structure (**5.7.1 TS2 start**) and the corresponding 3-D output structure (**5.7.1 TS2 end)** that was obtained is depicted below.



5.7.1 TS2 start



5.7.1 TS2 end

The output structure, **5.7.1 TS2 end**, shows the correct bond formation between atoms C9 and O27. However, the FREQ calculation for **5.7.1 TS2 end** at 1.5 Å again shows the "waving" of the O27-H28 group away from the cage with no movement for the

required reaction coordinate (C9–O27), confirming that this too is not the transition structure.

The third attempt to locate the transition structure **5.7.1** was carried out by performing another narrow-range relaxed scan (using a smaller step size of 0.05 Å) from 1.8 Å to 1.4 Å. The results of this scan are shown below in Figure 5.7.

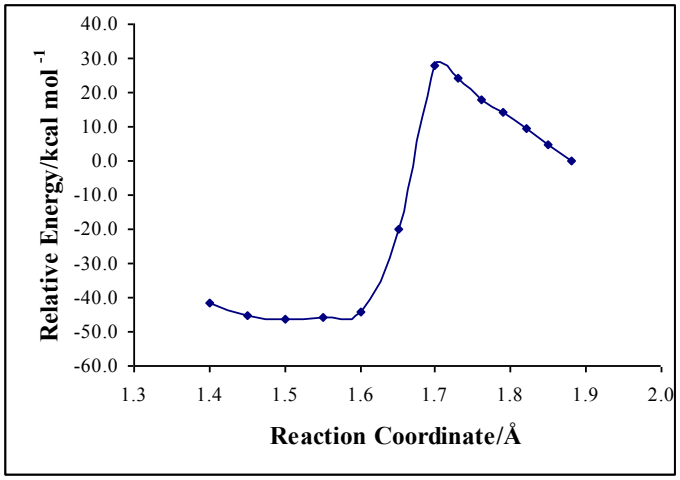
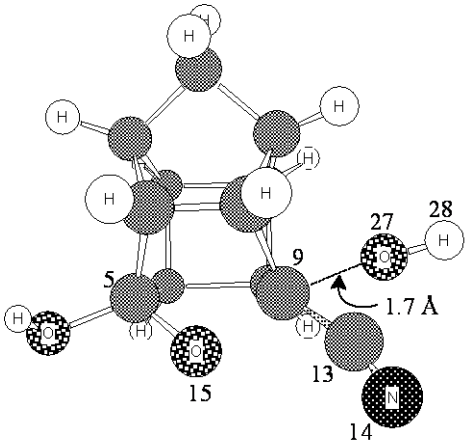
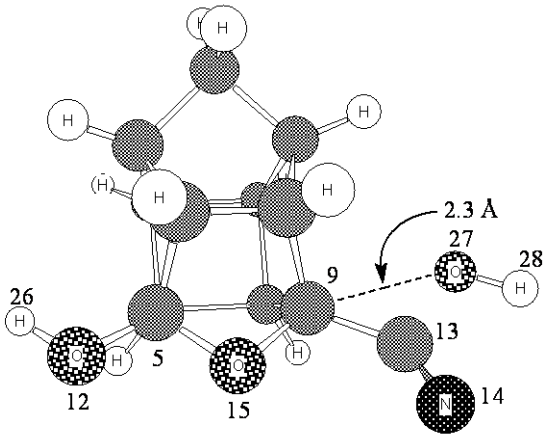


Figure 5.7 Graphical representation of energy vs. reaction coordinate of the zoomed in (1.83 Å to 1.35 Å) relaxed scan for structure 5.7.1.

The maximum in Figure 5.7 is at 1.7 Å. The corresponding structure closest to this maximum bond length was used in this transition structure optimization. The 3-D input structure (**5.7.1 TS3 start**) and the corresponding 3-D output structure (**5.7.1 TS3 end)** that was obtained is depicted below.



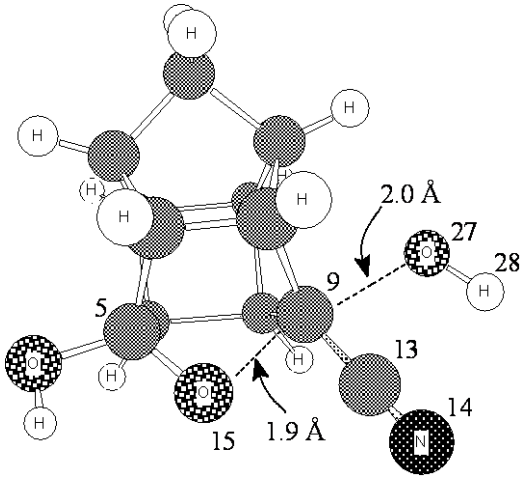
5.7.1 TS3 start



5.7.1 TS3 end

From the output, it can clearly be seen that the hydroxyl group O27-H28 has again moved away from atom C9 instead of moving closer to it. The FREQ calculation shows a vibration of the other hydroxyl group (O12-H26), on the left side of the cage. This is also not the transition structure.

Another transition structure optimization at 1.7 Å, using the same cartesian coordinates as **5.7.1 TS3 start,** was carried out, this time using CALCFC in the route section of the Gaussian input file. The 3-D output structure (**5.7.1 TS4 end**) that was obtained is shown below.

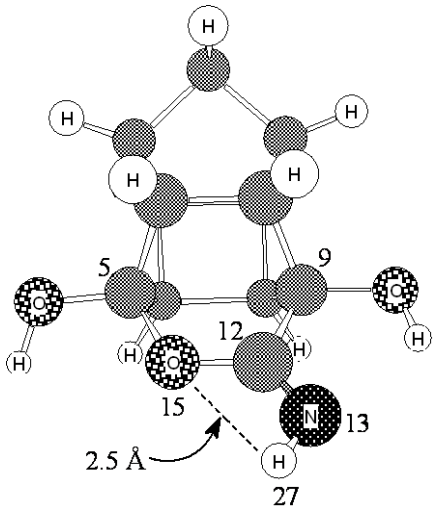


5.7.1 TS4 end

This output structure shows the correct orientation of the hydroxyl group (O27-H28). The negative eigenvalue of the frequency calculation of **5.7.1 TS4 end** shows the movement of the hydroxyl group (O27-H28) attaching to atom C9 on the cage and the formation dissociation of the bond between atoms O15–C9 and O27–C9 which is expected in the corresponding transition structure. The distance between O27–C9 in the start structure (**5.7.1 TS3 start**) was 2.3 Å. This distance was reduced to 2.0 Å in the **5.7.1 TS4 end** structure. However, this TS as well, produces a high energy value since O15 has a negative charge (ionic species) in a gas phase calculation (see Figure 5.2). An explanation for the high energy is presented in Section 5.4 at the end of this chapter.)

5.3.4 Transition Structure 5.10

The next transition structure on the reaction profile was then attempted, namely structure **5.10** in Figure 5.1. On closer inspection of the structure shown below, it can be seen that the structure is actually **5.11**. The 3-D input structure for the relaxed SCAN calculation is represented below. A relaxed scan from 2.5 Å to 1.2 Å between atoms O15 and H27 was performed to see if atom H27 is transferred to atom O15. If atom H27 moves closer to O15, this will result in the bond between atoms O15-C12 and N13-H27 breaking. The graphical presentation of the relaxed scan is also depicted below.



5.10 (Scan start)

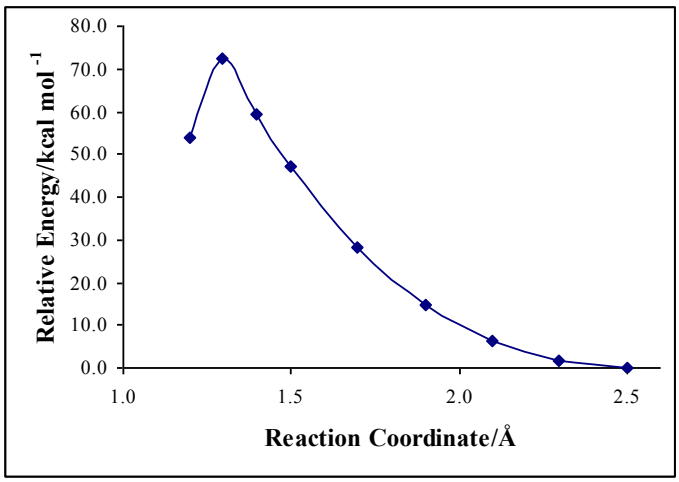
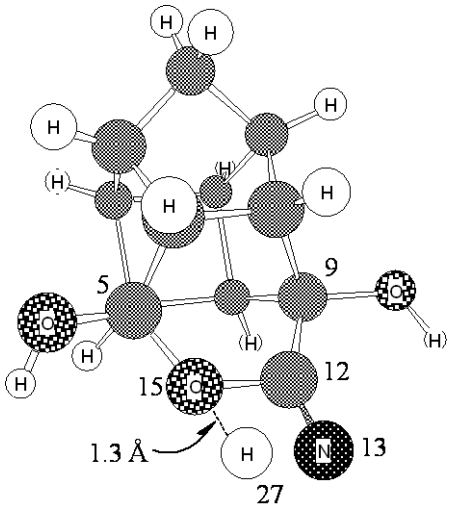
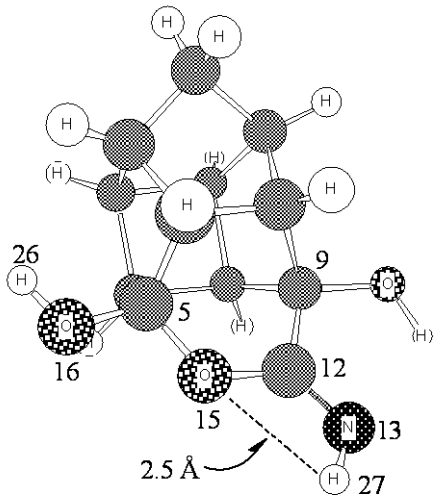


Figure 5.8 Graphical representation of energy vs. reaction coordinate for structure 5.10.

The maximum in Figure 5.8 is at 1.3 Å. Hence the structure closest to this maximum bond length was manually extracted from the scan output file and used in a transition-state optimization. The 3-D input structure **5.10 TS1 start** and the 3-D output structure **5.10 TS1 end** that was obtained is depicted below.

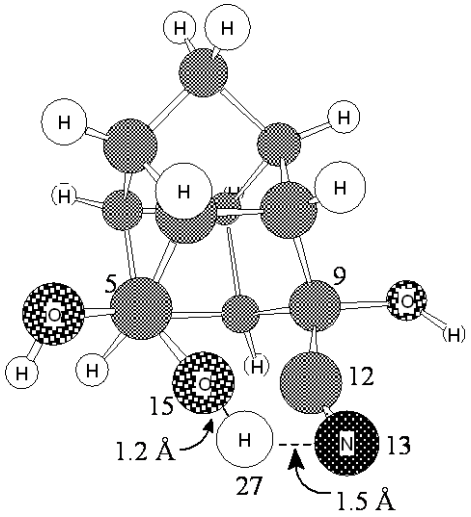


5.10 TS1 start



5.10 TS1 end

The end structure, above, shows the correct orientation of the atoms however, the expected O15-C12 bond break did not occur. The negative eigenvalue of the frequency calculation of **5.10 TS1 end** shows the vibration of the O16-H26 hydroxide confirming that this is the incorrect transition structure. In order to find the correct transition-state the same input file was used, **5.10 TS1 start**, but the search for the transition-state was changed to include CALCFC in the route section of the Gaussian input file. Shown below is the output structure, **5.10 TS2 end** that was obtained using CALCFC.

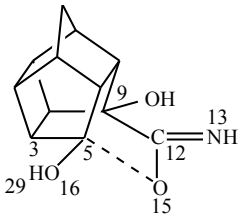


5.10 TS2 end

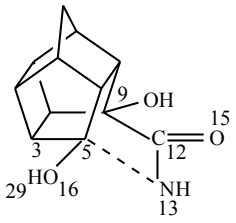
The output structure above clearly shows the bond break between atoms O15 and C12. The frequency calculation shows the intramolecular transfer of atom H27 between O15 and N13. As atom H27 is transferred to atom O15, there is a subtle movement of the bond C12-O15, verifying that this bond breaks/forms as well. This confirms that this is the expected TS.

5.3.5 Transition Structure 5.12 and 5.13

Shown below are diagrams of postulated transition structures **5.12** and **5.13**.

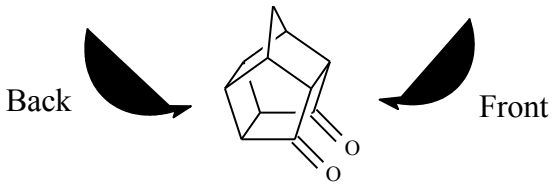


5.12



5.13

When referring to the above structures, in particular the nitrogen N13 and oxygen O15, with reference to its location on the cage, it was stated as either being at the "front" or "back" of the cage. "Front" is defined as closer to the CH_2 bridge at the top (see figure below) and "back" as closer to the cyclobutane ring.



5.1

Starting structures were constructed by setting the angles C9-C12-C13-O15 and C3-C5-C16-O29 (in **5.12** and **5.13**) at +90º and -90º. On closer examination of the above two structures, it was noted that in **5.12**, the transition structure had the nitrogen at back of the cage and in **5.13** the nitrogen was in front. The angle C3-C5-C16-O29 was fixed since it interfered with the SCAN calculation. When the transition structure optimization was performed for each structure no restraints were applied. These two transition structures were calculated simultaneously. First, a relaxed scan was performed for **5.12**. The bond length between atoms C5 and O15 was scanned from 3.2 Å to 1.9 Å. The graphical presentation of the relaxed scan is depicted below.

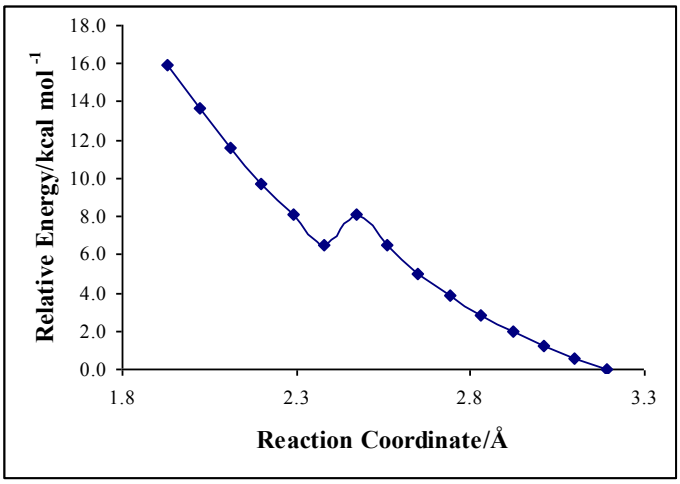
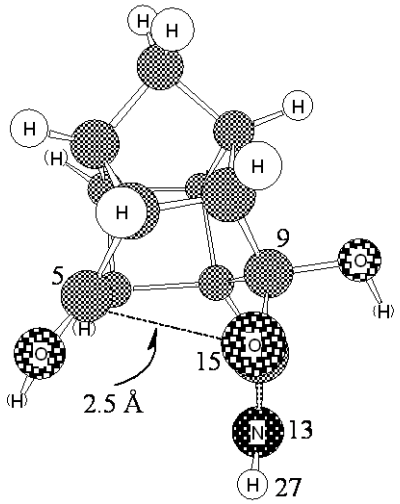
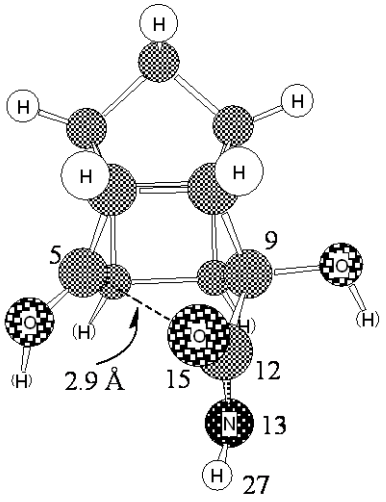


Figure 5.9 Graphical representation of energy vs. reaction coordinate for structure 5.12.

From Figure 5.9, it can be seen that there is a slight maximum at 2.5 Å. The structure closest to this maximum bond length was manually extracted and submitted for a transition-state optimization. The 3-D TS input structure and the 3-D TS output structures that were obtained for **5.12** are shown below.



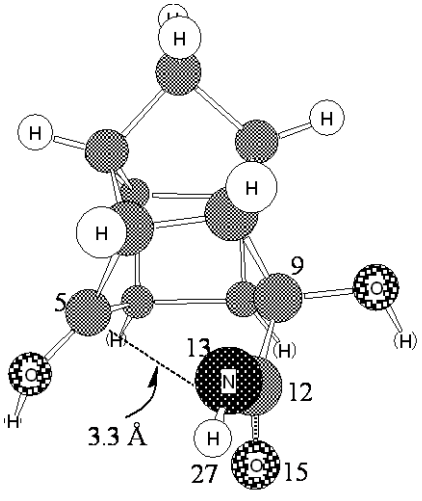
5.12 TS1 start



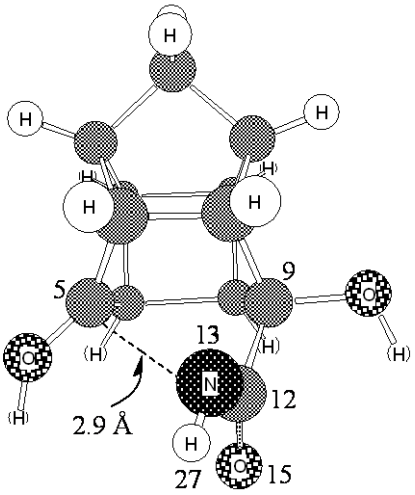
5.12 TS1 end

The output structure shows the correct orientation of the atoms. The frequency calculation when viewed enabling the vibration mode showed the C5–O15 bond break associated with the negative eigenvalue.

In the transition structure optimization of **5.13**, the same structure that was used as the input coordinates for **5.12 TS1 start**, was used but the atoms O15 and N13 were rotated so that N13 was now positioned at the front of the cage. The 3-D TS input structure and the 3-D TS output structures that were obtained for **5.13** are shown below.



5.13 TS1 start



5.13 TS1 end

The output TS structure shows the correct orientation of the atoms and the frequency calculation shows the C5–N13 bond formation corresponding to the single negative eigenvalue.

Further scans were performed and it was observed (see Figure 5.10 below) that there is a possibility that instead of just two transition structures, there may actually be four transition structures present. The two transition structures described thus far, have bond breakage for C5-O15 (**5.12 TS1 end**) and C5-N13 bond formation (**5.13 TS1 end**). These two transition structures occur with the movement of atoms on opposite sides of the cage moiety. It might be possible that two more transition structures exist, where C5-O15 bond breakage/formation (**5.12 TS2 end**) and C5-N13 bond breakage/formation (**5.13 TS2 end**) flip around to the back of the cage. In order to confirm the absence and or presence of these other two transition structures, a modified scan procedure involving steps wise variation of angles were used.

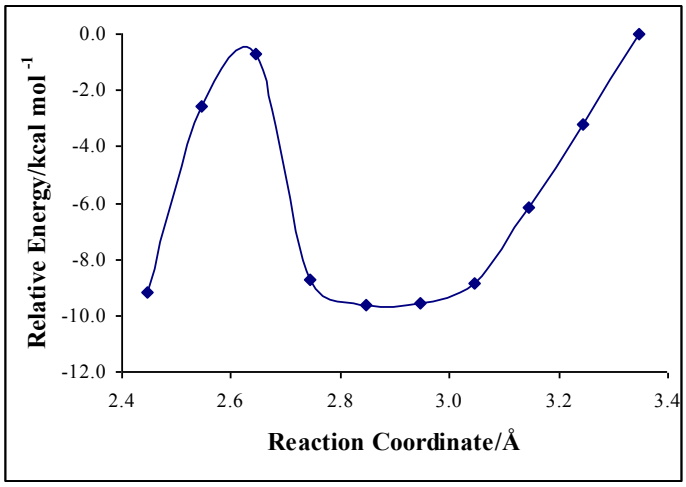
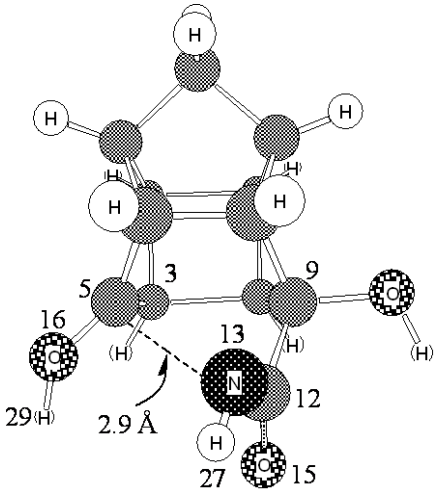


Figure 5.10 Graphical representation of energy vs. reaction coordinate for structures 5.12 and 5.13.

The above scan results in Figure 5.10 indicate a maximum and a minimum when scanning the bond lengths. This meant that it would be more feasible to use dihedral angles instead of bond lengths in the SCAN calculations. The first SCAN calculation was done using structure **5.13**. Shown below is the 3-D TS output structure (**5.13 TS1 end**) that was used for the scan.



5.13 TS1 end

The above TS structure was modified to have atoms 9, 12, 13, 15 fixed at an angle of 180°. Atoms 3, 5, 16, 29 were fixed at an angle of 0° away from the cyano group since the hydroxide (O16-H29) was interfering in the SCAN calculation. The scan of the angle between atoms 5, 9, 12, 13 was scanned from –60° to –110°.

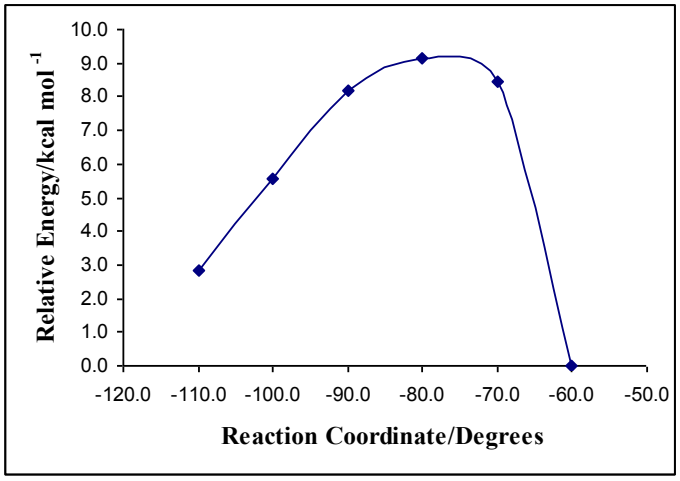
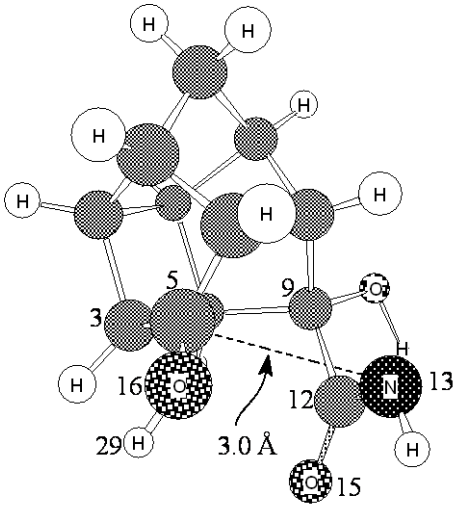
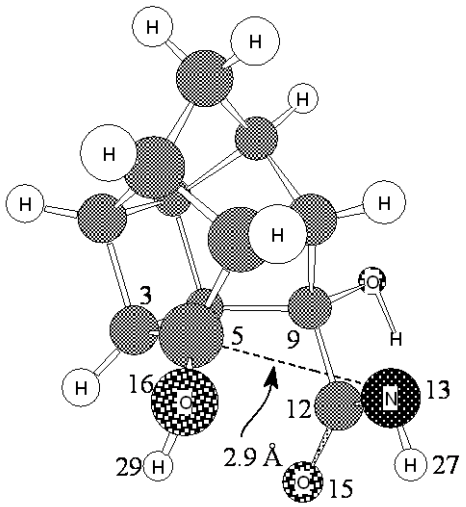


Figure 5.11 Graphical representation of energy vs. reaction coordinate for structure 5.13.

A maximum was observed at -80.0°. The structure closest to the maximum was extracted from the scan output file (**5.13 TS2 start**) and submitted for a TS search. The input and output structures (**5.13 TS2 end**) that were obtained are shown below.



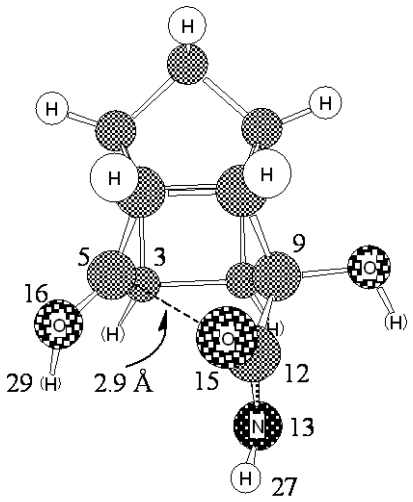
5.13 TS2 start



5.13 TS2 end

The frequency calculation produced one negative eigenvalue corresponding to the following: N13 moving towards C5 to "close" the cage (bond formation) and forming the lactam **5.2**.

The second SCAN calculation was done using structure **5.12**. Shown below is the 3-D TS output structure (**5.12 TS1 end**) that was obtained from the scan.



5.12 TS1 end

The above TS structure was modified to have atoms 9, 12, 13, 15 fixed at an angle of 180°. Atoms 3, 5, 16, 29 were fixed at an angle of 0° for the same reason as stated above. The scan for the atoms 5, 9, 12, 13 was carried out from 60° to 110°.

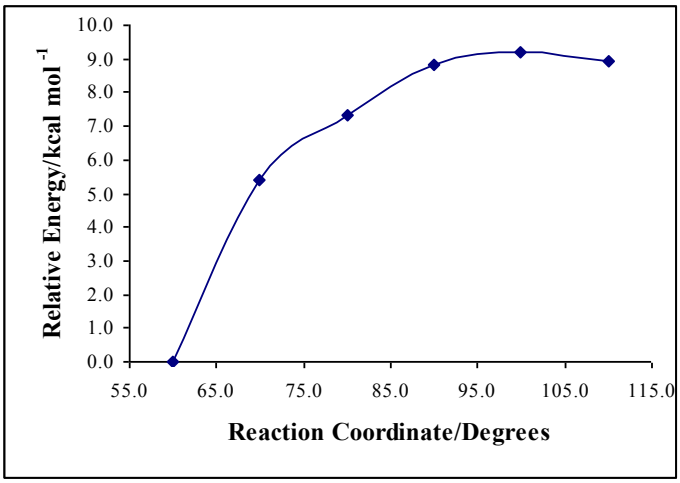
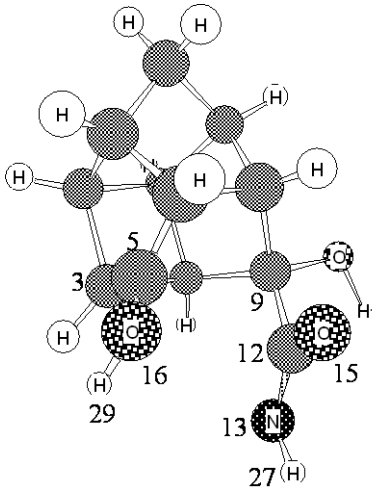
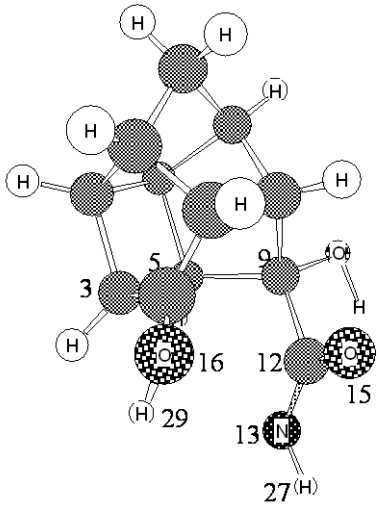


Figure 5.12 Graphical representation of energy vs. reaction coordinate for structure 5.12.

A maximum was observed at 100.0°. The structure closest to the maximum was extracted from the scan output file (**5.12 TS2 start** as shown below) and submitted for a TS optimization. The output structure (**5.12 TS2 output**) is also shown below.



5.12 TS2 start



5.12 TS2 end

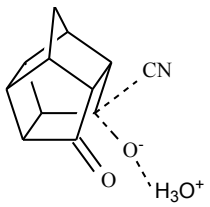
The negative eigenvalue of the frequency calculation corresponds to the correct vibration for above TS, that is, O15 breaking away from C5.

The energies of the four transition structures obtained namely, **5.12 TS1**, **5.12 TS2**, **5.13 TS1** and **5.13 TS2**, were compared and it was found there was no significant difference in the energy values and the geometry of the structures. Thus it was concluded that only two transition structures exist.

5.4 Transition structure modeling with solvent molecules

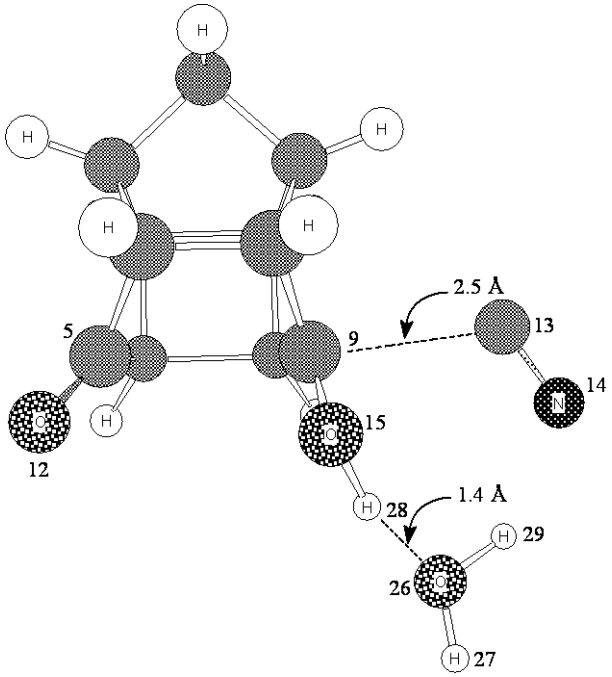
In the reaction profile Figure 5.2 (page 32) it can be seen that structures **5.3.1** and **5.7.1** have relatively high-energy values in comparison to the other transition-state structures in the profile. This is expected since the calculation was carried out in the gas phase. Ionic species in the gas phase have a much higher energies than when they are solvated in an aqueous medium. In aqueous solution the intermediate oxygen anion would instantly remove a proton from the solvent to become a neutral OH species (i.e., to form **5.4** and **5.9**). We therefore elected to perform the calculation for the relatively high energy transition state structures, with one solvent molecule present.

The first "solvated" transition structure **5.3.2** is shown below.



5.3.2

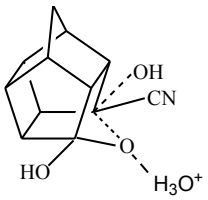
When H_3O^+ is added to the **5.3.1 TS end** (Page 38) structure, the total charge is zero and one could essentially obtain a non-ionic transition structure involving a solvent molecule, which should have a considerably lower energy. A starting structure for the "solvated" transition-state was obtained by fixing the bond length (C9-C13) of the incoming cyano group at 2.1 Å and H_3O^+ positioned about 2.0 Å away from O15. The structure was then allowed to partially optimize for 20 cycles using the normal restricted transition structure algorithm. The partially optimized structure was used as a starting structure for a "solvated" transition structure. Only the 3-D optimized TS end structure is shown below.



5.3.2 TS end

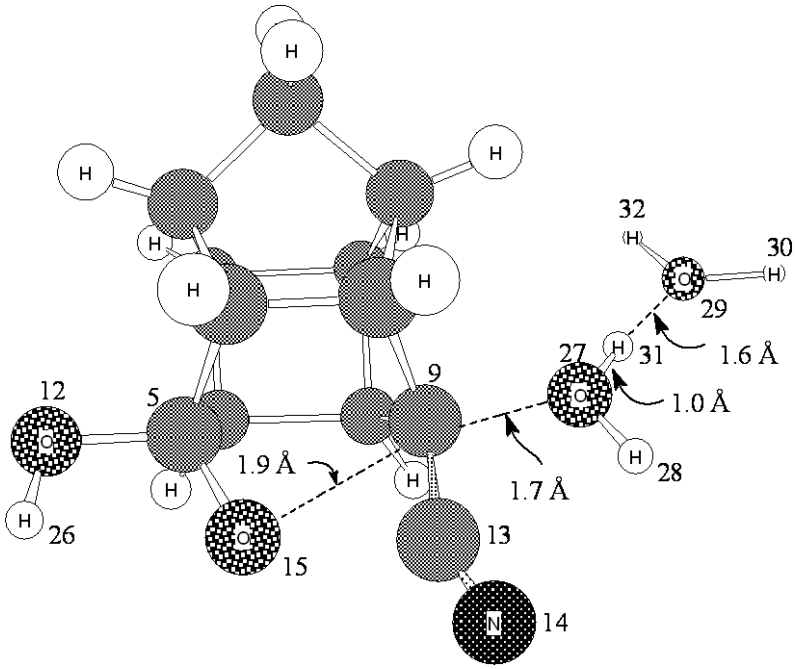
A frequency calculation was carried out on the **5.3.2 TS end** structure. The FREQ calculation produced one negative eigenvalue and when the vibration associated with that negative eigenvalue was viewed, it showed clearly the bond formation between C13 and C9 as well as the intramolecular transfer of hydrogen H28 between oxygen atoms O15 and O26. The relative energy obtained for this "solvated" neutral TS was much lower (110.1 kcal mol^{-1}) than the gas phase ionic transition-state obtained for **5.3.1 TS end**. Thus this lower energy was used to calculate the relative energies for the reaction profile shown in Figure 5.13. Since only one solvent molecule was used, it should be emphasized that this method provides an approximate answer. It is still not viable to use more solvent molecules at the *ab initio* level. In reality H_3O^+ is also not present, although the approximation is not too unusual since to remove a proton from an alcohol (the reverse of the reaction), H^+ will be released to form H_3O^+.

The second "solvated" transition structure to which a solvent molecule was added is **5.7.2** depicted below.



5.7.2

A TS optimization, using the same procedure that was employed for the location of **5.7.1 TS4 end** (Page 46), was used for **5.7.2** but this time it was carried out in the presence of a solvent molecule. The starting structure was obtained by fixing the reaction coordinate between C9-O15 at 1.9 Å An H_3O^+ ion was also placed about 2.0 Å away from the oxygen atom O27. This structure was then used for a TS optimization. The 3-D TS output structure for the optimized transition-state is presented below.



5.7.2 TS end

In the SCAN calculation, the reaction coordinate between C9-O15 was fixed at 1.9 Å. H_3O^+ was added close to the attacking OH^- (O27-H28) with the hope that the transfer of a proton between O27 and O29 could be observed. The molecule was partially optimized using a constrained transition-state optimization. The constraints were then released and a full transition-state optimization was performed followed by a frequency calculation. The FREQ calculation produces one negative eigenvalue and

when the vibration associated with that negative eigenvalue was viewed, it showed clearly the bond formation between C13 and O15. It is clearly visible that the OH^- (from O27) is attacking the quaternary carbon (C9) on the cage with C9-O15 bond braking. It is also clear that H is transferred between O27 and N14. The transition-state therefore leads to formation of product **5.11** thus eliminating the two intermediates **5.9** and **5.10**. The relative energy obtained for this "solvated" neutral TS was much lower (110.7 kcal mol^{-1}) than the gas phase ionic transition state structure obtained for **5.7.1 TS end**. Therefore this lower energy was used to calculate the relative energies for the reaction profile shown in Figure 5.13.

This argument of intramolecular hydrogen transfer vs. intermolcular hydrogen transfer can also be used to explain the higher energies that were obtained for **5.10**.

Solvated energies for both **5.12** and **5.13** should also exist thus making **5.7.2** the overall rate-determining step of the reaction. Due to time constraints the solvated transition structure for **5.13** was not calculated. It will be considered in future work.

The results in the reaction profile (Figure 5.13) show that a single solvent molecule results in the lowering of the energy by approximately 110 kcal mol^{-1} for transition structures **5.3.2** and **5.7.2**.

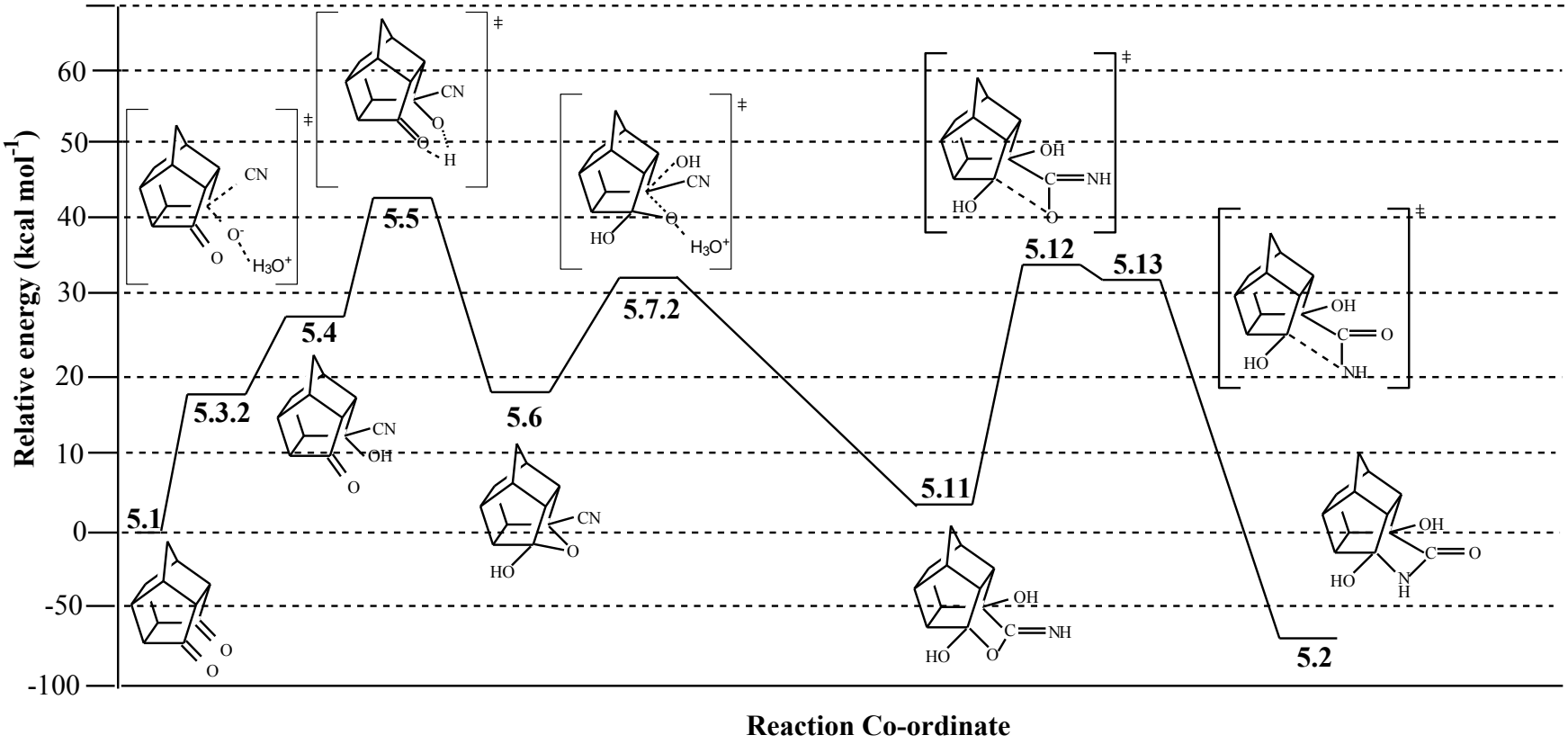


Figure 5.13 Calculated reaction profile for the proposed mechanism.

Martins and co-workers[23] have shown that structures **5.4** and **5.6** are intermediates in the conversion of the dione **5.1** to the lactam **5.2**. They successfully isolated an inseparable cyanohydrin mixture (**5.4** and **5.6**). Treatment of the mixture with aqueous sodium hydroxide yielded the hydroxylactam **5.2**.[23] The RHF (Restricted Hartree Fock) calculated energy barrier between **5.4** and **5.6** (i.e., **5.5**) was found to be 41 kcal mol^{-1} (21 kcal mol^{-1} if corrected to MP2 energy).[67] Since these compounds are found experimentally to co-exist and interchange at room temperature, the real energy barrier should be lower than approximately 15 kcal mol^{-1} and certainly lower than the rate-determining step in this reaction. A logical explanation for the higher than expected energy barrier for the conversion between the cyanohydrin mixture **5.4** and **5.6**, is that the intramolecular hydrogen transfer reported here is obviously less preferred than the intermolcular hydrogen transfer via the aqueous solvent which should also exist. The experimental results by Martins and co-workers[23] also imply that **5.7.2** should be the rate-determining step for the overall reaction. The theoretical approach followed in this investigation has therefore provided some valuable insight into this unique mechanism which correlates well with experimental results.

5.5 Calculation of Heats of Formation

In computing the heats of formation (ΔH_f) for each structure within the proposed mechanism, Hess's Law was applied. Hess's Law states:

$$\Delta H_f = \Delta H_{products} - \Delta H_{reactants} \qquad (5.1)$$

The combined energy values presented in Table 5.1 and Table 5.2 were used to calculate the heats of formation (see Appendix 1 for calculation details) for each structure depicted in the modified mechanism (see Figure 5. 1). These energy values (see Appendix 1) were used in the reaction profile (see Figure 5.2 and Figure 5.13).

This model has therefore enhanced our understanding of the formation of the lactam **5.2** in this one-pot reaction.

CHAPTER 6

6. CONCLUSION

One of the primary goals of this study was to get a better understanding of the conversion of the dione **1.1** to the lactam **1.2** (see Abstract). It was observed that high energies for the transition structures were obtained in the gas phase. In particular, two structures **5.3.1** and **5.7.1** which are both ionic species (see Chapter 5) resulted in abnormally high energies. These high energies are the result of calculating the energy of an ionic species (O^-) in the gas phase. In reality, the ionic species does not exist in solution since it will upon formation immediately abstract a proton from the solvent to form an alcohol (OH^-).

It is postulated that the energy of **5.5** will also be lowered considerably in the solvated state due to intermolecular H transfer. It should drop to below that of **5.7.2**.

This prompted an investigation to include a solvent molecule. However due to time constraints, only two "solvated" transition structures **5.3.1** and **5.7.1** (see Chapter 5) were found. This study has shown that the energy of an ionic transition structure decreased by about 110 kcal mol^{-1} for both "solvated" transition structures. This lowering of energy is due to the removal of a complete ionic species in the transition structure due to hydrogen transfer from solvent as the ionic species starts to form. Although this is generally accepted in organic textbooks, the theoretical results obtained in this investigation quantify the energy differences and reconfirm our basic knowledge in this regard. Since one solvent molecule lowers the energy of an ionic transition structure by about 110 kcal mol^{-1}, then the energy of the transition structures **5.12** and **5.13**, which also contains ionic atoms (carbocations), should also be lowered by at least 10-50 kcal mol^{-1} in solvent making **5.7.2** the overall rate determining step.

The rate-determining step in reality should involve a TS that is only 12 kcal mol^{-1}, which is lower than the inherent energy molecules have at room temperature. [68] Since the real experimental reaction is performed at 0 ^oC to 10 ^oC, the computational model therefore gave a reasonable answer.

APPENDIX 1

Table 1.1 Summary of Energies

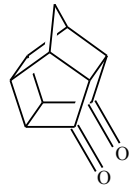
Structure number[b]	Energies[a] (RHF/3-21+G*)	
	Hartrees	**kcal mol^{-1}**
5.1	-568.9543	-357024.26
5.3.1	-660.7663	-414637.10
5.3.2	-736.9142	-462420.64
5.4	-661.3513	-415004.23
5.5	-661.2569	-414944.99
5.6	-661.3657	-415013.23
5.7.1	-736.3609	-462073.48
5.7.2	-812.5102	-509857.86
5.9	-736.9832	-492463.95
5.10	-736.8741	-462395.47
5.11	-737.0049	-462477.55
5.12	-736.8873	-462403.79
5.13	-736.8880	-462404.19
5.2	-737.0314	-462494.22
HCN	-92.3680	-57961.83
H_2O	-75.6193	-47451.85
H_3O^+	-75.8998	-47627.88
Na^+	-160.6757	-100825.51
NaCN	-252.6906	-158565.74
OH^-	-74.9957	-47060.54
NaOH	-235.8689	-148009.96

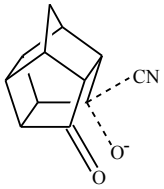
[a]Energies are expressed in Hartrees and kcal mol^{-1}, performed at the HF level using the 3-21+G* level of theory.

[b]Structure number as per proposed reaction mechanism shown in Figure 5.1.

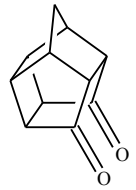
The cartesian coordinates of all the optimized structures presented are available on the CD accompanying this Thesis.

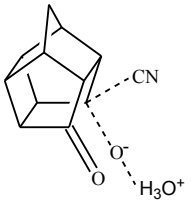
Scheme of reaction



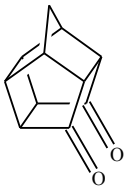
5.1 + NaCN ⟶  + Na^+ $\triangle H = 127.39$ kcal mol^{-1}

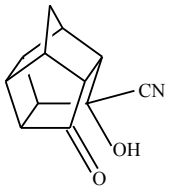
5.3.1



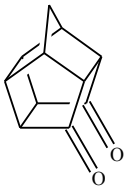
5.1 + HCN + H_2O ⟶  $\triangle H = 17.30$ kcal mol^{-1}

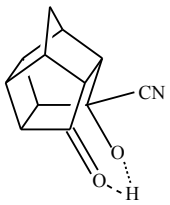
5.3.2



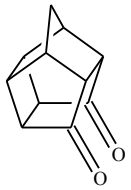
5.1 + NaCN + H_2O ⟶  + NaOH $\triangle H = 27.66$ kcal mol^{-1}

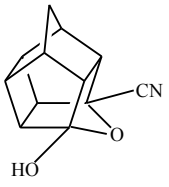
5.4



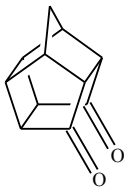
5.1 + HCN + H_2O ⟶  $\triangle H = 41.10$ kcal mol^{-1}

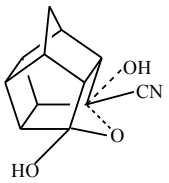
5.5



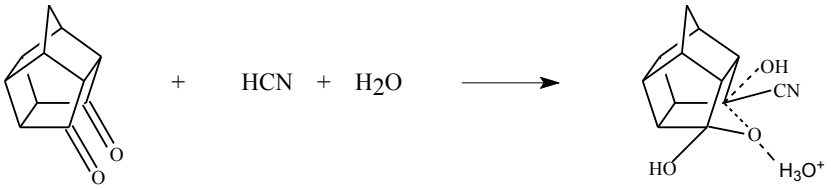
5.1 + NaCN + H_2O ⟶  + NaOH $\triangle H = 18.66$ kcal mol^{-1}

5.6

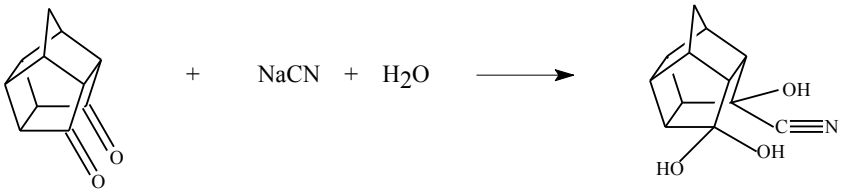


5.1 + HCN + H_2O ⟶  + H_3O^+ $\triangle H = 188.43$ kcal mol^{-1}

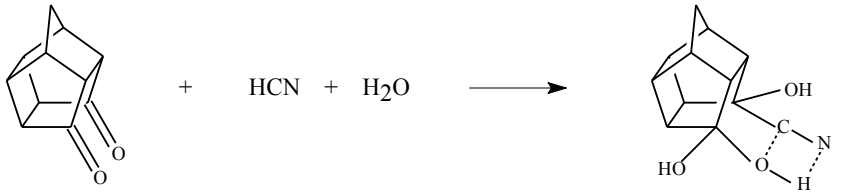
5.7.1



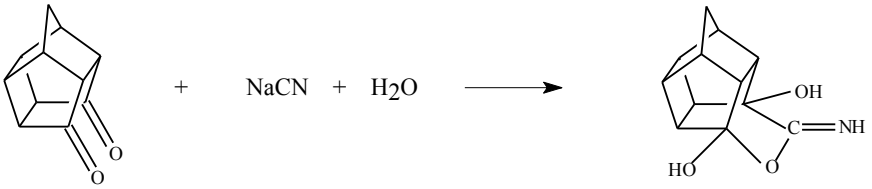
5.1 **5.7.2** $\triangle H = 31.90$ kcal mol^{-1}



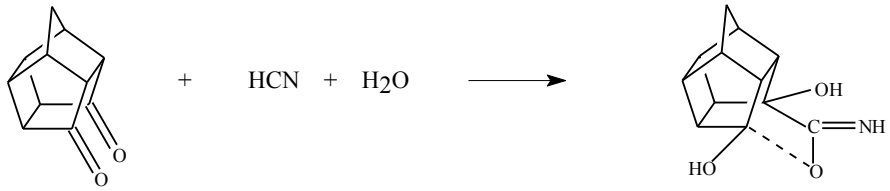
5.1 **5.9** $\triangle H = 19.79$ kcal mol^{-1}



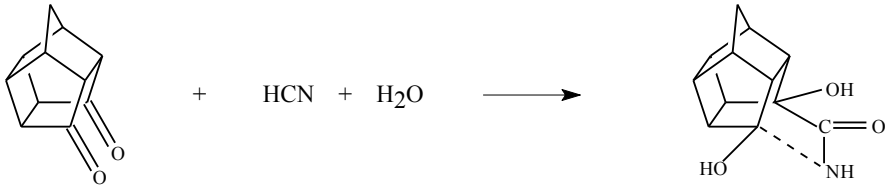
5.1 **5.10** $\triangle H = 42.50$ kcal mol^{-1}



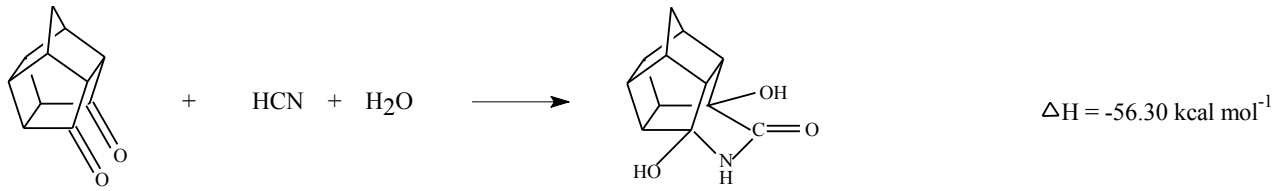
5.1 **5.11** $\triangle H = 6.19$ kcal mol^{-1}



5.1 **5.12** $\triangle H = 36.20$ kcal mol^{-1}



5.1 **5.13** $\triangle H = 33.70$ kcal mol^{-1}



5.1 **5.2**

Table 2.1 Heats of Formation

Structure number[b]	Relative Energies[a]/kcal mol^{-1}	Relative Energies[d]/kcal mol^{-1}
5.1	0	
5.3.1	127.39	
5.3.2[c]	63.11	17.3
5.4	27.66	
5.5	86.90	41.1
5.6	18.66	
5.7.1	188.43	
5.7.2[c]	77.74	31.9
5.9	19.79	
5.10	88.27	42.5
5.11	6.19	
5.12	79.95	36.2
5.13	79.55	33.7
5.2	-10.46	-56.3

[a]Relative energies are expressed in kcal mol^{-1}, performed at the HF level using the 3-21+G* level of theory and reported relative to structure **5.1**.

[b]Structure number as per proposed reaction mechanism shown in Figure 5.1.

[c]Relative energies of the "solvated" transition state structures.

[d]Relative energies of the transition state structures with solvent with included HCN.

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H,-1.8644580038,-1.7715030384,-0.7119838407
H,0.2884874212,0.3417554208,2.3763589788
H,-0.5591918037,1.1522322036,-2.448127526
H,1.4156645243,2.1018724018,-1.1605300358
H,2.1329054977,0.740357793,0.8658401205
H,0.0735879059,-1.3526645396,-2.2991785258
H,0.2621359072,2.9193543622,1.0904559401
H,-0.8791267586,3.1007745647,-0.2552076946
```

```
%chk=dionest
#N RHF/STO-3g OPT OPTCYC=1000

OPT- dione

0   1
C,-1.0737807073,1.1718277558,0.8184553036 L
C,-1.5302892204,0.4692352323,-0.493502841 L
C,-1.1355669789,-1.0351723711,-0.3935465005 L H
C,0.0187152109,0.1923364192,1.3470498693 L H
C,-0.6123643072,-1.1543691114,1.0248573543 H
C,-0.3369600322,0.7270971082,-1.4707747222 L
C,0.6623434126,1.5469770389,-0.6033382682 L
C,1.2331603314,0.4547629648,0.352476567 L H
C,1.3686306302,-0.7263146954,-0.5974688673 H
C,0.0719810422,-0.7742336537,-1.3824617232 L H
C,-0.2624428398,2.3659673152,0.3038828136 L
O,-0.6977419797,-2.1231389919,1.7637845031 H
O,2.3314391596,-1.4682569601,-0.7171881892 H
H,-1.8795103241,1.3995292904,1.5369692417 L
H,-2.5472963382,0.7114743354,-0.8340053929 L
H,-1.8683612194,-1.7912506757,-0.7162802831 L
H,0.3010281643,0.3411059552,2.4052739141 L
H,-0.5552861673,1.141916814,-2.4653529717 L
H,1.422909083,2.1131335283,-1.1675358047 L
H,2.158515996,0.7424851467,0.8840824844 L
H,0.0750517548,-1.3712997872,-2.3078255712 L
H,0.2727342764,2.908901213,1.1006377559 L
H,-0.8699219141,3.1064877801,-0.242507797 L
```

```
%chk=lactam
#N RHF/3-21+G* OPT OPTCYC=1000

Output of Opt STO-3G used for opt 3-21+G*

0   1
C,-1.28577607,1.4068047,1.0620296023
C,-1.9233846268,0.7333473671,-0.1860808449
C,-1.3923998481,-0.7244837345,-0.2636503432
C,-0.0457377405,0.4997079108,1.2920587776
C,-0.5767992911,-0.9472678294,1.0434784013
C,-0.9646168291,1.1444209834,-1.3443170139
C,0.1077552415,2.0096088829,-0.628127595
C,0.9176603952,0.9165678435,0.1215693386
C,1.0367308647,-0.2568754917,-0.9032923375
C,-0.4278576551,-0.3157943029,-1.4206184253
C,-0.6871899845,2.7071977556,0.4922166857
C,1.4547986801,-1.5479676174,-0.1544361903
O,2.5148343961,-2.1071294635,-0.3821172326
O,-1.3601029516,-1.349112364,2.1644726601
O,1.9757741158,0.0187388546,-1.9445226694
N,0.4786964612,-1.9634053883,0.7959279834
H,-1.9407099598,1.5000620199,1.9241313505
H,-2.9892005038,0.899269568,-0.3144681812
H,-2.1001379449,-1.5199126314,-0.4817881908
H,0.408951285,0.6122728113,2.2728656908
H,-1.3969764648,1.5782337337,-2.2414599122
H,0.7044760295,2.641807146,-1.2799983304
H,1.8856980393,1.2570462108,0.4806379535
H,-0.5412192977,-0.8519011523,-2.3589962711
H,-0.0528492445,3.2313385974,1.2024360052
H,-1.4433556579,3.3903164332,0.1139275624
H,-1.7593725453,-2.2107965155,1.8831309468
H,2.6787541623,-0.6650285905,-1.7925635649
H,0.8719235734,-2.3704449328,1.6530066608
```

```
%chk=lactamst
#N RHF/STO-3g OPT OPTCYC=1000

OPT - lactam

0   1
C,-1.2806022653,1.39249934,1.063683623 L
C,-1.9193223872,0.7209949537,-0.1802418909 L
C,-1.3844066666,-0.7378635777,-0.2463329946 L H
C,-0.0390414835,0.4824267616,1.3050083538 L H
C,-0.5874000706,-0.9339611858,1.0504703747 H
C,-0.9594471486,1.1331231543,-1.3449545866 L
C,0.1122444562,1.9958816984,-0.6310169963 L
C,0.9342807785,0.9046264399,0.1164562929 L H
C,1.0269543619,-0.2330015931,-0.9111844303 H
C,-0.409043389,-0.3242041101,-1.4185188135 L H
C,-0.6758891426,2.6799204693,0.4917353301 L
C,1.4448107655,-1.5265949172,-0.1556423207 H
O,2.5036350037,-2.0815701674,-0.3960415888 H
O,-1.3817376048,-1.3575601188,2.1665557639 H
O,1.9712982688,0.0325243703,-1.9596827999 H
N,0.4794306188,-1.9416332871,0.8037104454 H
H,-1.9478176959,1.5058859063,1.9352215745 L
H,-2.9994975558,0.8793765215,-0.3098104987 L
H,-2.110620048,-1.5323520321,-0.4889959312 L
H,0.4268627325,0.6196633786,2.2995396603 L
H,-1.3956004708,1.5644020047,-2.257120217 L
H,0.7062933699,2.6522437573,-1.2896910744 L
H,1.9150202187,1.2618758084,0.484041337 L
H,-0.5390415069,-0.8661496,-2.3698342297 L
H,-0.0377181502,3.2217556629,1.2092588475 L
H,-1.4320654278,3.3936508584,0.1252898387 L
H,-1.8047692543,-2.1915213196,1.8395161374 H
H,2.6611610701,-0.6622568949,-1.796003658 H
H,0.8773861921,-2.3253783147,1.669192444 H
```

```
%chk=mech1st6
#N RHF/3-21+G* OPT OPTCYC=1000

Output of Opt STO-3G used for opt 3-21+G*

0  1
C,-0.66993331,1.4575044116,1.3618722691
C,-1.7427744825,0.7417263513,0.4976171358
C,-1.3875700094,-0.767015532,0.4098017389
C,0.5211052453,0.4713229955,1.2648718793
C,-0.0412748214,-0.9852820576,1.1885767525
C,-1.2262910797,0.9460865999,-0.9617900627
C,0.0840464291,1.7547877622,-0.7713834704
C,1.0391448026,0.6762573189,-0.1994619236
C,0.6720728733,-0.7071283196,-0.8409277767
C,-0.8754886376,-0.5643641902,-1.0437527552
C,-0.227745618,2.6314542177,0.4611584077
C,1.4596032214,-1.1066338362,-2.0394329453
N,2.0646959431,-1.4061538091,-2.9769566697
O,0.8142898115,-1.6619581187,0.2326630231
O,-0.0706997106,-1.6558851802,2.4301947587
H,-0.9769722367,1.7049764572,2.3745589192
H,-2.773182504,1.009715853,0.7135882318
H,-2.1613304995,-1.5063702259,0.5949658313
H,1.2840307513,0.5962021505,2.0277899951
H,-1.9198386783,1.3443196984,-1.6969996932
H,0.4493912891,2.2668137249,-1.6578316982
H,2.0958205578,0.9198774268,-0.2653808575
H,-1.298702879,-1.1671664591,-1.8418563347
H,0.6457559858,3.1544152898,0.8423792727
H,-1.0238754222,3.3488942181,0.2781306279
H,-0.3520564513,-2.5781494073,2.2035946419
```

```
%chk=mech1st6st
#N RHF/sto-3g OPT OPTCYC=1000

OPT - mech1str6

0   1
C,-0.6653556589,1.4300495428,1.3639195227 L
C,-1.7351301339,0.7170739752,0.5064707701 L
C,-1.3693615675,-0.7849459223,0.4306173041 L H
C,0.5338310749,0.4559928276,1.2802134626 L H
C,-0.0352713246,-0.9774174532,1.1935647628 H
C,-1.2168614418,0.9219534513,-0.9660923631 L
C,0.0879333799,1.7266237161,-0.7773373433 L
C,1.0550760293,0.6586025429,-0.2115024498 L H
C,0.6712886949,-0.6981368197,-0.8319937005 H
C,-0.846624973,-0.5792149647,-1.0463194571 L H
C,-0.2238507381,2.5916501629,0.4564168679 L
C,1.4354976664,-1.04719389,-2.0636366589 H
N,2.024313808,-1.3138284854,-3.0210510028 H
O,0.8297687103,-1.6690383171,0.2404925745 H
O,-0.1048752091,-1.6229722284,2.449598724 H
H,-0.9794437062,1.6984839974,2.3869450889 L
H,-2.7804832553,0.9779710692,0.7269998372 L
H,-2.1631007707,-1.5246217343,0.6098483306 L
H,1.3048677678,0.6093560772,2.0561375522 L
H,-1.9218413746,1.3152437392,-1.7129589571 L
H,0.4501544778,2.2621251862,-1.6714500239 L
H,2.1246354559,0.9242469595,-0.2821366696 L
H,-1.28975464,-1.1856262926,-1.8493107196 L
H,0.6531174954,3.1384047258,0.8404902863 L
H,-1.0185283516,3.3347836758,0.2787138463 L
H,-0.4959938096,-2.5077066563,2.2374237552 H
```

```
%chk=mech1s10H2

#N RHF/3-21G** OPT OPTCYC=1000

Output from mech1s10opt2-open str-H added 3A to O-optimisation

-1  2
 C                  0.587658   -0.489304    1.294949
 C                  1.342863   -0.876705    0.026126
 C                  0.253413   -0.719018   -1.053721
 C                 -0.905612   -1.568952   -0.440747
 C                 -0.841018   -1.110846    1.046462
 C                 -0.031010    0.945071    1.240781
 C                  0.368228    1.644656   -0.078878
 C                 -0.357231    0.727451   -1.096679
 C                 -1.774117    0.534997   -0.512519
 C                 -1.450766    0.342968    1.002688
 C                 -2.183945   -0.880875   -0.963845
 C                  2.668111   -0.310276   -0.232950
 O                  1.595603   -2.316149    0.202576
 O                 -0.448217    2.895339   -0.089854
 N                  3.783387   -0.177583   -0.441509
 O                  1.646028    1.881796   -0.269276
 H                  1.114168   -0.785697    2.184974
 H                  0.586101   -1.070867   -2.019400
 H                 -0.808827   -2.628536   -0.590351
 H                 -1.219480   -1.818371    1.764462
 H                  0.133829    1.562572    2.105169
 H                 -0.337113    1.151540   -2.086087
 H                 -2.436911    1.352348   -0.728371
 H                 -2.254722    0.582792    1.678493
 H                 -2.298211   -0.965099   -2.037742
 H                 -3.079195   -1.246059   -0.474202
 H                  2.031429   -2.635364   -0.569601
 H                  0.219985    3.546623   -0.229163
 H                  2.618856    2.062337   -0.414232
```

```
%chk=mech1s10H2
#N RHF/3-21+G* OPT OPTCYC=1000

Output from mech1s10opt2-open str-H added 3A to O-optimisation
Energy = -731.9821

0  1
 C                  0.367945   -0.587192    1.305726
 C                  1.090632   -1.019199    0.033236
 C                  0.000861   -0.776088   -1.032778
 C                 -1.179937   -1.594564   -0.415391
 C                 -1.082363   -1.156085    1.077143
 C                 -0.199125    0.874336    1.273194
 C                  0.077608    1.607157   -0.028165
 C                 -0.578328    0.694110   -1.055260
 C                 -2.000468    0.526001   -0.451118
 C                 -1.650029    0.310826    1.054671
 C                 -2.440644   -0.869949   -0.916642
 C                  2.438543   -0.504838   -0.192127
 O                  1.253310   -2.455720    0.213818
 O                 -0.645932    2.836867    0.083785
 N                  3.534903   -0.240182   -0.349060
 O                  1.414551    1.864636   -0.384467
 H                  0.888953   -0.884656    2.196961
 H                  0.297802   -1.108216   -2.014440
 H                 -1.112762   -2.652267   -0.576992
 H                 -1.468059   -1.858819    1.792189
 H                 -0.018602    1.472959    2.148358
 H                 -0.561487    1.113201   -2.047921
 H                 -2.655127    1.354045   -0.644665
 H                 -2.417112    0.586355    1.754471
 H                 -2.569404   -0.936932   -1.988305
 H                 -3.338852   -1.212869   -0.422524
 H                  1.631493   -2.835115   -0.562032
 H                 -0.542358    3.333123   -0.711273
 H                  1.877595    2.317096    0.299568
```

```
%chk=mech1str11
#N RHF/3-21+G* OPT OPTCYC=1000

Output of Opt STO-3G used for opt 3-21+G*

0   1
C,-1.0049803267,1.9116707934,0.3263251816
C,-1.5373947152,1.0599844684,-0.8612518696
C,-1.4358188903,-0.4397697401,-0.4651058841
C,-0.1425847501,0.8667750425,1.0846977068
C,-0.9924815244,-0.4381386553,1.0322368158
C,-0.2861175277,0.9033784787,-1.7782652261
C,0.8179561287,1.6810881169,-1.0117845385
C,1.11525259,0.7035207465,0.1585653545
C,1.0934405105,-0.7164478309,-0.4888418823
C,-0.1805193218,-0.5957309134,-1.378001174
C,0.0396357312,2.82849632,-0.3392080709
C,0.8665539798,-1.7889158559,0.5931237799
N,1.6925174352,-2.7529728719,0.7052145758
O,2.2732221434,-0.9859576068,-1.2451943715
O,-0.2556562278,-1.6291691102,1.3909169006
O,-2.0669082397,-0.3347562824,1.9578179994
H,-1.7687521778,2.3900747617,0.9335100297
H,-2.4643946915,1.4083336022,-1.3078395342
H,-2.2822961752,-1.0871248554,-0.6777295084
H,0.1103921108,1.1512160054,2.1024307425
H,-0.3871643565,1.145928378,-2.8322614861
H,1.6888243992,1.9523053795,-1.6022967509
H,2.0470161795,0.9088429122,0.6791747733
H,-0.2388009969,-1.3425512519,-2.1651044673
H,0.6359000466,3.3854553888,0.378949073
H,-0.3994651116,3.5193043939,-1.0543940799
H,1.3897560406,-3.3818291792,1.4801182226
H,2.6166730247,-1.820768244,-0.8369707435
H,-2.5182230501,-1.2147790157,1.9026463127
```

```
%chk=mech1str11st
#N RHF/sto-3g OPT OPTCYC=1000

Optimisation mech1str11

0   1
C,-1.0022813894,1.8983732951,0.3314481848 L
C,-1.5387655802,1.0494697351,-0.8514218176 L
C,-1.4344027813,-0.4483645655,-0.4418226684 L H
C,-0.1405472954,0.8542539739,1.101055236 L H
C,-0.999287305,-0.422575198,1.0360496732 H
C,-0.2853565861,0.8912330474,-1.7757964201 L
C,0.8193331407,1.6650878376,-1.0128387348 L
C,1.129123238,0.6865425207,0.1588758355 L H
C,1.0904761763,-0.6966808286,-0.5042593295 H
C,-0.167275508,-0.6063766035,-1.3694528938 L H
C,0.0442222974,2.8004375127,-0.3337974432 L
C,0.8633450263,-1.7666844214,0.5869430644 H
N,1.6964102212,-2.7238060329,0.69460017 H
O,2.2709686926,-0.9801465603,-1.2685215742 H
O,-0.2557403327,-1.6128654212,1.3914388878 H
O,-2.0885664581,-0.3317177449,1.9569934532 H
H,-1.772699638,2.4025884121,0.9395868726 L
H,-2.4816431361,1.393316356,-1.3001452543 L
H,-2.2900943859,-1.1018485917,-0.6782632508 L
H,0.132599514,1.1634330911,2.1276854515 L
H,-0.3886150654,1.1277510493,-2.8443580474 L
H,1.6957184791,1.9560593036,-1.6167011648 L
H,2.0766658272,0.9076385739,0.6855362272 L
H,-0.2441540699,-1.3564068547,-2.1736397377 L
H,0.6488822526,3.3755064454,0.3868577136 L
H,-0.3887575188,3.522939578,-1.0451277864 L
H,1.4044206455,-3.3546614323,1.472066662 H
H,2.6088610014,-1.8064659588,-0.8381545636 H
H,-2.5608512686,-1.1936677635,1.8332734349 H
```

```
%chk=mech1str2st
#N RHF/sto-3g OPT OPTCYC=1000

Optimisation mech1str2

0   1
C,-1.4277634695,1.561961221,0.3412375935 L
C,-1.0961086913,1.1837786952,-1.133417646 L
C,-1.1584213381,-0.3697833834,-1.2515523967 L H
C,-1.1238698869,0.2268965056,1.0900368424 L H
C,-1.699419361,-0.7818488293,0.105998653 H
C,0.4658301216,1.1297279145,-1.1426422294 L
C,0.8441138155,1.4854743818,0.3200445759 L
C,0.4663005734,0.1664414152,1.0645199459 L H
C,0.9625152476,-0.9181121352,0.0984082301 H
C,0.4203824594,-0.4253442126,-1.2474503837 L H
C,-0.2563900297,2.4655840143,0.7378990349 L
O,-2.4911844398,-1.6799158334,0.3421762752 H
C,2.4776507432,-0.9304024185,0.0608445107 H
N,3.6314321428,-0.977199256,0.0308895176 H
O,0.4550581407,-2.2048074345,0.4981798818 H
H,-2.4397822386,1.9685638373,0.5074360874 L
H,-1.6049106359,1.7793333164,-1.9047981031 L
H,-1.6526709069,-0.8053278366,-2.1342165372 L
H,-1.5296651142,0.1677916987,2.116456235 L
H,1.0045192886,1.6815625099,-1.9265397726 L
H,1.8833485909,1.8252512173,0.4713848415 L
H,0.8857434352,0.082471878,2.0851142863 L
H,0.8734145544,-0.8886867131,-2.1400686129 L
H,-0.2377986197,2.7136895711,1.8121940348 L
H,-0.2281497653,3.418035065,0.1830157547 L
H,0.6660156996,-2.7907426178,-0.2726144774 H
```

```
%chk=mech1str2st
#N RHF/STO-3g OPT OPTCYC=1000

Optimisation mech1str2
Energy = -656.7586

0  1
 C                 -1.422468    1.571371    0.347873
 C                 -1.092430    1.194852   -1.129007
 C                 -1.149166   -0.356625   -1.257884
 C                 -1.111847    0.234022    1.079960
 C                 -1.699936   -0.816385    0.109080
 C                  0.463800    1.149320   -1.143367
 C                  0.845091    1.505735    0.321809
 C                  0.463561    0.188668    1.056186
 C                  0.963900   -0.934816    0.093746
 C                  0.415096   -0.401588   -1.267477
 C                 -0.256262    2.494048    0.744248
 O                 -2.491333   -1.705039    0.344379
 C                  2.473718   -0.970506    0.066328
 N                  3.627653   -1.013260    0.037762
 O                  0.438126   -2.202301    0.502987
 H                 -2.427990    1.949911    0.512453
 H                 -1.597014    1.790241   -1.884724
 H                 -1.646840   -0.785735   -2.122558
 H                 -1.513506    0.167831    2.086936
 H                  0.989700    1.705644   -1.914172
 H                  1.873643    1.823704    0.470608
 H                  0.885376    0.096621    2.053970
 H                  0.873107   -0.856923   -2.142038
 H                 -0.236693    2.724708    1.806213
 H                 -0.234186    3.419058    0.173769
 H                  0.708150   -2.832092   -0.212675
```

```
%nproc=2
# opt=(gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity optcyc=100

TS1

0  1
 C                  0.000000    0.000000    0.000000
 C                  0.000000    0.000000    1.564294
 C                  1.517144    0.000000    2.038806
 C                  1.436890   -0.540715   -0.304289
 C                  2.221254    0.135213    0.748749
 C                 -0.123205   -1.520023    1.927097
 C                 -0.167799   -2.206040    0.532617
 C                  1.310973   -2.090147    0.090384
 C                  2.100326   -2.382876    1.361721
 C                  1.367325   -1.538218    2.394993
 C                 -0.910211   -1.187900   -0.344616
 C                  3.605591   -2.086876    1.262106
 N                  4.168257   -1.917341    2.424190
 O                  1.859940   -3.778523    1.672640
 O                  4.089783   -2.006755    0.082034
 O                  3.249095    0.865163    0.494894
 H                 -0.226679    0.950520   -0.461245
 H                 -0.657020    0.713054    2.034921
 H                  1.846673    0.652474    2.829337
 H                  1.822823   -0.389274   -1.296553
 H                 -0.890485   -1.818984    2.622258
 H                 -0.533653   -3.219144    0.535487
 H                  1.615126   -2.710506   -0.734159
 H                  1.618420   -1.774189    3.411949
 H                 -0.893687   -1.440937   -1.398261
 H                 -1.934841   -1.020282   -0.031359
 H                  5.172893   -1.805492    2.354776
 H                  2.547789   -4.119215    2.264045
 H                  3.802110    1.164417    1.238979

 1  2 1.0  4 1.0  11 1.0  17 1.0
 2  3 1.0  6 1.0  18 1.0
 3  5 1.0  10 1.0  19 1.0
 4  5 1.0  8 1.0  20 1.0
 5  16 2.0
 6  7 1.0  10 1.0  21 1.0
 7  8 1.0  11 1.0  22 1.0
 8  9 1.0  23 1.0
 9  10 1.0  12 1.0  14 1.0
 10  24 1.0
 11  25 1.0  26 1.0
 12  13 2.0  15 2.0
 13  27 1.0
 14  28 1.0
 15
 16  29 1.0
 17
 18
```

```
 Entering Gaussian System, Link 0=g98
 Input=mech1s13ts1F.gjf
 Output=mech1s13ts1F.out
 Initial command:
 /usr/g98/l1.exe /usr/scratch/Singh/Gau-1426.inp -
scrdir=/usr/scratch/Singh/
 Default is to use a total of   2 processors:
                                2 via shared-memory
                                1 via Linda
 Entering Link 1 = /usr/g98/l1.exe PID=      1432.
```

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

Cite this work as:
Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

```
**********************************************
Gaussian 98:  DEC-AXP-OSF/1-G98RevA.7 11-Apr-1999
                  11-Oct-2001
**********************************************
%nproc=2
Will use up to    2 processors via shared memory.
%chk=mech1s13ts1F
%nosave
-------------------
#N RHF/3-21+G* FREQ
-------------------
1/10=4,30=1,38=1/1,3;
2/17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
```

```
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;
------------------------------
Freq calc of output str of TS1
------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                    -2.12266   0.90143  -0.00033
C                    -1.54943   0.51691   1.40344
C                    -0.00112   0.87687   1.39856
C                    -0.81773   0.93178  -0.86397
C                     0.13535   1.53917   0.08667
C                    -1.20567  -1.00484   1.25051
C                    -1.61154  -1.30515  -0.21995
C                    -0.4585   -0.62562  -0.99746
C                     0.78457  -0.95859  -0.17955
C                     0.31998  -0.6683    1.24111
C                    -2.82155  -0.38911  -0.45247
C                     2.04895  -0.18979  -0.59628
N                     2.94857  -0.14322   0.34409
O                     0.97678  -2.39034  -0.30376
O                     2.03817   0.32586  -1.76564
O                     0.81864   2.59382  -0.18634
H                    -2.69867   1.81522  -0.0288
H                    -2.12345   0.84869   2.25316
H                     0.44869   1.38439   2.23483
H                    -0.86384   1.43581  -1.81281
H                    -1.58262  -1.69091   1.99116
H                    -1.72702  -2.3498   -0.45575
H                    -0.35352  -0.89625  -2.0333
H                     0.97017  -1.05578   2.00271
H                    -3.13901  -0.35695  -1.48816
H                    -3.67057  -0.63429   0.17614
H                     3.80954   0.29201   0.03438
H                     1.88892  -2.63204  -0.0834
H                     1.52882   2.85906   0.42549

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  97 maximum allowed number of steps= 174.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

--------------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
--------------------------------------------------------------------------
  1   1  C     0  -2.122661          0.901428         -0.000334
  2   2  C     0  -1.549435          0.516906          1.403436
  3   3  C     0  -0.001116          0.876871          1.398560
```

4	4	C	0	-0.817734	0.931784	-0.863967
5	5	C	0	0.135347	1.539167	0.086674
6	6	C	0	-1.205665	-1.004841	1.250511
7	7	C	0	-1.611540	-1.305147	-0.219953
8	8	C	0	-0.458504	-0.625616	-0.997458
9	9	C	0	0.784569	-0.958586	-0.179554
10	10	C	0	0.319978	-0.668295	1.241107
11	11	C	0	-2.821550	-0.389105	-0.452472
12	12	C	0	2.048950	-0.189793	-0.596279
13	13	N	0	2.948565	-0.143224	0.344093
14	14	O	0	0.976784	-2.390337	-0.303758
15	15	O	0	2.038171	0.325862	-1.765645
16	16	O	0	0.818640	2.593824	-0.186337
17	17	H	0	-2.698669	1.815224	-0.028804
18	18	H	0	-2.123452	0.848689	2.253162
19	19	H	0	0.448693	1.384388	2.234831
20	20	H	0	-0.863837	1.435806	-1.812811
21	21	H	0	-1.582617	-1.690905	1.991164
22	22	H	0	-1.727021	-2.349800	-0.455752
23	23	H	0	-0.353515	-0.896254	-2.033295
24	24	H	0	0.970167	-1.055780	2.002711
25	25	H	0	-3.139006	-0.356951	-1.488164
26	26	H	0	-3.670565	-0.634286	0.176139
27	27	H	0	3.809539	0.292007	0.034383
28	28	H	0	1.888917	-2.632041	-0.083401
29	29	H	0	1.528821	2.859062	0.425488

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.122661	0.901428	-0.000334
2	6	0	-1.549435	0.516906	1.403436
3	6	0	-0.001116	0.876871	1.398560
4	6	0	-0.817734	0.931784	-0.863967
5	6	0	0.135347	1.539167	0.086674
6	6	0	-1.205665	-1.004841	1.250511
7	6	0	-1.611540	-1.305147	-0.219953
8	6	0	-0.458504	-0.625616	-0.997458
9	6	0	0.784569	-0.958586	-0.179554
10	6	0	0.319978	-0.668295	1.241107
11	6	0	-2.821550	-0.389105	-0.452472
12	6	0	2.048950	-0.189793	-0.596279
13	7	0	2.948565	-0.143224	0.344093
14	8	0	0.976784	-2.390337	-0.303758
15	8	0	2.038171	0.325862	-1.765645
16	8	0	0.818640	2.593824	-0.186337
17	1	0	-2.698669	1.815224	-0.028804
18	1	0	-2.123452	0.848689	2.253162
19	1	0	0.448693	1.384388	2.234831
20	1	0	-0.863837	1.435806	-1.812811
21	1	0	-1.582617	-1.690905	1.991164
22	1	0	-1.727021	-2.349800	-0.455752

23	1	0	-0.353515	-0.896254	-2.033295
24	1	0	0.970167	-1.055780	2.002711
25	1	0	-3.139006	-0.356951	-1.488164
26	1	0	-3.670565	-0.634286	0.176139
27	1	0	3.809539	0.292007	0.034383
28	1	0	1.888917	-2.632041	-0.083401
29	1	0	1.528821	2.859062	0.425488

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.564294	0.000000			
3	C	2.541350	1.589619	0.000000		
4	C	1.565125	2.418393	2.406015	0.000000	
5	C	2.347952	2.370099	1.475907	1.476819	0.000000
6	C	2.457510	1.567570	2.239129	2.893445	3.102387
7	C	2.275621	2.441132	3.158204	2.459420	3.351978
8	C	2.468914	2.873983	2.864886	1.603858	2.492847
9	C	3.455974	3.182845	2.544925	2.570855	2.594443
10	C	3.157798	2.219404	1.586011	2.878537	2.497937
11	C	1.535693	2.425599	3.603313	2.435027	3.571015
12	C	4.352959	4.176919	3.052855	3.089898	2.667884
13	N	5.189148	4.667974	3.294406	4.098788	3.287994
14	O	4.531483	4.212879	3.811669	3.817148	4.037506
15	O	4.556327	4.790666	3.804536	3.055546	2.919578
16	O	3.398536	3.528278	2.476252	2.428843	1.285973
17	H	1.080564	2.248929	3.192908	2.239615	2.849769
18	H	2.254113	1.077781	2.288111	3.380576	3.205090
19	H	3.441086	2.331579	1.076685	3.378052	2.176401
20	H	2.270521	3.414479	3.371883	1.075392	2.148742
21	H	3.313292	2.284941	3.073402	3.951623	4.124542
22	H	3.306724	3.421420	4.102271	3.429612	4.345883
23	H	3.239516	3.903635	3.878890	2.219133	3.265659
24	H	4.172341	3.029993	2.245780	3.919801	3.331947
25	H	2.197752	3.413460	4.438676	2.727410	4.098385
26	H	2.187595	2.707526	4.152441	3.416584	4.383705
27	H	5.963522	5.535656	4.089516	4.756891	3.880442
28	H	5.346500	4.893753	4.252164	4.542697	4.528014
29	H	4.164970	3.989704	2.686384	3.299002	1.949023

		6	7	8	9	10
6	C	0.000000				
7	C	1.554729	0.000000			
8	C	2.399046	1.547827	0.000000		
9	C	2.451175	2.421379	1.524817	0.000000	
10	C	1.562350	2.504204	2.370449	1.522626	0.000000
11	C	2.427007	1.535358	2.436582	3.660996	3.579854
12	C	3.829812	3.845104	2.576473	1.537323	2.567936
13	N	4.338388	4.739491	3.693316	2.371055	2.826624
14	O	3.016361	2.807860	2.378132	1.449926	2.404877
15	O	4.624980	4.285994	2.780074	2.395205	3.602928
16	O	4.371811	4.594440	3.557219	3.552579	3.595508
17	H	3.437800	3.309849	3.451713	4.455299	4.110081
18	H	2.298525	3.319242	3.938548	4.200112	3.048909
19	H	3.068258	4.183794	3.912904	3.381064	2.284199

20	H	3.931608	3.257158	2.253565	3.334349	3.892951
21	H	1.077657	2.244702	3.366056	3.294219	2.286522
22	H	2.234291	1.077143	2.208029	2.884415	3.145948
23	H	3.394309	2.244555	1.075744	2.176115	3.350711
24	H	2.302747	3.415791	3.350695	2.192299	1.073746
25	H	3.414367	2.200133	2.738259	4.179577	4.417060
26	H	2.714280	2.201484	3.419758	4.481061	4.130344
27	H	5.321002	5.657181	4.485859	3.280274	3.815155
28	H	3.742131	3.745997	3.220502	2.007308	2.841160
29	H	4.804980	5.255388	4.256433	3.936296	3.816908

		11	12	13	14	15
11	C	0.000000				
12	C	4.876698	0.000000			
13	N	5.830026	1.302219	0.000000		
14	O	4.295857	2.465260	3.058946	0.000000	
15	O	5.084535	1.278058	2.345176	3.262115	0.000000
16	O	4.713775	3.070869	3.508471	4.988052	3.020781
17	H	2.248035	5.184786	5.988808	5.592074	5.260463
18	H	3.056130	5.158168	5.509428	5.161453	5.808895
19	H	4.589267	3.613039	3.486811	4.579505	4.432913
20	H	3.002243	3.550613	4.656177	4.506051	3.107387
21	H	3.033315	4.704942	5.063573	3.508049	5.593842
22	H	2.245513	4.352395	5.231619	2.708377	4.801214
23	H	2.974458	2.887203	4.137966	2.644481	2.699142
24	H	4.566125	2.944224	2.738217	2.664749	4.153320
25	H	1.083729	5.266715	6.360925	4.741013	5.229378
26	H	1.084478	5.788528	6.639446	4.991179	6.105906
27	H	6.683734	1.931202	1.013224	3.915842	2.525666
28	H	5.230247	2.500647	2.738579	0.969003	3.406085
29	H	5.499740	3.257309	3.322051	5.328484	3.387862

		16	17	18	19	20
16	O	0.000000				
17	H	3.605897	0.000000			
18	H	4.201495	2.544097	0.000000		
19	H	2.731602	3.900711	2.627402	0.000000	
20	H	2.610967	2.587130	4.296914	4.255442	0.000000
21	H	5.372751	4.197474	2.609729	3.693646	4.976263
22	H	5.567081	4.298117	4.210191	5.090887	4.113090
23	H	4.118961	4.107291	4.954918	4.905279	2.397404
24	H	4.258462	5.082329	3.641457	2.506040	4.912207
25	H	5.105368	2.653671	4.059856	5.455688	2.914750
26	H	5.541214	2.643234	2.984426	5.028076	4.014838
27	H	3.780550	6.684381	6.358716	4.162998	5.153722
28	H	5.335331	6.389608	5.802941	4.855939	5.207293
29	H	0.974187	4.378087	4.552043	2.571976	3.572178

		21	22	23	24	25
21	H	0.000000				
22	H	2.538187	0.000000			
23	H	4.282340	2.547147	0.000000		
24	H	2.630631	3.872124	4.250521	0.000000	
25	H	4.038255	2.651608	2.889113	5.436898	0.000000
26	H	2.961467	2.668265	3.994127	5.005039	1.769004
27	H	6.069291	6.154095	4.797737	3.708488	7.142939
28	H	4.152241	3.646000	3.441446	2.771383	5.694683

29	H	5.730148	6.205590	4.867361	4.257431	5.982760

		26	27	28	29
26	H	0.000000			
27	H	7.538573	0.000000		
28	H	5.913225	3.500389	0.000000	
29	H	6.268914	3.456069	5.526378	0.000000

Interatomic angles:

C1-C2-C3=107.3679	C2-C1-C4=101.2107	C1-C4-C3= 76.3287
C2-C3-C4= 71.1837	C2-C1-C5= 71.4039	C1-C5-C3= 79.7547
C2-C3-C5=101.2097	C1-C4-C5=101.0024	C2-C5-C4= 73.8283
C3-C5-C4=109.1441	C1-C2-C6=103.382	C1-C6-C3= 65.324
C3-C2-C6= 90.3395	C4-C1-C6= 89.1289	C4-C2-C6= 90.4997
C4-C3-C6= 76.9629	C5-C1-C6= 80.3855	C5-C2-C6=102.0414
C5-C3-C6=111.5971	C5-C4-C6= 83.7647	C2-C1-C7= 76.4642
C3-C1-C7= 81.7351	C3-C2-C7=101.0555	C4-C1-C7= 77.1903
C4-C2-C7= 60.807	C3-C4-C7= 80.941	C5-C1-C7= 92.9203
C5-C2-C7= 88.3126	C5-C4-C7=114.4444	C1-C7-C6= 77.2945
C2-C6-C7=102.8576	C3-C6-C7=111.4259	C4-C7-C6= 89.2964
C2-C1-C8= 87.902	C3-C1-C8= 69.735	C2-C3-C8= 74.2346
C1-C4-C8=102.3472	C2-C4-C8= 88.8092	C3-C4-C8= 88.8589
C5-C1-C8= 62.2729	C2-C5-C8= 72.4056	C3-C5-C8= 88.5592
C5-C4-C8=107.9625	C1-C6-C8= 61.0962	C2-C6-C8= 90.3586
C3-C6-C8= 76.2063	C4-C8-C6= 90.3294	C5-C8-C6= 78.6941
C1-C7-C8= 77.8832	C2-C7-C8= 89.2788	C3-C8-C7= 85.9324
C4-C8-C7=102.5709	C5-C8-C7=109.8921	C6-C7-C8=101.2928
C1-C3-C9= 85.6045	C2-C3-C9= 98.0067	C1-C4-C9=111.0069
C2-C4-C9= 79.2122	C4-C3-C9= 62.4917	C1-C5-C9= 88.5878
C2-C5-C9= 79.6098	C5-C3-C9= 75.1616	C5-C4-C9= 74.2656
C1-C6-C9= 89.5061	C2-C6-C9=102.5128	C3-C6-C9= 65.5389
C4-C9-C6= 70.3143	C5-C9-C6= 75.8253	C1-C7-C9= 94.696
C2-C7-C9= 81.7728	C3-C9-C7= 78.9344	C4-C7-C9= 63.5637
C5-C9-C7= 83.793	C6-C7-C9= 72.4367	C1-C8-C9=117.8998
C2-C8-C9= 87.0286	C3-C9-C8= 85.6095	C4-C8-C9=110.4867
C5-C8-C9= 76.2402	C6-C8-C9= 73.5464	C7-C8-C9=104.0037
C1-C2-C10=111.9804	C1-C3-C10= 97.1102	C2-C3-C10= 88.6753
C1-C4-C10= 85.1367	C4-C2-C10= 76.5965	C4-C3-C10= 89.8622
C1-C5-C10= 81.2675	C5-C2-C10= 65.8545	C5-C3-C10=109.2821
C4-C5-C10= 88.9538	C1-C6-C10=101.199	C2-C6-C10= 90.3221
C3-C10-C6= 90.6628	C4-C10-C6= 74.8224	C5-C10-C6= 96.9479
C1-C7-C10= 82.5499	C7-C2-C10= 64.7987	C3-C10-C7= 98.5998
C4-C7-C10= 70.8842	C5-C10-C7= 84.1508	C7-C6-C10=106.9082
C1-C8-C10= 81.4367	C2-C10-C8= 77.4574	C3-C10-C8= 90.5571
C4-C8-C10= 90.7128	C5-C8-C10= 61.7513	C6-C10-C8= 71.8725
C7-C8-C10= 76.2532	C2-C10-C9=115.2813	C3-C10-C9=109.8856
C4-C9-C10= 85.2984	C5-C10-C9= 76.1033	C6-C10-C9=105.2187
C7-C9-C10= 74.9841	C8-C9-C10=102.128	C2-C1-C11=102.9678
C3-C1-C11=122.2669	C3-C2-C11=126.3747	C4-C1-C11=103.4901
C4-C2-C11= 60.3561	C3-C4-C11= 96.2006	C5-C1-C11=132.5963
C5-C2-C11= 96.2476	C5-C4-C11=130.1953	C1-C11-C6= 72.7592
C6-C2-C11= 71.2021	C3-C6-C11=101.0319	C4-C11-C6= 73.0407
C1-C11-C7= 95.6318	C2-C11-C7= 72.1612	C4-C11-C7= 72.5845
C6-C7-C11=103.5168	C1-C11-C8= 72.906	C2-C11-C8= 72.4683
C3-C8-C11= 85.2313	C8-C4-C11= 70.8307	C5-C8-C11= 92.8354
C8-C6-C11= 60.6436	C8-C7-C11=104.4228	C9-C4-C11= 93.9581

C9-C6-C11= 97.2633 C9-C7-C11=134.1872 C9-C8-C11=133.7764
C10-C2-C11=100.7381 C10-C4-C11= 84.2686 C10-C6-C11=126.2477
C10-C7-C11=122.9901 C10-C8-C11= 96.259 C1-C5-C12=120.284
C2-C5-C12=111.8745 C3-C5-C12= 90.1747 C4-C5-C12= 91.8099
C1-C8-C12=119.2406 C2-C8-C12= 99.9097 C3-C8-C12= 68.018
C4-C8-C12= 92.3362 C5-C8-C12= 63.4838 C6-C8-C12=100.599
C7-C8-C12=136.1396 C3-C9-C12= 93.5163 C4-C9-C12= 94.1702
C5-C9-C12= 75.6512 C6-C9-C12=146.6554 C7-C9-C12=151.7542
C8-C9-C12=114.5751 C2-C10-C12=121.3284 C3-C10-C12= 91.4787
C4-C10-C12= 68.8556 C5-C10-C12= 63.5396 C6-C10-C12=134.5812
C7-C10-C12= 98.5832 C8-C10-C12= 62.7457 C10-C9-C12=114.1124
C11-C8-C12=153.201 C3-C9-N13= 84.0766 C4-C9-N13=112.0098
C5-C9-N13= 82.7993 C6-C9-N13=128.2203 C7-C9-N13=162.9503
C8-C9-N13=141.9438 C2-C10-N13=135.0159 C3-C10-N13= 92.2236
C4-C10-N13= 91.8463 C5-C10-N13= 75.9904 C6-C10-N13=161.8078
C7-C10-N13=125.4055 C8-C10-N13= 90.1357 C10-C9-N13= 90.3929
C5-C12-N13=106.7073 C8-C12-N13=142.262 C9-C12-N13=112.974
C10-C12-N13= 87.4268 C1-C7-O14=125.7806 C2-C7-O14=106.5508
C4-C7-O14= 92.6468 C6-C7-O14= 82.0814 C1-C8-O14=138.415
C2-C8-O14=106.2848 C3-C8-O14= 92.8004 C4-C8-O14=146.2498
C5-C8-O14=111.9483 C6-C8-O14= 78.3072 C7-C8-O14= 88.6986
C3-C9-O14=143.7291 C4-C9-O14=141.805 C5-C9-O14=173.0384
C6-C9-O14= 97.9889 C7-C9-O14= 89.3367 C8-C9-O14=106.1262
C2-C10-O14=131.2557 C3-C10-O14=144.7547 C4-C10-O14= 92.0747
C5-C10-O14=110.8608 C6-C10-O14= 96.6796 C7-C10-O14= 69.7422
C10-C8-O14= 60.8539 C10-C9-O14=107.9771 C11-C7-O14=162.2782
C11-C8-O14=126.3066 C5-C12-O14=103.6595 C7-O14-C12= 93.4091
C8-O14-C12= 64.2459 C12-C9-O14=111.1963 C10-O14-C12= 63.6298
N13-C9-O14=103.7389 N13-C10-O14= 71.0452 N13-C12-O14=104.2814
C1-C5-O15=119.3664 C2-C5-O15=129.5336 C3-C5-O15=115.9582
C4-C5-O15= 80.8683 C1-C8-O15=120.3477 C2-C8-O15=115.8279
C3-C8-O15= 84.7343 C4-C8-O15= 83.789 C5-C8-O15= 66.9848
C6-C8-O15=126.3496 C7-C8-O15=163.3466 C3-C9-O15=100.6873
C4-C9-O15= 75.8534 C5-C9-O15= 71.4971 C6-C9-O15=145.2268
C7-C9-O15=125.7057 C8-C9-O15= 87.385 C10-C5-O15= 82.9803
C10-C8-O15= 88.4055 C10-C9-O15=132.478 C11-C8-O15=154.0977
C5-C12-O15= 88.0916 C8-C12-O15= 85.272 C9-C12-O15=116.2859
C10-C12-O15=136.3992 C5-O15-N13= 76.4306 C8-O15-N13= 91.8103
C9-N13-O15= 61.0404 C10-N13-O15= 87.8016 N13-C12-O15=130.7012
O14-C8-O15= 78.0276 O14-C9-O15=113.7926 O14-C12-O15=117.7129
C1-C3-O16= 85.2591 C2-C3-O16=118.7782 C1-C4-O16=114.9006
C2-C4-O16= 93.4201 C3-C4-O16= 61.6144 C1-C5-O16=136.5421
C2-C5-O16=148.1448 C3-C5-O16=127.2904 C4-C5-O16=122.9255
C6-C3-O16=135.9274 C6-C4-O16=110.1484 C7-C4-O16=140.0661
C8-C3-O16= 83.1771 C8-C4-O16=122.4655 C8-C5-O16=138.2832
C9-C3-O16= 90.0561 C9-C4-O16= 90.515 C9-C5-O16=129.4061
C10-C3-O16=123.0212 C10-C4-O16= 84.8401 C10-C5-O16=141.5911
C11-C4-O16=151.4581 C12-C5-O16= 95.5105 O15-C5-O16= 81.9423
C2-C1-H17=115.2682 C3-C1-H17=117.8838 C3-C2-H17=111.4109
C4-C1-H17=114.425 C2-H17-C4= 65.2026 C3-C4-H17= 86.7546
C5-C1-H17=106.4945 C5-C2-H17= 76.1391 C3-C5-H17= 89.286
C5-C4-H17= 98.0322 C6-C1-H17=150.2609 C6-C2-H17=127.616
C6-C4-H17= 83.0447 C7-C1-H17=159.5855 C7-C2-H17= 89.678
C7-C4-H17= 89.4304 C8-C1-H17=150.6589 C8-C2-H17= 83.7686

C8-C4-H17=127.0261 C8-C5-H17= 80.1886 C9-C4-H17=135.579
C9-C5-H17=109.7523 C10-C2-H17=133.7997 C10-C4-H17=106.1709
C10-C5-H17=100.2438 C11-C1-H17=117.4071 C2-H17-C11= 65.2837
C4-H17-C11= 65.7222 C5-H17-C11= 88.1095 C6-C11-H17= 94.5964
C7-C11-H17=120.8913 C8-C11-H17= 94.8369 C12-C5-H17=139.9705
O15-C5-H17=131.5055 O16-C4-H17=101.0615 O16-C5-H17=116.1267
C1-C2-H18=115.8912 C1-H18-C3= 68.037 C3-C2-H18=116.8377
C4-C1-H18=123.5314 C4-C2-H18=147.9418 C4-C3-H18= 92.1025
C5-C1-H18= 88.2606 C5-C2-H18=133.1438 C5-C3-H18=115.0417
C1-H18-C6= 65.3314 C6-C2-H18=119.5085 C6-C3-H18= 61.0115
C4-C6-H18= 80.362 C7-C1-H18= 94.2366 C7-C2-H18=137.7758
C7-C6-H18=117.6517 C8-C1-H18=112.9251 C8-C2-H18=169.4727
C8-C3-H18= 99.0806 C8-C6-H18=113.9307 C9-C3-H18=120.6027
C9-C6-H18=124.2973 C10-C2-H18=132.1181 C10-C3-H18=102.2903
C10-C6-H18=102.6404 C11-C1-H18=105.9333 C11-C2-H18=116.0336
C11-C6-H18= 80.5406 O16-C3-H18=123.6869 H17-C1-H18= 92.633
H17-C2-H18= 92.9933 C3-H18-H17= 82.5318 C4-H17-H18= 89.6983
C5-H17-H18= 72.6627 C6-H18-H17= 90.3078 C11-H17-H18= 78.9816
C1-C2-H19=122.8587 C1-C3-H19=140.5111 C2-C3-H19=120.7489
C4-C2-H19= 90.642 C4-C3-H19=149.4769 C1-C5-H19= 98.9585
C2-H19-C5= 63.3283 C5-C3-H19=116.1193 C4-C5-H19=134.3486
C6-C2-H19=102.007 C6-C3-H19=132.2391 C7-C2-H19=122.455
C8-C2-H19= 96.9204 C8-C3-H19=164.4722 C8-C5-H19=113.6904
C9-C3-H19=133.8382 C9-C5-H19= 89.816 C2-C10-H19= 62.3385
C10-C3-H19=116.8567 C4-C10-H19= 80.8449 C5-H19-C10= 68.0621
C6-C10-H19=104.2401 C7-C10-H19=121.7237 C8-C10-H19=114.4038
C9-C10-H19=124.0588 C11-C2-H19=149.4575 C12-C5-H19= 95.9298
C12-C10-H19= 96.0782 N13-C10-H19= 85.3381 O14-C10-H19=155.1706
O15-C5-H19=120.187 C2-H19-O16= 87.9792 O16-C3-H19= 91.8331
C4-O16-H19= 81.5508 O16-C5-H19=101.0327 C10-H19-O16= 91.1409
H17-C2-H19=116.7584 H17-C5-H19=100.9565 C1-H18-H19= 89.3073
H18-C2-H19= 93.4835 H18-C3-H19= 95.9242 C5-H19-H18= 83.1333
C6-H18-H19= 76.731 C10-H19-H18= 76.3875 O16-H19-H18=103.2406
H17-H18-H19= 97.9105 C2-C1-H20=124.8226 C3-C1-H20= 88.7879
C1-C4-H20=117.4007 C2-C4-H20=153.466 C3-C4-H20=148.7544
C1-H20-C5= 64.1171 C2-C5-H20= 98.0378 C3-C5-H20=136.1517
C5-C4-H20=113.7575 C6-C1-H20=112.4572 C6-C4-H20=162.3143
C7-C1-H20= 91.5269 C7-C4-H20=130.0527 C1-H20-C8= 66.1474
C2-C8-H20= 82.5495 C3-C8-H20= 81.4643 C8-C4-H20=113.0339
C5-H20-C8= 68.9322 C6-C8-H20=115.3154 C7-C8-H20=116.7018
C9-C4-H20=127.3182 C9-C5-H20= 88.8162 C9-C8-H20=122.7142
C10-C4-H20=157.3261 C10-C5-H20=113.6035 C10-C8-H20=114.6589
C11-C1-H20=102.4198 C2-C11-H20= 77.1532 C11-C4-H20=111.5963
C5-H20-C11= 86.0962 C6-C11-H20= 92.1775 C7-C11-H20= 85.2606
C11-C8-H20= 79.4962 C12-C5-H20= 94.3627 C12-C8-H20= 94.396
O14-C8-H20=153.238 O15-C5-H20= 73.8727 O15-C8-H20= 75.4329
C1-H20-O16= 87.9585 C3-O16-H20= 82.9843 O16-C4-H20= 87.3822
O16-C5-H20= 95.6734 C8-H20-O16= 93.6936 C11-H20-O16=114.0498
H17-C1-H20= 94.3286 C2-H17-H20= 89.5457 H17-C4-H20= 96.2081
C5-H20-H17= 73.331 C8-H20-H17= 90.7003 C11-H17-H20= 76.4087
O16-H20-H17= 87.8455 H18-C1-H20=143.4894 H18-H17-H20=113.7315
H19-C5-H20=159.3992 H19-O16-H20=105.5752 C1-C2-H21=117.5819
C3-C2-H21=103.5172 C4-C2-H21=114.2874 C5-C2-H21=124.749
C1-C6-H21=135.4896 C2-C6-H21=118.3111 C3-C6-H21=132.6668

C4-C6-H21=167.2268 C1-C7-H21= 94.2706 C2-H21-C7= 65.2137
C4-C7-H21=114.2102 C7-C6-H21=115.8329 C8-C2-H21= 80.5765
C8-C6-H21=148.6024 C8-C7-H21=124.101 C9-C6-H21=134.1867
C9-C7-H21= 89.7371 C10-C2-H21= 60.9911 C3-C10-H21=103.5734
C4-C10-H21= 99.1847 C5-C10-H21=119.0339 C10-C6-H21=118.8712
C7-H21-C10= 67.0913 C8-C10-H21= 92.5544 C9-C10-H21=118.3394
C11-C2-H21= 80.1121 C11-C6-H21=114.26 C11-C7-H21=105.1807
C12-C10-H21=151.4367 N13-C10-H21=163.9397 O14-C7-H21= 87.1974
O14-C10-H21= 96.7613 H17-C2-H21=135.5783 C1-H18-H21= 85.5454
H18-C2-H21= 94.9866 C3-H18-H21= 77.424 H18-C6-H21= 94.2383
C7-H21-H18= 85.9278 C10-H21-H18= 76.7123 H17-H18-H21=109.0571
H19-C2-H21=106.2737 H19-C10-H21=107.8234 H19-H18-H21= 89.7038
C1-C6-H22= 89.4939 C2-C6-H22=127.4229 C3-C6-H22=132.992
C4-C6-H22= 82.8834 C1-C7-H22=159.6289 C2-C7-H22=150.7141
C4-C7-H22=149.2473 C6-C7-H22=114.984 C1-C8-H22= 89.8082
C2-C8-H22= 83.5349 C3-C8-H22=107.2214 C4-C8-H22=127.5285
C5-C8-H22=135.0943 C6-H22-C8= 65.3701 C8-C7-H22=113.3086
C3-C9-H22= 97.9563 C4-C9-H22= 77.6704 C5-C9-H22=104.8495
C9-C6-H22= 75.8348 C9-C7-H22=104.3919 C9-C8-H22= 99.5691
C10-C6-H22=110.6668 C10-C7-H22=117.1974 C10-C8-H22= 86.7283
C10-C9-H22= 85.1591 C1-C11-H22=120.8219 C2-C11-H22= 94.1074
C4-C11-H22= 94.1456 C6-H22-C11= 65.6074 C11-C7-H22=117.451
C8-H22-C11= 66.3319 C9-H22-C11= 90.1801 C12-C8-H22=130.7681
C12-C9-H22=158.6534 N13-C9-H22=169.0261 C6-H22-O14= 74.5263
C7-H22-O14= 83.9844 O14-C8-H22= 72.2848 C9-O14-H22= 81.818
C10-O14-H22= 75.681 C11-H22-O14=119.9731 C12-O14-H22=114.4662
O15-C8-H22=148.3185 O15-C9-H22=130.6148 H17-C11-H22=146.0799
H18-C6-H22=136.5 H20-C8-H22=134.4048 H20-C11-H22=102.2539
C2-H21-H22= 90.2113 H21-C6-H22= 93.4405 H21-C7-H22= 92.8859
C8-H22-H21= 90.0641 C9-H22-H21= 74.5107 C10-H21-H22= 81.2108
C11-H22-H21= 78.443 O14-H22-H21= 83.8568 H18-H21-H22=109.7312
C1-C4-H23=116.692 C2-C4-H23=114.5827 C3-C4-H23=113.9353
C5-C4-H23=122.8869 C6-C4-H23= 82.0541 C1-C7-H23= 91.5593
C2-C7-H23=112.7694 C4-H23-C7= 66.8662 C6-C7-H23=125.6331
C1-C8-H23=127.6097 C2-C8-H23=160.298 C3-C8-H23=157.172
C4-C8-H23=110.261 C5-C8-H23=127.8784 C6-C8-H23=153.2389
C7-C8-H23=116.4834 C3-C9-H23=110.2502 C4-H23-C9= 71.5866
C5-C9-H23= 85.9266 C6-C9-H23= 94.18 C7-H23-C9= 66.4033
C9-C8-H23=112.4573 C10-C4-H23= 81.0695 C10-C7-H23= 89.5831
C10-C8-H23=150.7796 C10-C9-H23=129.0334 C1-C11-H23= 85.5346
C2-C11-H23= 92.0153 C11-C4-H23= 79.3002 C6-C11-H23= 77.128
C11-C7-H23=102.1618 C11-C8-H23=109.5386 C9-H23-C11= 89.2034
C4-H23-C12= 73.1565 C5-C12-H23= 71.8886 C7-H23-C12= 96.2493
C12-C8-H23= 95.5956 C12-C9-H23=100.6551 C10-C12-H23= 75.5389
C11-H23-C12=112.5938 N13-C9-H23=130.9652 N13-C12-H23=160.5643
C4-H23-O14=103.0629 C7-H23-O14= 69.5526 O14-C8-H23= 92.0221
O14-C9-H23= 91.4122 C10-O14-H23= 83.0029 C11-H23-O14= 99.5636
C12-O14-H23= 68.7069 C4-H23-O15= 76.121 C5-O15-H23= 70.9477
C7-H23-O15=119.9344 C8-H23-O15= 82.9397 O15-C9-H23= 72.1977
C11-H23-O15=127.2524 C12-O15-H23= 85.1539 N13-O15-H23=110.0366
O14-H23-O15= 75.239 O16-C4-H23=124.7341 H17-C4-H23=134.1967
H17-C11-H23=102.8261 C1-H20-H23= 87.8504 H20-C4-H23= 85.9936
C5-H20-H23= 91.668 C7-H23-H20= 89.0603 H20-C8-H23= 84.2206
C9-H23-H20= 93.4883 C11-H23-H20= 66.9612 C12-H23-H20= 83.8769

O14-H23-H20=126.6207 O15-H23-H20= 74.8741 O16-H20-H23=110.5824
H17-H20-H23=110.9187 H21-C7-H23=145.073 C4-H23-H22= 91.7728
C6-H22-H23= 90.208 H22-C7-H23= 93.4347 H22-C8-H23= 95.5003
C9-H23-H22= 74.816 C11-H22-H23= 76.4359 C12-H23-H22=106.2648
O14-H23-H22= 62.8573 O15-H23-H22=132.4368 H20-H23-H22=112.542
H21-H22-H23=114.7241 C1-C3-H24=121.161 C2-C3-H24=103.0356
C4-C3-H24=114.797 C5-C3-H24=125.8243 C1-C6-H24=122.4115
C2-C6-H24=101.3511 C6-C3-H24= 61.7867 C4-C6-H24= 97.2868
C7-C6-H24=123.4594 C8-C3-H24= 80.9505 C8-C6-H24= 90.8769
C3-H24-C9= 69.9676 C4-C9-H24=110.5097 C5-C9-H24= 87.8063
C6-H24-C9= 66.0379 C7-C9-H24= 95.396 C8-C9-H24=127.7804
C2-C10-H24=130.6077 C3-C10-H24=113.8131 C4-C10-H24=163.4628
C5-C10-H24=133.7465 C6-C10-H24=120.6173 C7-C10-H24=142.1027
C8-C10-H24=151.068 C9-C10-H24=114.0939 C11-C6-H24=149.7592
C3-H24-C12= 70.6023 C5-C12-H24= 72.6522 C6-H24-C12= 92.9437
C8-C12-H24= 74.4015 C12-C9-H24=102.8485 C12-C10-H24= 99.6164
C3-H24-N13= 82.1102 C6-H24-N13=118.5194 N13-C9-H24= 73.6288
C10-H24-N13= 83.5462 C12-N13-H24= 85.777 C3-H24-O14=101.4912
C6-H24-O14= 74.3768 C7-O14-H24= 77.1922 C8-O14-H24= 83.0699
O14-C9-H24= 91.7345 O14-C10-H24= 91.8256 C12-O14-H24= 69.9245
N13-H24-O14= 68.9504 O15-C9-H24=129.6897 O15-C12-H24=157.4061
O15-N13-H24=109.3356 O16-C3-H24=128.7333 H18-C3-H24=106.8629
H18-C6-H24=104.6334 C2-H19-H24= 77.4683 H19-C3-H24= 90.9177
C5-H19-H24= 90.446 C6-H24-H19= 79.1697 C9-H24-H19= 91.8002
H19-C10-H24= 88.9457 C12-H24-H19= 82.6233 N13-H24-H19= 83.2201
O14-H24-H19=124.6347 O16-H19-H24=108.7137 H18-H19-H24= 90.3338
C2-H21-H24= 75.7444 C3-H24-H21= 77.6957 H21-C6-H24= 95.2743
C7-H21-H24= 88.5867 C9-H24-H21= 85.6517 H21-C10-H24= 96.3033
C12-H24-H21=115.0053 N13-H24-H21=141.1632 O14-H24-H21= 82.9749
H18-H21-H24= 88.0354 H19-H24-H21= 91.9236 H22-C6-H24=117.1693
H22-C9-H24= 98.4907 H22-O14-H24= 92.2121 H22-H21-H24= 97.0142
H23-C9-H24=153.317 H23-C12-H24= 93.5832 H23-O14-H24=106.3725
C2-C1-H25=129.5108 C3-C1-H25=138.8655 C4-C1-H25= 91.3246
C2-C4-H25= 82.8775 C3-C4-H25=119.5573 C5-C1-H25=128.7071
C5-C4-H25=152.9883 C6-C1-H25= 94.1857 C6-C4-H25= 74.7447
C1-H25-C7= 62.3207 C2-C7-H25= 94.5493 C4-C7-H25= 71.4069
C6-C7-H25=130.0293 C8-C1-H25= 71.5882 C2-C8-H25= 74.8776
C3-C8-H25=104.7561 C8-C4-H25= 73.3067 C5-C8-H25=103.0575
C6-C8-H25= 83.0246 C8-C7-H25= 92.2021 C9-C4-H25=104.1188
C9-C7-H25=129.4162 C9-C8-H25=156.2884 C10-C4-H25=103.9513
C10-C7-H25=139.6584 C10-C8-H25=119.504 C1-C11-H25=112.9387
C2-C11-H25=150.899 C4-C11-H25= 93.6385 C6-C11-H25=150.825
C7-C11-H25=113.1593 C8-C11-H25= 94.1986 C12-C8-H25=164.5775
O14-C7-H25=142.1237 O14-C8-H25=135.7159 O15-C8-H25=142.7518
O16-C4-H25=163.8607 H17-C1-H25=102.7007 C2-H17-H25= 87.8492
C4-H17-H25= 67.1324 C5-H17-H25= 96.2006 C7-H25-H17= 85.4444
C8-H25-H17= 79.591 H17-C11-H25= 99.615 H18-C1-H25=131.547
H18-H17-H25=102.6982 H20-C1-H25= 81.416 H20-C4-H25= 89.0284
C5-H20-H25=107.1035 C7-H25-H20= 77.7228 H20-C8-H25= 70.6914
C11-H25-H20= 84.0328 O16-H20-H25=134.9428 H20-H17-H25= 67.5682
H21-C7-H25=130.6026 C1-H25-H22= 85.4395 C4-H25-H22= 79.2111
C6-H22-H25= 88.2339 H22-C7-H25=102.5537 C8-H22-H25= 67.8847
C9-H22-H25= 97.9588 H22-C11-H25= 99.6305 O14-H22-H25=124.3816
H17-H25-H22=108.2228 H20-H25-H22= 95.1619 H21-H22-H25=102.1544

C1-H25-H23= 77.8047 H23-C4-H25= 70.6224 H23-C7-H25= 81.0787
H23-C8-H25= 87.0002 C9-H23-H25=110.4167 C11-H25-H23= 83.8207
C12-H23-H25=131.5043 O14-H23-H25=117.844 O15-H23-H25=138.6841
H17-H25-H23= 95.5422 H20-H23-H25= 66.1614 H23-H22-H25= 67.4876
C2-C1-H26= 90.8213 C3-C1-H26=122.6502 C3-C2-H26=149.088
C4-C1-H26=130.3969 C4-C2-H26= 83.3952 C5-C1-H26=150.246
C5-C2-H26=119.2384 C6-C1-H26= 71.2417 C6-C2-H26= 73.431
C3-C6-H26=113.5764 C4-C6-H26= 74.9964 C1-H26-C7= 62.4589
C2-C7-H26= 71.137 C4-C7-H26= 94.1188 C6-C7-H26= 90.8672
C8-C1-H26= 94.3198 C8-C2-H26= 75.5033 C8-C6-H26= 83.7049
C8-C7-H26=130.7929 C9-C6-H26=120.2547 C9-C7-H26=151.5114
C10-C2-H26=113.5575 C10-C6-H26=148.7593 C10-C7-H26=122.6107
C1-C11-H26=112.0625 C2-C11-H26= 92.9535 C4-C11-H26=149.8638
C6-C11-H26= 93.2764 C7-C11-H26=113.2232 C8-C11-H26=150.1066
O14-C7-H26=170.1659 H17-C1-H26=102.6271 C2-H17-H26= 66.6419
C4-H17-H26= 88.4052 C5-H17-H26=105.8278 C6-H26-H17= 79.8221
C7-H26-H17= 85.6728 H17-C11-H26= 98.9307 H18-C1-H26= 84.4151
H18-C2-H26= 94.0726 C3-H18-H26=103.1218 H18-C6-H26= 72.5403
C7-H26-H18= 77.9825 C11-H26-H18= 83.4093 H18-H17-H26= 70.2157
H19-C2-H26=172.3961 H19-H18-H26=127.1534 H20-C1-H26=128.4562
H20-C11-H26=155.5839 H20-H17-H26=100.2726 C1-H26-H21= 78.5237
H21-C2-H26= 72.205 H21-C6-H26= 92.3671 H21-C7-H26= 83.5227
C10-H21-H26=103.0642 C11-H26-H21= 83.3362 H17-H26-H21= 96.8299
H18-H21-H26= 64.4192 C1-H26-H22= 85.2299 C2-H26-H22= 79.0515
C6-H22-H26= 66.5527 H22-C7-H26=103.5712 C8-H22-H26= 88.5397
C9-H22-H26=107.5458 H22-C11-H26=100.6634 O14-H22-H26=136.3439
H17-H26-H22=108.0367 H18-H26-H22= 96.1248 H21-H22-H26= 69.2824
H23-C7-H26=127.8831 H23-C11-H26=156.7952 H23-H22-H26= 99.9361
H24-C6-H26=172.0497 H24-H21-H26=126.9217 C1-H26-H25= 66.5111
C2-H26-H25= 97.146 C4-H25-H26= 96.575 C6-H26-H25= 96.9452
C7-H25-H26= 66.3431 C8-H25-H26= 96.325 H25-C11-H26=109.3496
H17-H26-H25= 70.8091 H18-H26-H25=114.9035 H20-H25-H26=115.834
H21-H26-H25=114.878 H22-H25-H26= 71.0874 H23-H25-H26=115.9738
C5-C12-H27=114.1187 C8-C12-H27=168.6035 C9-C12-H27=141.8166
C10-C12-H27=115.2544 C9-N13-H27=148.8415 C10-N13-H27=165.2393
C12-N13-H27=112.4362 O14-C12-H27=125.4809 C5-O15-H27= 90.6018
C8-O15-H27=115.3619 C9-O15-H27= 83.566 O15-C12-H27=101.8777
O15-N13-H27= 88.2216 H23-C12-H27=169.1666 H23-O15-H27=133.319
H24-C12-H27= 96.8428 H24-N13-H27=160.4335 C3-C9-H28=137.8521
C4-C9-H28=165.6174 C5-C9-H28=159.2875 C6-C9-H28=113.7676
C7-C9-H28=115.2077 C8-C9-H28=131.0146 C2-C10-H28=150.2656
C3-C10-H28=146.2487 C4-C10-H28=105.1614 C5-C10-H28=115.8598
C6-C10-H28=113.1515 C7-C10-H28= 88.7487 C8-C10-H28= 75.7325
C10-C9-H28=106.3866 C5-C12-H28=122.3116 C8-C12-H28= 78.7231
C12-C9-H28= 88.7056 C10-C12-H28= 68.1718 N13-C9-H28= 76.9377
C10-N13-H28= 61.3731 N13-C12-H28= 86.0451 C7-O14-H28=163.202
C8-O14-H28=145.0394 C9-O14-H28=110.5863 C10-O14-H28=106.8349
C12-O14-H28= 80.8076 N13-H28-O14= 99.9644 O15-C9-H28=101.002
O15-C12-H28=125.5322 O15-N13-H28= 83.7506 H19-C10-H28=142.4494
H21-C10-H28=107.6561 H22-C9-H28= 94.6769 H22-O14-H28=162.983
H23-C9-H28=110.6351 H23-C12-H28= 79.0388 H23-O14-H28=139.7452
C3-H24-H28=115.4892 C6-H24-H28= 94.5852 H24-C9-H28= 82.4599
C10-H24-H28= 82.6507 C12-H28-H24= 67.6737 H24-N13-H28= 60.7985
H24-O14-H28= 86.0106 H19-H24-H28=133.8298 H21-H24-H28=100.4327

```
   H27-C12-H28=103.5929    H27-N13-H28=132.1793      C1-C3-H29=105.6
     C2-C3-H29=136.2959      C4-C3-H29= 80.5513      C1-C5-H29=151.3965
     C2-C5-H29=134.7278      C3-C5-H29=102.4434      C4-C5-H29=148.4112
     C6-C3-H29=154.4898      C8-C3-H29=100.0761      C8-C5-H29=146.5127
     C9-C3-H29= 97.5693      C9-C5-H29=119.3998     C10-C3-H29=124.5832
    C10-C5-H29=117.7279     C12-C5-H29= 88.3126     O15-C5-H29= 85.7418
    C3-O16-H29= 91.6128     C4-O16-H29=148.5037     C5-O16-H29=118.5098
    H17-C5-H29=130.7267     H18-C3-H29=132.2705     C2-H19-H29=108.8066
    C3-H19-H29= 84.2212     H19-C5-H29= 76.9173    C10-H19-H29=103.466
   O16-H29-H19= 88.8285    H18-H19-H29=122.2042     H20-C5-H29=121.2458
   H20-O16-H29=169.035      H24-C3-H29=119.0858    H24-H19-H29=113.9377
Stoichiometry    C12H13NO3
Framework group  C1[X(C12H13NO3)]
Deg. of freedom   81
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6              0       -2.072443    0.945731   -0.358931
   2          6              0       -1.734815    0.596337    1.127994
   3          6              0       -0.195701    0.923016    1.354480
   4          6              0       -0.648720    0.919480   -1.008499
   5          6              0        0.160452    1.537988    0.060932
   6          6              0       -1.411388   -0.936625    1.076024
   7          6              0       -1.591309   -1.277303   -0.430212
   8          6              0       -0.313982   -0.648785   -1.037804
   9          6              0        0.777589   -0.980483   -0.026115
  10          6              0        0.105426   -0.633017    1.295193
  11          6              0       -2.726028   -0.344098   -0.876154
  12          6              0        2.111084   -0.253060   -0.262775
  13          7              0        2.854380   -0.194135    0.804846
  14          8              0        0.949246   -2.419345   -0.076095
  15          8              0        2.295832    0.223279   -1.434270
  16          8              0        0.905261    2.568186   -0.133177
  17          1              0       -2.612897    1.870073   -0.504259
  18          1              0       -2.425139    0.968475    1.867302
  19          1              0        0.131677    1.448584    2.235305
  20          1              0       -0.533461    1.392325   -1.967457
  21          1              0       -1.916786   -1.589365    1.768735
  22          1              0       -1.696006   -2.326579   -0.649976
  23          1              0       -0.056264   -0.956106   -2.035983
  24          1              0        0.618866   -1.008497    2.160251
  25          1              0       -2.877566   -0.339901   -1.949227
  26          1              0       -3.668613   -0.550040   -0.380961
  27          1              0        3.764142    0.212128    0.620707
  28          1              0        1.809359   -2.672830    0.291217
  29          1              0        1.518323    2.838632    0.573968
---------------------------------------------------------------------
Rotational constants (GHZ):      0.9453982      0.6570898      0.5382844
```

```
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,N-
14,O-16,
 O-16,O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1
 Standard basis: 3-21+G* (6D, 7F)
 There are   234 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    131072 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
   234 basis functions      343 primitive gaussians
    58 alpha electrons       58 beta electrons
       nuclear repulsion energy      1230.5338231209 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   234 RedAO= T  NBF=   234
 NBsUse=   234 1.00D-04 NBFU=   234
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -736.887327232     A.U. after   17 cycles
             Convg  =    0.7297D-08             -V/T =  2.0022
             S**2   =   0.0000
 Range of M.O.s used for correlation:     1   234
 NBasis=   234 NAE=    58 NBE=    58 NFC=     0 NFV=     0
 NROrb=    234 NOA=    58 NOB=    58 NVA=   176 NVB=   176

 **** Warning!!: The largest alpha MO coefficient is  0.10564505D+03

          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   3 vectors were produced by pass 12.
   3 vectors were produced by pass 13.
 Inv2:  IOpt= 1 Iter= 1 AM= 7.79D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  42 with in-core refinement.
 PrsmSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 G2DrvN: will do   10 atoms at a time, making    3 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
```

```
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  45 IRICut=      45 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
          There are  90 degrees of freedom in the 1st order CPHF.
  87 vectors were produced by pass  0.
 AX will form  44 AO Fock derivatives at one time.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  1.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  3.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  4.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  5.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  6.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  46 vectors were produced by pass  7.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
   3 vectors were produced by pass  8.
   1 vectors were produced by pass  9.
 Inv2:  IOpt= 1 Iter= 1 AM= 4.90D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 659 with in-core refinement.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.

 ******************************************************************

           Population analysis using the SCF density.

 ******************************************************************

 Alpha  occ. eigenvalues --  -20.63375 -20.47525 -20.37555 -15.41271 -
11.40708
 Alpha  occ. eigenvalues --  -11.24220 -11.24087 -11.24030 -11.23563 -
11.23261
 Alpha  occ. eigenvalues --  -11.22923 -11.21110 -11.20520 -11.20310 -
11.19687
```

```
 Alpha  occ. eigenvalues --  -11.19440  -1.55531  -1.36926  -1.30633  -
1.27881
 Alpha  occ. eigenvalues --   -1.13779  -1.12411  -1.11289  -1.07945  -
0.96960
 Alpha  occ. eigenvalues --   -0.96014  -0.93208  -0.89612  -0.82862  -
0.81906
 Alpha  occ. eigenvalues --   -0.77126  -0.76849  -0.75107  -0.71799  -
0.70212
 Alpha  occ. eigenvalues --   -0.68867  -0.66906  -0.65695  -0.63830  -
0.61960
 Alpha  occ. eigenvalues --   -0.60476  -0.58186  -0.56367  -0.56197  -
0.53556
 Alpha  occ. eigenvalues --   -0.52739  -0.51527  -0.50826  -0.49989  -
0.49012
 Alpha  occ. eigenvalues --   -0.48468  -0.47466  -0.46628  -0.45738  -
0.43125
 Alpha  occ. eigenvalues --   -0.37861  -0.34917  -0.30795
 Alpha virt. eigenvalues --    0.02309   0.04122   0.05375   0.06394
0.06993
 Alpha virt. eigenvalues --    0.08169   0.08634   0.09374   0.10468
0.10569
 Alpha virt. eigenvalues --    0.11700   0.12391   0.13782   0.14052
0.14560
 Alpha virt. eigenvalues --    0.14697   0.15697   0.16774   0.17147
0.17629
 Alpha virt. eigenvalues --    0.17955   0.18706   0.19058   0.19306
0.19770
 Alpha virt. eigenvalues --    0.20124   0.20244   0.22773   0.23038
0.23417
 Alpha virt. eigenvalues --    0.23481   0.23831   0.24321   0.24666
0.25146
 Alpha virt. eigenvalues --    0.25609   0.26117   0.26289   0.26965
0.27267
 Alpha virt. eigenvalues --    0.27467   0.28015   0.28174   0.29484
0.29935
 Alpha virt. eigenvalues --    0.30470   0.31103   0.31384   0.32083
0.33084
 Alpha virt. eigenvalues --    0.33365   0.34346   0.34855   0.35126
0.36897
 Alpha virt. eigenvalues --    0.37187   0.37926   0.38903   0.39192
0.39786
 Alpha virt. eigenvalues --    0.41612   0.41972   0.42613   0.43473
0.44084
 Alpha virt. eigenvalues --    0.44345   0.45768   0.46168   0.47142
0.47432
 Alpha virt. eigenvalues --    0.47988   0.48840   0.49588   0.49872
0.51027
 Alpha virt. eigenvalues --    0.51158   0.51580   0.52636   0.53585
0.54714
 Alpha virt. eigenvalues --    0.54996   0.56379   0.56565   0.57177
0.58401
 Alpha virt. eigenvalues --    0.59159   0.60500   0.60769   0.61351
0.62955
```

```
 Alpha virt. eigenvalues --    0.63265   0.65174   0.65881   0.66598
0.67611
 Alpha virt. eigenvalues --    0.71161   0.73226   0.77298   0.86820
1.07366
 Alpha virt. eigenvalues --    1.08714   1.10315   1.11237   1.11716
1.12382
 Alpha virt. eigenvalues --    1.13783   1.15012   1.16259   1.16971
1.17523
 Alpha virt. eigenvalues --    1.17962   1.19200   1.19800   1.20567
1.21263
 Alpha virt. eigenvalues --    1.22192   1.22939   1.25208   1.25755
1.26611
 Alpha virt. eigenvalues --    1.28778   1.31414   1.33796   1.36191
1.38134
 Alpha virt. eigenvalues --    1.39490   1.43214   1.43459   1.44603
1.47668
 Alpha virt. eigenvalues --    1.48846   1.50705   1.52164   1.52470
1.53415
 Alpha virt. eigenvalues --    1.55938   1.57664   1.57826   1.58673
1.62421
 Alpha virt. eigenvalues --    1.65390   1.68901   1.69652   1.72397
1.76032
 Alpha virt. eigenvalues --    1.76824   1.83053   1.85964   1.91762
1.93340
 Alpha virt. eigenvalues --    2.00376   2.04450   2.10423   2.13464
2.21000
 Alpha virt. eigenvalues --    2.22125   2.22911   2.25308   2.29291
2.31003
 Alpha virt. eigenvalues --    2.34747   2.36862   2.40484   2.46031
2.50567
 Alpha virt. eigenvalues --    2.54786   2.69079   2.89902   3.01864
3.15603
 Alpha virt. eigenvalues --    3.19975   3.38996   3.74489   3.80144
3.89515
 Alpha virt. eigenvalues --    3.95524
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   15.180200  -9.193594   6.141701  -5.330544  -1.954677   5.672068
  2  C   -9.193594  24.335759 -16.591500   2.359963   7.648944 -13.775234
  3  C    6.141701 -16.591500  41.379178   8.408140 -29.948164  11.200808
  4  C   -5.330544   2.359963   8.408140  27.078587 -21.785922  -2.170386
  5  C   -1.954677   7.648944 -29.948164 -21.785922  50.413150  -3.952820
  6  C    5.672068 -13.775234  11.200808  -2.170386  -3.952820  23.114600
  7  C   -2.370003   4.523348  -1.878133   3.501145  -0.520292  -7.929162
  8  C    3.314836  -3.576442  -3.128637 -10.958974   8.749742   3.825388
  9  C    0.160961  -0.289607   5.593153   6.940279 -12.192594   4.405939
 10  C   -3.344301   9.963401 -15.710528  -3.662503  12.454421 -13.739533
 11  C   -2.137822   0.527888  -0.204921  -0.301154   0.765138  -0.131572
 12  C   -0.405178  -0.088363  -0.307200   0.915406  -2.682240  -0.868799
 13  N    0.102498  -0.259220   0.721379  -0.120974   0.078140   0.158108
 14  O    0.059177  -0.135062   0.096763  -0.132605   0.162155   0.102801
 15  O   -0.062608   0.023194   0.114571   0.278388  -0.241848   0.015308
 16  O   -0.058281  -0.138230   0.987685   0.818407  -1.359328   0.063627
 17  H    0.507851  -0.140099   0.016612  -0.128965   0.021103   0.028309
```

18	H	-0.086484	0.540724	-0.110175	0.017731	0.007838	-0.103132
19	H	0.033215	-0.073785	0.540549	-0.012934	-0.133837	0.044624
20	H	0.005484	-0.034488	0.051073	0.529686	-0.154773	0.008033
21	H	-0.019791	-0.079862	0.047768	0.005863	0.014107	0.559037
22	H	-0.026865	0.029713	-0.002524	0.054201	0.003868	-0.095621
23	H	0.031357	-0.002833	0.010610	-0.094268	0.010811	-0.029338
24	H	-0.004156	0.020386	-0.005246	0.005028	-0.007275	-0.091933
25	H	-0.074825	0.015450	0.015841	0.057631	-0.030547	0.025980
26	H	-0.069132	0.000762	-0.006221	0.014573	0.005902	0.051365
27	H	-0.001566	0.004560	-0.027497	0.020036	-0.038099	-0.003448
28	H	-0.004497	0.010248	-0.007607	0.003419	-0.013102	-0.025289
29	H	0.028546	-0.048525	0.107578	0.015919	-0.075063	0.021336

		7	8	9	10	11	12
1	C	-2.370003	3.314836	0.160961	-3.344301	-2.137822	-0.405178
2	C	4.523348	-3.576442	-0.289607	9.963401	0.527888	-0.088363
3	C	-1.878133	-3.128637	5.593153	-15.710528	-0.204921	-0.307200
4	C	3.501145	-10.958974	6.940279	-3.662503	-0.301154	0.915406
5	C	-0.520292	8.749742	-12.192594	12.454421	0.765138	-2.682240
6	C	-7.929162	3.825388	4.405939	-13.739533	-0.131572	-0.868799
7	C	17.502031	-8.553897	1.267571	4.502283	-3.730774	-0.690782
8	C	-8.553897	29.749088	-27.232693	9.415896	0.954619	2.379340
9	C	1.267571	-27.232693	79.707582	-35.392489	-0.621807	-15.060101
10	C	4.502283	9.415896	-35.392489	38.367871	0.358146	2.838831
11	C	-3.730774	0.954619	-0.621807	0.358146	12.371934	-0.940646
12	C	-0.690782	2.379340	-15.060101	2.838831	-0.940646	20.850471
13	N	-0.046395	0.603132	-1.195973	0.308798	0.009134	-1.382886
14	O	-0.039443	0.841565	-3.023960	1.195052	-0.044694	0.419091
15	O	-0.042176	0.444863	-0.885343	0.176343	0.004018	-0.033287
16	O	-0.009006	-0.072354	-0.163895	-0.148358	-0.013263	0.126253
17	H	0.016358	0.050617	-0.001019	-0.000560	-0.027256	0.005123
18	H	-0.000751	0.009113	-0.003900	0.070762	0.020945	0.000856
19	H	-0.005243	0.012792	-0.011539	-0.043385	-0.004760	0.000531
20	H	0.030995	-0.081538	-0.012008	-0.004566	-0.008490	0.015576
21	H	-0.104447	0.043000	-0.038938	-0.104550	0.050275	-0.010724
22	H	0.549024	-0.166353	-0.000227	0.027985	-0.029556	0.003788
23	H	-0.039442	0.569802	-0.291584	0.136829	0.026698	0.006308
24	H	0.015714	0.081533	-0.361232	0.667135	0.002236	0.004047
25	H	-0.106827	0.035520	-0.024544	0.006246	0.392570	0.004922
26	H	-0.168171	0.066975	-0.013078	-0.013060	0.448174	-0.000636
27	H	0.002647	-0.031425	0.053917	0.014320	-0.000275	0.080532
28	H	0.022163	-0.021135	0.219025	-0.112395	0.001115	-0.037861
29	H	-0.003000	0.001024	0.034769	-0.042333	0.002507	-0.050151

		13	14	15	16	17	18
1	C	0.102498	0.059177	-0.062608	-0.058281	0.507851	-0.086484
2	C	-0.259220	-0.135062	0.023194	-0.138230	-0.140099	0.540724
3	C	0.721379	0.096763	0.114571	0.987685	0.016612	-0.110175
4	C	-0.120974	-0.132605	0.278388	0.818407	-0.128965	0.017731
5	C	0.078140	0.162155	-0.241848	-1.359328	0.021103	0.007838
6	C	0.158108	0.102801	0.015308	0.063627	0.028309	-0.103132
7	C	-0.046395	-0.039443	-0.042176	-0.009006	0.016358	-0.000751
8	C	0.603132	0.841565	0.444863	-0.072354	0.050617	0.009113
9	C	-1.195973	-3.023960	-0.885343	-0.163895	-0.001019	-0.003900
10	C	0.308798	1.195052	0.176343	-0.148358	-0.000560	0.070762
11	C	0.009134	-0.044694	0.004018	-0.013263	-0.027256	0.020945

12	C	-1.382886	0.419091	-0.033287	0.126253	0.005123	0.000856
13	N	8.941569	0.138094	-0.069900	0.024885	0.000027	0.000135
14	O	0.138094	8.915344	0.037613	0.002214	0.000062	0.000037
15	O	-0.069900	0.037613	9.099989	0.026619	0.000055	-0.000004
16	O	0.024885	0.002214	0.026619	8.335850	0.000068	0.000305
17	H	0.000027	0.000062	0.000055	0.000068	0.370863	-0.000401
18	H	0.000135	0.000037	-0.000004	0.000305	-0.000401	0.355778
19	H	0.004198	0.000320	0.000549	0.001124	-0.000028	0.000043
20	H	0.000029	0.000373	-0.001184	0.003679	-0.000030	-0.000012
21	H	0.000006	0.003527	0.000002	-0.000056	-0.000005	-0.000475
22	H	-0.000020	0.004389	0.000150	-0.000017	-0.000013	-0.000008
23	H	0.001450	0.014516	-0.000669	0.001013	-0.000003	0.000000
24	H	0.020304	0.007870	0.001629	0.001239	0.000000	-0.000031
25	H	0.000015	-0.000053	0.000022	0.000235	-0.000182	-0.000020
26	H	-0.000018	-0.000112	-0.000001	-0.000037	-0.000446	0.000190
27	H	0.203316	-0.004180	-0.022176	-0.000881	0.000000	0.000000
28	H	0.008549	0.178587	-0.000425	0.000127	0.000000	0.000000
29	H	0.005853	-0.000046	-0.002446	0.231616	-0.000003	0.000003

		19	20	21	22	23	24
1	C	0.033215	0.005484	-0.019791	-0.026865	0.031357	-0.004156
2	C	-0.073785	-0.034488	-0.079862	0.029713	-0.002833	0.020386
3	C	0.540549	0.051073	0.047768	-0.002524	0.010610	-0.005246
4	C	-0.012934	0.529686	0.005863	0.054201	-0.094268	0.005028
5	C	-0.133837	-0.154773	0.014107	0.003868	0.010811	-0.007275
6	C	0.044624	0.008033	0.559037	-0.095621	-0.029338	-0.091933
7	C	-0.005243	0.030995	-0.104447	0.549024	-0.039442	0.015714
8	C	0.012792	-0.081538	0.043000	-0.166353	0.569802	0.081533
9	C	-0.011539	-0.012008	-0.038938	-0.000227	-0.291584	-0.361232
10	C	-0.043385	-0.004566	-0.104550	0.027985	0.136829	0.667135
11	C	-0.004760	-0.008490	0.050275	-0.029556	0.026698	0.002236
12	C	0.000531	0.015576	-0.010724	0.003788	0.006308	0.004047
13	N	0.004198	0.000029	0.000006	-0.000020	0.001450	0.020304
14	O	0.000320	0.000373	0.003527	0.004389	0.014516	0.007870
15	O	0.000549	-0.001184	0.000002	0.000150	-0.000669	0.001629
16	O	0.001124	0.003679	-0.000056	-0.000017	0.001013	0.001239
17	H	-0.000028	-0.000030	-0.000005	-0.000013	-0.000003	0.000000
18	H	0.000043	-0.000012	-0.000475	-0.000008	0.000000	-0.000031
19	H	0.345856	-0.000011	-0.000068	0.000000	-0.000001	-0.000526
20	H	-0.000011	0.326286	0.000000	-0.000007	0.000360	-0.000001
21	H	-0.000068	0.000000	0.360776	-0.000380	-0.000005	-0.000242
22	H	0.000000	-0.000007	-0.000380	0.346441	0.000256	0.000013
23	H	-0.000001	0.000360	-0.000005	0.000256	0.329641	-0.000006
24	H	-0.000526	-0.000001	-0.000242	0.000013	-0.000006	0.332083
25	H	0.000000	0.000097	-0.000029	-0.000345	0.000143	0.000000
26	H	0.000000	-0.000019	0.000023	-0.000363	-0.000058	0.000000
27	H	0.000015	0.000000	0.000000	0.000000	-0.000001	-0.000122
28	H	0.000000	0.000000	0.000010	-0.000055	-0.000027	0.000549
29	H	-0.000489	0.000026	0.000000	0.000000	-0.000001	0.000003

		25	26	27	28	29
1	C	-0.074825	-0.069132	-0.001566	-0.004497	0.028546
2	C	0.015450	0.000762	0.004560	0.010248	-0.048525
3	C	0.015841	-0.006221	-0.027497	-0.007607	0.107578
4	C	0.057631	0.014573	0.020036	0.003419	0.015919
5	C	-0.030547	0.005902	-0.038099	-0.013102	-0.075063

6	C	0.025980	0.051365	-0.003448	-0.025289	0.021336
7	C	-0.106827	-0.168171	0.002647	0.022163	-0.003000
8	C	0.035520	0.066975	-0.031425	-0.021135	0.001024
9	C	-0.024544	-0.013078	0.053917	0.219025	0.034769
10	C	0.006246	-0.013060	0.014320	-0.112395	-0.042333
11	C	0.392570	0.448174	-0.000275	0.001115	0.002507
12	C	0.004922	-0.000636	0.080532	-0.037861	-0.050151
13	N	0.000015	-0.000018	0.203316	0.008549	0.005853
14	O	-0.000053	-0.000112	-0.004180	0.178587	-0.000046
15	O	0.000022	-0.000001	-0.022176	-0.000425	-0.002446
16	O	0.000235	-0.000037	-0.000881	0.000127	0.231616
17	H	-0.000182	-0.000446	0.000000	0.000000	-0.000003
18	H	-0.000020	0.000190	0.000000	0.000000	0.000003
19	H	0.000000	0.000000	0.000015	0.000000	-0.000489
20	H	0.000097	-0.000019	0.000000	0.000000	0.000026
21	H	-0.000029	0.000023	0.000000	0.000010	0.000000
22	H	-0.000345	-0.000363	0.000000	-0.000055	0.000000
23	H	0.000143	-0.000058	-0.000001	-0.000027	-0.000001
24	H	0.000000	0.000000	-0.000122	0.000549	0.000003
25	H	0.420727	-0.015385	0.000000	0.000000	0.000000
26	H	-0.015385	0.425680	0.000000	0.000000	0.000000
27	H	0.000000	0.000000	0.398345	-0.000065	0.000088
28	H	0.000000	0.000000	-0.000065	0.307993	0.000000
29	H	0.000000	0.000000	0.000088	0.000000	0.237154

Total atomic charges:

		1
1	C	-0.093567
2	C	0.422504
3	C	-1.505055
4	C	-0.325173
5	C	0.755261
6	C	-0.381064
7	C	0.304663
8	C	-1.325396
9	C	4.433336
10	C	-2.185758
11	C	-1.738406
12	C	0.907782
13	N	-1.254234
14	O	-0.799393
15	O	-0.861244
16	O	-0.661240
17	H	0.281962
18	H	0.280934
19	H	0.302792
20	H	0.325431
21	H	0.275178
22	H	0.302528
23	H	0.318442
24	H	0.310999
25	H	0.277358
26	H	0.273091
27	H	0.351959
28	H	0.470674

```
29  H    0.535635
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  C    0.188395
 2  C    0.703439
 3  C   -1.202263
 4  C    0.000257
 5  C    0.755261
 6  C   -0.105886
 7  C    0.607191
 8  C   -1.006954
 9  C    4.433336
10  C   -1.874758
11  C   -1.187958
12  C    0.907782
13  N   -0.902276
14  O   -0.328719
15  O   -0.861244
16  O   -0.125604
17  H    0.000000
18  H    0.000000
19  H    0.000000
20  H    0.000000
21  H    0.000000
22  H    0.000000
23  H    0.000000
24  H    0.000000
25  H    0.000000
26  H    0.000000
27  H    0.000000
28  H    0.000000
29  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  2442.9859
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=    -7.9223    Y=     4.5708    Z=     4.0045  Tot=     9.9846
Quadrupole moment (Debye-Ang):
  XX=  -105.0853   YY=   -89.2381   ZZ=   -99.5653
  XY=     2.3331   XZ=     7.3952   YZ=     5.5627
Octapole moment (Debye-Ang**2):
 XXX=   -29.6503  YYY=    33.9852  ZZZ=     4.4064  XYY=    20.3784
 XXY=     4.9708  XXZ=    12.1945  XZZ=   -30.4278  YZZ=     3.6752
 YYZ=    19.8026  XYZ=    11.4890
Hexadecapole moment (Debye-Ang**3):
XXXX= -1701.7963 YYYY=  -917.5775 ZZZZ=  -600.9154 XXXY=    21.7431
XXXZ=    12.4871 YYYX=    28.2738 YYYZ=    26.5987 ZZZX=    11.8319
ZZZY=     5.9103 XXYY=  -376.4382 XXZZ=  -453.6948 YYZZ=  -246.8084
XXYZ=    26.4285 YYXZ=    29.7342 ZZXY=     3.2996
N-N= 1.230533823121D+03 E-N=-4.184489588108D+03  KE= 7.353025820100D+02
 Exact polarizability: 134.232   5.469 119.059   7.722  -0.855 116.567
Approx polarizability: 113.413   5.737 114.085   5.623  -2.384 118.238
Full mass-weighted force constant matrix:
```

```
 Low frequencies ---  -93.7907   -1.4712   -1.1416   -0.1731   -0.0008
-0.0006
 Low frequencies ---   -0.0003  128.1822  146.1274
 ******    1 imaginary frequencies (negative Signs) ******
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                      1                      2                      3
                    ?A                     ?A                     ?A
 Frequencies --   -93.7907               128.1822               146.1274
 Red. masses --     8.7091                 5.2370                 6.2087
 Frc consts  --     0.0451                 0.0507                 0.0781
 IR Inten    --     2.4715                 6.2993                 2.5530
 Raman Activ --     1.7437                 0.1965                 0.2723
 Depolar     --     0.7479                 0.6932                 0.7432
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.02   0.01   0.05     0.15   0.06  -0.04     0.03   0.00  -
0.08
   2   6    -0.03  -0.04   0.04     0.10   0.06  -0.02    -0.09  -0.01  -
0.05
   3   6    -0.05  -0.02   0.06     0.14  -0.10  -0.01    -0.12   0.03
0.08
   4   6    -0.02   0.05   0.06     0.15  -0.11  -0.03     0.08   0.00
0.04
   5   6     0.00  -0.02   0.08     0.13  -0.08  -0.02     0.00   0.01
0.11
   6   6    -0.01  -0.04  -0.02    -0.04   0.02   0.01    -0.05   0.00  -
0.03
   7   6     0.00   0.01  -0.03    -0.07   0.01   0.02     0.03  -0.01  -
0.04
   8   6    -0.01   0.04  -0.01    -0.01  -0.12   0.01     0.05  -0.02
0.04
   9   6     0.00   0.03  -0.01    -0.02  -0.13   0.01     0.01   0.02
0.08
  10   6    -0.01  -0.02   0.00    -0.01  -0.11   0.01    -0.05   0.04
0.06
  11   6    -0.01   0.02   0.00     0.03   0.11  -0.01     0.07   0.00  -
0.13
  12   6    -0.01   0.05  -0.05    -0.11   0.03   0.01    -0.02   0.00  -
0.11
  13   7    -0.19   0.48   0.06    -0.12   0.20   0.01     0.17   0.00  -
0.25
  14   8    -0.01   0.03  -0.06     0.07  -0.11  -0.01     0.03   0.02
0.23
  15   8     0.16  -0.37  -0.18    -0.19   0.07   0.01    -0.22  -0.03  -
0.16
  16   8     0.15  -0.14   0.07    -0.10   0.10   0.04     0.08  -0.04
0.20
  17   1    -0.03   0.00   0.07     0.24   0.11  -0.07     0.04   0.00  -
0.12
  18   1    -0.05  -0.08   0.04     0.13   0.14  -0.04    -0.16  -0.03  -
0.11
```

19	1	-0.05	-0.06	0.07	0.18	-0.12	-0.02	-0.21	0.03	0.11
20	1	-0.02	0.08	0.07	0.20	-0.13	-0.04	0.18	0.00	0.05
21	1	0.00	-0.07	-0.04	-0.11	0.09	0.02	-0.07	-0.01	-0.05
22	1	0.01	0.02	-0.07	-0.17	0.01	0.04	0.04	-0.01	-0.04
23	1	0.01	0.08	-0.01	-0.03	-0.17	0.02	0.10	0.00	0.05
24	1	-0.01	-0.04	-0.01	-0.05	-0.16	0.01	-0.10	0.04	0.08
25	1	0.00	0.05	0.00	0.04	0.10	-0.02	0.17	-0.01	-0.15
26	1	-0.01	-0.01	-0.01	0.00	0.21	-0.02	0.02	0.01	-0.22
27	1	-0.18	0.46	0.04	-0.19	0.36	0.00	0.14	-0.01	-0.42
28	1	0.01	-0.02	-0.14	0.06	-0.09	0.01	0.08	0.09	0.18
29	1	0.21	-0.26	0.07	-0.20	0.21	0.08	0.00	-0.06	0.29

	4	5	6
	?A	?A	?A
Frequencies --	166.7836	268.0564	305.3770
Red. masses --	6.3054	5.2632	4.7272
Frc consts --	0.1033	0.2228	0.2597
IR Inten --	17.9906	24.0594	1.1262
Raman Activ --	0.5750	1.3907	0.8013
Depolar --	0.4827	0.6881	0.6031

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.03	-0.01	0.00	-0.01	0.06	0.00	0.02	0.01	0.07
2	6	-0.02	0.00	-0.01	-0.04	0.05	0.01	0.04	-0.07	0.03
3	6	-0.03	-0.01	-0.03	-0.03	-0.02	0.02	0.02	-0.02	0.00
4	6	-0.05	0.00	-0.01	-0.01	-0.04	0.00	0.00	-0.01	0.01
5	6	0.05	-0.08	-0.05	-0.02	-0.04	0.02	0.01	-0.01	0.01
6	6	-0.03	0.00	0.01	-0.10	0.04	0.00	0.07	-0.06	-0.08
7	6	-0.04	-0.01	0.01	-0.13	0.03	0.02	-0.04	0.00	-0.09
8	6	-0.04	-0.02	0.00	-0.08	-0.06	0.00	-0.03	-0.04	-0.12
9	6	-0.02	0.00	0.01	-0.01	0.02	-0.02	-0.01	-0.01	-0.12
10	6	-0.03	-0.02	0.01	-0.07	-0.02	-0.01	0.05	0.02	-0.13
11	6	-0.04	-0.01	0.02	-0.09	0.10	0.02	-0.05	0.07	0.05

12	6	-0.07	0.11	0.04	-0.01	0.03	-0.03	0.00	0.01	-0.11
13	7	-0.04	0.07	0.03	-0.02	-0.13	0.00	-0.14	-0.01	0.00
14	8	0.10	0.03	-0.03	0.42	0.08	0.00	-0.04	-0.04	0.33
15	8	-0.15	0.27	0.10	0.12	-0.09	-0.04	0.13	0.13	-0.04
16	8	0.33	-0.29	-0.09	-0.05	-0.03	0.01	0.00	-0.01	0.02
17	1	-0.04	-0.01	0.00	0.05	0.10	-0.01	0.06	0.04	0.13
18	1	-0.01	0.01	0.00	-0.04	0.08	0.00	0.04	-0.13	0.07
19	1	-0.01	0.01	-0.04	-0.01	-0.03	0.02	0.06	-0.07	0.01
20	1	-0.05	-0.03	-0.02	0.02	-0.04	0.01	-0.04	0.04	0.03
21	1	-0.04	0.01	0.02	-0.11	0.06	0.02	0.14	-0.11	-0.08
22	1	-0.04	-0.02	0.02	-0.21	0.03	0.03	-0.12	0.01	-0.12
23	1	-0.04	-0.02	0.00	-0.12	-0.08	-0.01	-0.08	0.02	-0.15
24	1	-0.03	-0.01	0.01	-0.09	-0.05	-0.01	0.10	-0.01	-0.18
25	1	-0.05	-0.02	0.02	-0.11	0.11	0.02	-0.16	0.14	0.06
26	1	-0.03	-0.01	0.03	-0.09	0.16	0.04	-0.01	0.06	0.13
27	1	-0.07	0.13	0.04	0.05	-0.28	0.04	-0.13	0.03	0.15
28	1	0.09	0.09	0.03	0.49	0.42	0.08	-0.13	0.09	0.62
29	1	0.52	-0.53	-0.16	-0.09	0.03	0.02	-0.01	0.00	0.03

	7			8			9		
	?A			?A			?A		
Frequencies --	329.3096			372.7432			385.8320		
Red. masses --	4.1254			6.2966			3.2881		
Frc consts --	0.2636			0.5154			0.2884		
IR Inten --	9.8174			16.8710			28.4644		
Raman Activ --	0.6125			2.8379			1.1783		
Depolar --	0.4724			0.2859			0.6598		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.02	0.05	0.12	0.01	0.04	-0.05	0.06	-0.02	0.02
2 6	0.00	-0.08	0.08	-0.05	0.05	-0.02	-0.04	0.00	0.05
3 6	0.02	-0.06	0.05	-0.05	-0.06	0.03	-0.04	0.05	0.13
4 6	-0.05	0.05	0.08	0.02	-0.12	-0.03	0.08	-0.07	0.11

```
    5   6    -0.02  -0.01   0.01    -0.03  -0.14   0.01     0.01  -0.03
0.11
    6   6    -0.03  -0.07  -0.08    -0.11   0.03   0.02    -0.01   0.01
0.07
    7   6     0.00   0.06  -0.13    -0.13   0.01   0.04     0.00  -0.03
0.07
    8   6     0.05   0.06   0.01    -0.05  -0.08   0.03    -0.01  -0.05
0.05
    9   6     0.02  -0.02   0.07     0.04  -0.01   0.02    -0.02   0.03  -
0.03
   10   6    -0.03  -0.08   0.03    -0.06  -0.04   0.03     0.01   0.03
0.03
   11   6     0.02   0.14  -0.09    -0.10   0.08   0.03     0.12   0.01  -
0.12
   12   6     0.02  -0.01   0.07     0.20   0.07  -0.01    -0.03   0.03  -
0.09
   13   7     0.13   0.05   0.00     0.29   0.15  -0.09    -0.12  -0.05  -
0.03
   14   8     0.03  -0.02   0.09    -0.14  -0.04  -0.02    -0.04   0.04  -
0.09
   15   8    -0.08  -0.05   0.04     0.26   0.15   0.01     0.07   0.07  -
0.06
   16   8    -0.08  -0.02  -0.25    -0.09  -0.12   0.02    -0.03  -0.04  -
0.13
   17   1     0.01   0.08   0.21     0.11   0.09  -0.10     0.10   0.00  -
0.02
   18   1     0.02  -0.15   0.14    -0.07   0.10  -0.06    -0.10  -0.01
0.00
   19   1     0.05  -0.08   0.05    -0.04  -0.03   0.01    -0.08   0.02
0.16
   20   1    -0.11   0.09   0.09     0.10  -0.12  -0.01     0.15  -0.05
0.13
   21   1    -0.05  -0.14  -0.16    -0.14   0.08   0.04     0.03   0.01
0.10
   22   1    -0.04   0.08  -0.22    -0.22   0.01   0.07    -0.02  -0.03
0.10
   23   1     0.13   0.15   0.00    -0.08  -0.16   0.04    -0.06  -0.06
0.04
   24   1    -0.10  -0.12   0.05    -0.12  -0.08   0.05     0.04   0.02
0.00
   25   1     0.14   0.31  -0.10    -0.17   0.04   0.04     0.44   0.05  -
0.17
   26   1    -0.03   0.04  -0.22    -0.08   0.17   0.11    -0.04   0.04  -
0.41
   27   1     0.09   0.08  -0.12     0.23   0.23  -0.25    -0.07  -0.09
0.09
   28   1     0.11   0.00  -0.08    -0.11  -0.22  -0.21    -0.25  -0.02
0.35
   29   1     0.11   0.08  -0.45    -0.15  -0.05   0.04    -0.04   0.20  -
0.22
                     10                    11                    12
                     ?A                    ?A                    ?A
 Frequencies --    414.4176              451.0759              478.4651
 Red. masses --      1.2023                2.4026                5.8462
```

Frc consts	--	0.1217			0.2880			0.7885		
IR Inten	--	120.3892			11.7984			14.2628		
Raman Activ	--	1.2555			1.1810			5.9821		
Depolar	--	0.7448			0.0885			0.1886		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.09	0.00	-0.05	0.03	-0.01	0.00
2	6	-0.01	0.00	0.01	-0.02	-0.02	-0.05	0.12	-0.02	0.00
3	6	-0.01	0.02	0.01	-0.06	0.02	0.09	0.17	-0.17	-0.05
4	6	0.01	0.00	0.02	0.12	-0.06	0.01	-0.03	-0.03	-0.11
5	6	0.00	0.01	0.02	0.03	-0.04	0.08	0.06	-0.20	-0.11
6	6	0.01	0.01	0.01	0.02	-0.03	-0.07	0.00	-0.05	0.03
7	6	0.00	0.00	0.02	0.04	-0.01	-0.07	0.01	-0.02	0.02
8	6	-0.01	-0.01	0.00	0.05	0.02	-0.04	-0.04	0.06	0.01
9	6	-0.01	-0.01	-0.02	-0.02	0.06	0.01	-0.09	0.22	0.06
10	6	0.01	0.01	-0.01	-0.02	0.02	0.02	0.00	-0.05	0.07
11	6	0.02	0.00	-0.03	-0.04	0.00	0.15	0.06	0.00	-0.06
12	6	-0.01	0.00	-0.02	-0.03	0.03	0.01	-0.06	0.13	0.03
13	7	-0.05	-0.02	0.00	-0.03	-0.03	0.01	-0.02	-0.05	0.00
14	8	-0.02	-0.03	0.07	-0.04	0.08	-0.02	-0.12	0.30	0.08
15	8	0.03	0.03	-0.01	-0.04	-0.02	-0.01	0.00	-0.04	-0.03
16	8	0.01	0.00	-0.01	-0.02	-0.04	-0.08	-0.09	-0.09	0.07
17	1	0.00	-0.01	-0.01	0.15	0.03	-0.08	0.02	-0.01	0.05
18	1	-0.02	0.00	0.00	-0.11	-0.07	-0.11	0.21	0.06	0.04
19	1	-0.02	0.01	0.02	-0.13	0.02	0.12	0.24	-0.05	-0.16
20	1	0.02	0.00	0.02	0.21	0.00	0.05	-0.07	0.00	-0.10
21	1	0.02	0.01	0.02	0.00	-0.05	-0.10	-0.07	0.00	0.03
22	1	0.00	-0.01	0.03	0.03	0.00	-0.11	0.04	-0.01	-0.02
23	1	-0.04	0.00	-0.01	0.13	0.01	-0.01	0.07	-0.07	0.08
24	1	0.04	0.00	-0.03	-0.02	-0.03	0.00	0.07	-0.16	-0.02

25	1	0.08	0.00	-0.04	-0.47	-0.08	0.21	0.25	0.03	-0.09
26	1	-0.01	0.00	-0.08	0.15	0.05	0.54	-0.03	0.00	-0.24
27	1	-0.05	0.01	0.04	0.00	-0.08	0.03	0.09	-0.29	0.01
28	1	0.40	0.04	-0.89	0.02	0.06	-0.18	-0.01	0.29	-0.18
29	1	-0.01	0.04	-0.01	-0.10	0.20	-0.10	-0.09	-0.20	0.11

	13	14	15
	?A	?A	?A
Frequencies --	523.6577	543.6447	597.9248
Red. masses --	3.2157	6.3976	5.0692
Frc consts --	0.5195	1.1140	1.0678
IR Inten --	8.1331	1.9620	5.4405
Raman Activ --	2.9830	5.6300	1.7302
Depolar --	0.3489	0.2464	0.6825

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.06	0.01	0.09	-0.07	0.08	-0.03	0.05	0.07	-0.02
2	6	-0.01	-0.08	0.06	0.00	0.21	0.04	-0.01	-0.10	-0.05
3	6	-0.12	0.12	-0.06	0.05	-0.01	0.06	-0.13	-0.06	-0.11
4	6	0.02	-0.11	-0.06	-0.06	0.01	0.00	0.01	0.10	-0.11
5	6	-0.08	-0.02	-0.08	-0.17	-0.19	0.05	-0.09	0.02	-0.14
6	6	0.11	-0.04	0.02	0.07	0.22	-0.04	-0.02	-0.12	0.07
7	6	-0.03	0.00	-0.01	0.18	0.14	-0.03	0.07	0.08	0.03
8	6	0.01	-0.09	-0.04	0.11	0.07	-0.07	0.09	0.08	0.18
9	6	0.03	0.02	-0.02	0.08	-0.05	-0.04	0.05	-0.04	0.16
10	6	0.08	0.13	-0.05	0.06	0.06	-0.01	0.03	-0.06	0.21
11	6	0.02	0.16	-0.01	0.09	-0.02	0.02	0.06	0.13	0.07
12	6	0.02	-0.01	0.05	0.03	-0.08	-0.04	-0.01	0.00	-0.12
13	7	0.03	0.00	0.05	-0.07	-0.02	0.03	-0.15	-0.05	-0.04
14	8	-0.01	0.03	-0.05	0.04	-0.09	0.01	0.02	-0.09	-0.01
15	8	-0.09	-0.04	0.04	-0.07	0.01	-0.02	0.08	0.08	-0.11
16	8	0.00	-0.08	0.05	-0.21	-0.26	0.05	-0.03	-0.01	0.00
17	1	0.17	0.09	0.16	-0.09	0.04	-0.19	0.05	0.09	0.10

18	1	-0.07	-0.15	0.04	0.02	0.19	0.07	-0.04	-0.07	-0.09
19	1	-0.11	0.19	-0.11	0.19	0.07	-0.04	-0.25	0.12	-0.17
20	1	-0.08	-0.13	-0.08	0.04	0.14	0.08	-0.01	-0.03	-0.17
21	1	0.26	-0.12	0.05	0.01	0.18	-0.12	-0.13	-0.14	-0.02
22	1	-0.19	0.03	-0.04	0.24	0.11	0.12	0.07	0.12	-0.16
23	1	0.01	-0.15	-0.02	0.09	0.12	-0.09	0.20	0.02	0.23
24	1	0.16	0.25	-0.04	-0.01	-0.02	-0.01	-0.03	0.08	0.30
25	1	0.14	0.25	-0.03	0.03	-0.02	0.03	-0.07	0.05	0.09
26	1	-0.05	0.18	-0.14	0.15	-0.19	0.07	0.12	0.17	0.20
27	1	0.02	0.03	0.05	-0.09	0.08	0.18	-0.11	-0.04	0.17
28	1	-0.01	-0.03	-0.10	0.03	-0.08	0.02	-0.01	-0.14	0.01
29	1	-0.38	0.06	0.31	-0.16	-0.30	0.01	0.03	-0.21	0.02

	16	17	18
	?A	?A	?A
Frequencies --	633.0333	674.5728	692.6278
Red. masses --	3.3843	2.8829	2.0441
Frc consts --	0.7990	0.7729	0.5778
IR Inten --	11.3742	83.1662	86.0291
Raman Activ --	1.2212	3.4162	7.1442
Depolar --	0.6622	0.2890	0.1257

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.04	-0.05	0.19	0.05	0.02	0.03	0.08	-0.01	0.03
2	6	-0.03	0.08	0.12	-0.06	0.01	0.06	-0.01	0.01	0.03
3	6	0.02	0.06	-0.04	-0.11	-0.08	-0.05	-0.02	0.02	0.00
4	6	-0.02	-0.13	0.02	0.06	0.09	-0.06	0.01	-0.01	-0.02
5	6	0.08	-0.01	-0.09	0.02	-0.01	-0.04	-0.06	0.02	-0.01
6	6	-0.11	0.07	-0.07	-0.08	-0.04	0.09	0.00	0.00	0.01
7	6	0.08	-0.01	-0.13	0.07	0.05	0.11	0.04	-0.02	-0.01
8	6	0.10	-0.07	-0.02	-0.02	0.09	-0.07	0.02	-0.05	-0.05
9	6	-0.01	-0.01	0.07	-0.05	-0.01	-0.09	-0.06	-0.01	-0.02
10	6	-0.15	0.02	0.04	-0.09	-0.06	-0.09	-0.04	0.04	-0.02

11	6	0.04	-0.05	0.02	0.14	-0.03	0.08	0.09	0.02	0.04
12	6	-0.02	0.04	-0.03	-0.03	-0.02	0.03	-0.13	-0.03	0.03
13	7	-0.04	-0.02	-0.04	0.04	0.02	-0.03	0.00	0.02	-0.09
14	8	-0.01	0.00	-0.03	0.01	-0.01	0.03	0.00	0.01	-0.01
15	8	0.06	0.03	-0.04	0.01	-0.01	0.05	0.06	-0.01	0.09
16	8	0.07	0.04	0.02	0.04	-0.04	-0.05	-0.06	0.03	0.03
17	1	-0.01	-0.05	0.07	-0.03	-0.03	0.03	0.09	-0.01	0.00
18	1	0.05	0.08	0.21	-0.06	0.11	0.00	-0.04	0.03	-0.02
19	1	0.15	0.07	-0.09	-0.05	-0.19	-0.01	0.02	0.03	-0.03
20	1	-0.27	-0.16	-0.03	0.02	0.17	-0.03	-0.03	0.00	-0.01
21	1	-0.18	0.00	-0.19	-0.06	-0.10	0.04	0.03	-0.04	-0.01
22	1	0.06	-0.03	-0.03	0.16	0.05	0.08	-0.02	-0.01	0.00
23	1	0.30	-0.05	0.03	-0.21	0.03	-0.10	0.04	-0.05	-0.04
24	1	-0.30	0.01	0.13	0.02	-0.03	-0.15	-0.01	0.04	-0.04
25	1	-0.03	0.19	0.04	0.18	-0.11	0.07	0.06	0.05	0.05
26	1	0.09	-0.27	0.04	0.13	-0.01	0.05	0.10	0.04	0.07
27	1	-0.03	-0.03	-0.01	-0.04	0.12	-0.16	-0.04	-0.02	-0.41
28	1	-0.01	-0.05	-0.06	0.03	0.12	0.09	0.02	0.06	-0.01
29	1	-0.28	0.20	0.25	-0.50	0.42	0.23	0.57	-0.53	-0.28

	19	20	21
	?A	?A	?A
Frequencies --	712.3662	794.5186	816.8180
Red. masses --	2.8587	4.9361	3.5720
Frc consts --	0.8547	1.8359	1.4041
IR Inten --	124.9449	19.6661	4.2107
Raman Activ --	0.5187	2.6385	7.5747
Depolar --	0.1350	0.7469	0.1385

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.06	-0.01	0.03	0.08	0.01	-0.01	-0.07	-0.01	-0.07
2	6	-0.06	0.03	0.05	0.19	0.01	-0.09	-0.13	0.00	0.16
3	6	-0.04	-0.06	-0.03	0.02	0.07	0.04	0.04	-0.04	-0.04

4	6	0.02	-0.01	-0.01	-0.10	0.08	0.00	0.13	-0.05	-0.02
5	6	-0.04	0.04	-0.01	-0.19	0.14	0.06	0.00	0.00	-0.01
6	6	-0.08	-0.01	0.02	0.01	0.05	-0.08	0.05	-0.04	0.09
7	6	0.01	-0.02	0.06	-0.01	-0.09	0.00	0.01	0.13	-0.01
8	6	0.04	-0.06	-0.03	-0.02	-0.10	-0.01	0.06	0.05	0.03
9	6	0.06	0.02	-0.05	-0.03	0.00	0.02	0.00	-0.01	0.01
10	6	-0.08	-0.03	-0.11	-0.01	-0.11	-0.01	0.03	0.03	-0.07
11	6	0.08	0.02	0.05	0.11	0.01	0.05	-0.12	-0.02	-0.08
12	6	0.16	0.08	-0.02	-0.12	0.33	0.08	-0.12	0.23	0.07
13	7	0.02	-0.02	0.13	0.03	-0.03	0.01	0.01	-0.02	-0.01
14	8	-0.03	0.02	0.01	-0.02	-0.13	0.00	-0.01	-0.10	0.00
15	8	-0.10	-0.01	-0.12	0.03	-0.04	-0.04	0.02	-0.04	-0.01
16	8	-0.02	0.06	0.01	0.02	-0.08	-0.02	0.01	0.01	0.00
17	1	0.07	-0.01	-0.03	-0.04	-0.05	0.06	0.05	0.05	-0.14
18	1	-0.07	0.12	0.00	0.14	-0.07	-0.11	-0.07	0.09	0.17
19	1	0.04	-0.16	0.00	-0.04	0.06	0.07	0.28	-0.17	-0.05
20	1	-0.05	-0.02	-0.02	-0.09	0.08	0.00	0.23	-0.10	-0.03
21	1	-0.04	-0.04	0.02	-0.14	0.24	-0.02	0.26	-0.28	0.02
22	1	-0.05	-0.02	0.09	-0.12	-0.08	0.03	0.13	0.12	-0.02
23	1	-0.05	-0.08	-0.05	0.02	-0.03	-0.02	0.08	0.00	0.05
24	1	-0.10	-0.04	-0.10	-0.05	-0.16	0.00	0.11	0.13	-0.07
25	1	0.07	0.02	0.06	0.12	0.04	0.05	-0.19	-0.11	-0.07
26	1	0.08	0.04	0.06	0.08	0.08	0.03	-0.07	-0.06	0.01
27	1	0.17	-0.18	0.51	0.21	-0.45	-0.07	0.16	-0.42	-0.14
28	1	-0.02	-0.07	-0.07	-0.04	-0.13	0.06	-0.02	-0.11	0.03
29	1	0.46	-0.36	-0.23	-0.32	0.15	0.19	0.06	-0.06	-0.02

	22	23	24
	?A	?A	?A

Frequencies --		824.4286			829.0606			849.9716		
Red. masses --		3.8993			4.9237			4.5266		
Frc consts --		1.5615			1.9939			1.9268		
IR Inten --		21.3093			1.8863			5.5881		
Raman Activ --		9.0289			7.3060			5.2716		
Depolar --		0.0658			0.0497			0.0310		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.10	0.07	0.06	0.16	-0.19	0.01	-0.08	0.04	-0.08
2	6	-0.06	-0.03	-0.05	0.13	-0.02	0.13	-0.01	0.04	0.15
3	6	-0.09	0.01	0.10	0.04	0.17	0.07	-0.02	-0.09	0.20
4	6	-0.01	0.05	-0.10	0.09	0.09	-0.13	-0.02	0.00	-0.22
5	6	0.22	-0.16	-0.04	-0.06	0.00	0.00	-0.13	0.14	0.00
6	6	0.08	0.03	-0.01	-0.12	-0.02	0.18	0.03	0.04	0.03
7	6	0.05	0.03	0.02	-0.08	-0.02	-0.10	0.01	0.06	0.01
8	6	-0.09	-0.05	-0.18	0.00	0.12	-0.18	0.11	-0.18	-0.12
9	6	-0.04	0.00	-0.02	-0.06	0.00	-0.02	0.04	0.02	0.01
10	6	0.03	0.03	0.17	-0.05	0.00	0.13	0.09	-0.17	0.08
11	6	0.03	-0.01	0.04	-0.12	-0.07	-0.09	-0.04	0.02	-0.02
12	6	-0.01	0.11	0.03	0.07	-0.03	-0.02	-0.01	-0.07	-0.01
13	7	0.03	0.01	0.04	0.02	0.01	0.04	-0.02	-0.01	-0.03
14	8	0.01	-0.11	-0.01	0.02	-0.07	0.00	-0.02	0.10	0.01
15	8	0.00	-0.01	-0.03	-0.02	0.02	-0.04	0.00	0.00	0.03
16	8	-0.02	0.08	0.01	-0.04	-0.04	0.01	0.09	0.05	-0.03
17	1	-0.17	0.04	0.10	0.18	-0.15	0.19	-0.09	0.03	-0.13
18	1	-0.12	-0.22	0.00	0.08	0.23	-0.04	-0.08	-0.02	0.13
19	1	-0.37	0.28	0.04	0.08	0.35	-0.05	0.00	-0.11	0.22
20	1	-0.04	0.21	-0.03	0.05	0.34	-0.02	-0.02	0.02	-0.22
21	1	-0.02	0.03	-0.09	-0.19	-0.02	0.15	-0.05	-0.03	-0.09
22	1	-0.01	0.03	0.08	0.12	-0.03	-0.12	-0.16	0.04	0.18
23	1	-0.16	-0.17	-0.17	0.05	0.08	-0.16	0.23	-0.38	-0.03

24	1	0.06	-0.08	0.10	0.05	0.06	0.10	0.13	-0.39	-0.03
25	1	0.17	-0.01	0.01	-0.15	0.05	-0.08	-0.02	-0.03	-0.03
26	1	-0.02	-0.12	-0.11	-0.13	0.06	-0.05	-0.04	-0.05	-0.04
27	1	0.17	-0.30	0.04	0.04	0.03	0.16	-0.13	0.23	-0.04
28	1	0.02	-0.05	0.01	0.05	0.08	0.04	-0.06	-0.01	-0.01
29	1	0.22	-0.01	-0.16	0.04	-0.13	-0.02	-0.04	0.07	0.07

	25			26			27		
	?A			?A			?A		
Frequencies --	872.7579			884.4725			906.5575		
Red. masses --	3.0758			2.4068			2.7729		
Frc consts --	1.3804			1.1093			1.3427		
IR Inten --	3.7456			20.1720			6.3992		
Raman Activ --	9.6888			2.1660			1.8835		
Depolar --	0.0126			0.5180			0.5867		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.07	-0.09	0.00	-0.03	0.03	-0.11	0.05	0.07
2	6	-0.12	0.07	0.05	0.02	0.14	-0.06	0.12	0.00	0.02
3	6	0.12	0.00	0.04	-0.10	-0.11	-0.05	-0.07	-0.03	-0.10
4	6	-0.06	0.16	-0.01	-0.07	-0.03	0.08	0.18	0.16	-0.02
5	6	0.02	-0.03	0.01	0.04	0.00	0.03	0.00	-0.02	0.05
6	6	0.03	-0.14	0.05	-0.04	-0.02	0.14	-0.03	0.02	-0.03
7	6	-0.06	-0.16	-0.07	0.01	-0.06	-0.09	-0.06	-0.05	0.01
8	6	-0.01	-0.09	-0.03	0.07	-0.01	-0.05	0.08	-0.11	0.00
9	6	-0.01	0.00	0.06	0.01	0.00	-0.03	0.04	-0.01	0.05
10	6	-0.04	0.12	0.04	0.13	0.00	0.03	-0.02	0.05	-0.05
11	6	0.11	0.03	0.03	-0.02	0.04	-0.02	-0.04	-0.06	0.01
12	6	0.01	-0.01	-0.01	-0.02	0.03	0.01	-0.02	0.00	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	-0.01	-0.02
14	8	0.01	-0.02	-0.02	-0.01	0.00	0.00	-0.01	0.04	-0.01
15	8	0.00	0.01	-0.01	0.00	-0.01	0.01	0.00	0.00	0.00
16	8	0.00	-0.02	-0.01	0.01	0.01	-0.01	-0.04	-0.04	-0.01

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  17   1    -0.21  -0.06  -0.22     0.02  -0.03  -0.07    -0.26  -0.01
0.20
  18   1    -0.15   0.15  -0.01     0.15   0.46  -0.09     0.34  -0.02
0.23
  19   1     0.41  -0.07  -0.03    -0.37  -0.14   0.06    -0.21  -0.05  -
0.04
  20   1     0.00   0.23   0.03    -0.20   0.01   0.08     0.50   0.23
0.06
  21   1     0.26  -0.22   0.15    -0.13   0.07   0.16    -0.03   0.08
0.03
  22   1    -0.28  -0.11  -0.23    -0.05  -0.05  -0.13    -0.16  -0.06
0.09
  23   1     0.14   0.00  -0.02     0.20   0.12  -0.06     0.18  -0.11
0.03
  24   1    -0.08   0.16   0.08     0.45   0.14  -0.10    -0.06   0.18
0.03
  25   1    -0.02  -0.02   0.04    -0.10   0.19  -0.01     0.05   0.00
0.00
  26   1     0.12   0.15   0.12     0.01   0.00   0.02    -0.08  -0.16  -
0.09
  27   1    -0.01   0.04   0.04     0.02  -0.07  -0.05    -0.04   0.06  -
0.01
  28   1     0.01  -0.05  -0.03    -0.01  -0.02   0.01    -0.03  -0.10  -
0.05
  29   1    -0.15   0.13   0.06     0.01   0.09  -0.04     0.06   0.03  -
0.13
                     28                    29                    30
                     ?A                    ?A                    ?A
 Frequencies --   912.7387              939.0234              969.6642
 Red. masses --     2.5164                1.4243                2.9780
 Frc consts  --     1.2352                0.7399                1.6497
 IR Inten    --     7.3152               66.1000               17.5049
 Raman Activ --     2.8544                0.3988                3.4499
 Depolar     --     0.3526                0.5128                0.5381
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.08  -0.11   0.05    -0.01   0.01  -0.01     0.08  -0.01
0.04
   2   6    -0.08  -0.07  -0.08    -0.01  -0.01  -0.01     0.06   0.18
0.06
   3   6     0.02  -0.09   0.01     0.01   0.03  -0.01    -0.13  -0.09
0.08
   4   6    -0.05   0.09  -0.01     0.00  -0.02   0.02     0.01  -0.01  -
0.09
   5   6     0.03  -0.02   0.00     0.01  -0.02   0.00     0.00   0.00  -
0.05
   6   6     0.05   0.13   0.02     0.00  -0.01   0.02     0.14  -0.02  -
0.12
   7   6    -0.02  -0.01   0.08     0.01   0.01   0.00    -0.07  -0.08  -
0.02
   8   6     0.13   0.00  -0.06    -0.01   0.00  -0.01    -0.07   0.12
0.07
   9   6     0.05   0.01   0.05     0.00  -0.01  -0.02     0.01   0.03
0.05
```

10	6	-0.04	0.05	-0.04	0.00	-0.01	0.01	-0.02	0.02	-0.03
11	6	-0.10	0.04	-0.01	0.01	0.01	0.00	-0.05	-0.07	0.04
12	6	-0.03	0.02	0.01	-0.04	0.11	0.04	-0.01	0.01	0.01
13	7	-0.02	-0.02	-0.03	0.04	-0.11	-0.01	0.00	-0.02	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	0.01	-0.05	0.00
15	8	0.01	0.00	0.00	0.01	-0.04	-0.03	0.01	0.00	-0.01
16	8	0.00	-0.01	-0.01	0.00	0.01	0.01	0.00	0.02	0.00
17	1	0.14	-0.05	0.22	0.00	0.01	-0.01	0.10	-0.01	-0.10
18	1	-0.28	-0.12	-0.25	0.01	0.00	0.00	0.03	0.27	-0.01
19	1	0.13	-0.22	0.04	-0.01	0.07	-0.03	-0.20	-0.11	0.12
20	1	-0.28	0.26	0.05	0.01	-0.01	0.02	-0.04	-0.09	-0.13
21	1	0.17	0.20	0.16	-0.02	-0.02	0.01	0.46	-0.13	0.02
22	1	0.00	-0.06	0.30	0.00	0.01	-0.03	0.09	-0.08	-0.09
23	1	0.28	0.01	-0.02	-0.03	0.01	-0.02	0.04	0.12	0.10
24	1	-0.21	-0.01	0.03	0.03	0.02	0.00	-0.32	-0.19	0.05
25	1	-0.02	0.08	-0.02	-0.01	0.00	0.00	0.24	0.04	-0.01
26	1	-0.16	0.20	-0.07	0.02	0.00	0.01	-0.21	0.02	-0.24
27	1	-0.07	0.08	-0.03	-0.36	0.88	0.19	-0.08	0.18	0.04
28	1	-0.02	-0.10	-0.02	-0.02	-0.01	0.03	0.02	-0.02	0.02
29	1	-0.06	0.09	0.00	0.08	-0.05	-0.05	0.05	-0.06	-0.01

	31			32			33		
	?A			?A			?A		
Frequencies --	986.1077			999.1806			1012.1917		
Red. masses --	3.0339			2.7821			2.5319		
Frc consts --	1.7382			1.6365			1.5283		
IR Inten --	11.1640			24.1098			10.3821		
Raman Activ --	4.9238			3.9244			8.7230		
Depolar --	0.4230			0.1271			0.3638		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.12	-0.03	0.03	0.04	0.07	0.06	0.08	0.19	-0.03
2 6	0.03	-0.03	0.06	-0.12	0.01	0.08	0.04	0.01	0.04

3	6	-0.02	-0.16	0.03	-0.03	0.03	0.02	-0.03	0.04	-0.02
4	6	-0.03	0.07	-0.01	0.08	0.09	0.02	-0.08	0.02	0.06
5	6	-0.02	0.03	-0.01	0.01	-0.04	-0.12	0.02	-0.01	0.00
6	6	-0.05	0.07	-0.07	-0.04	0.11	-0.02	-0.01	-0.08	0.00
7	6	0.02	0.09	-0.06	-0.05	-0.17	-0.05	0.12	-0.09	0.09
8	6	-0.15	-0.11	0.07	-0.02	0.03	0.09	0.03	-0.05	-0.05
9	6	-0.03	-0.01	0.04	0.04	0.00	-0.05	0.04	0.00	-0.02
10	6	0.08	0.18	0.04	0.14	-0.10	-0.01	-0.06	-0.02	0.00
11	6	0.03	-0.07	-0.10	0.02	-0.04	-0.06	-0.12	-0.03	-0.11
12	6	0.00	0.01	0.00	-0.02	0.02	0.01	-0.01	0.00	0.00
13	7	0.02	-0.01	0.02	0.00	0.00	0.00	-0.01	0.00	-0.01
14	8	0.01	-0.01	-0.02	-0.01	0.02	0.02	0.00	0.01	0.00
15	8	0.00	0.00	-0.01	0.00	-0.01	0.02	0.00	0.00	0.01
16	8	0.01	0.00	-0.01	-0.02	0.01	-0.01	-0.01	0.00	0.00
17	1	0.14	0.00	0.15	0.04	0.05	-0.01	0.40	0.41	0.08
18	1	-0.03	0.00	-0.01	-0.31	-0.30	0.06	0.17	0.06	0.14
19	1	0.04	-0.30	0.09	0.09	0.24	-0.14	-0.07	0.10	-0.04
20	1	-0.12	0.06	-0.03	0.08	-0.03	-0.03	-0.20	0.09	0.08
21	1	-0.17	-0.03	-0.25	-0.12	0.33	0.13	0.03	-0.18	-0.06
22	1	0.11	0.06	0.07	0.05	-0.20	0.03	0.35	-0.16	0.24
23	1	-0.33	-0.22	0.05	0.02	0.24	0.03	-0.05	-0.02	-0.08
24	1	0.16	0.30	0.04	0.22	-0.27	-0.13	-0.11	0.01	0.04
25	1	-0.32	-0.09	-0.05	-0.25	0.03	-0.01	-0.21	-0.25	-0.10
26	1	0.22	-0.14	0.23	0.10	0.06	0.15	-0.08	0.08	0.02
27	1	-0.03	0.13	0.06	-0.01	0.00	-0.04	0.00	-0.04	-0.04
28	1	0.00	-0.03	-0.02	-0.02	-0.02	0.02	-0.02	-0.07	-0.02
29	1	-0.02	0.03	0.01	-0.06	-0.22	0.12	-0.02	0.01	0.00

		34			35			36		
		?A			?A			?A		
Frequencies --		1013.1297			1031.9600			1041.1157		
Red. masses --		2.3968			2.0298			2.1522		
Frc consts --		1.4495			1.2736			1.3745		
IR Inten --		28.6400			1.4826			45.1342		
Raman Activ --		6.1963			4.6545			5.2804		
Depolar --		0.4252			0.6047			0.6017		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.05	-0.12	-0.08	-0.04	0.00	0.01	0.02	-0.06	0.09
2	6	0.01	0.02	0.09	0.04	-0.02	-0.02	-0.07	0.10	-0.09
3	6	-0.07	0.04	-0.08	-0.03	0.00	0.01	0.04	0.09	0.02
4	6	-0.04	0.07	0.12	-0.01	0.01	-0.02	0.02	0.07	-0.03
5	6	0.05	-0.05	-0.03	0.01	-0.01	0.00	0.00	-0.02	0.01
6	6	0.07	0.03	-0.04	0.11	0.07	0.14	-0.01	-0.09	-0.02
7	6	-0.10	0.12	0.01	0.07	0.00	-0.08	0.05	0.06	0.00
8	6	0.00	-0.05	-0.02	-0.04	-0.05	0.06	-0.03	-0.08	0.07
9	6	0.05	-0.04	0.01	-0.06	-0.01	0.00	0.10	-0.03	-0.02
10	6	0.01	-0.10	0.02	-0.11	-0.05	-0.05	0.03	-0.07	-0.02
11	6	0.06	-0.01	-0.04	0.03	0.04	-0.10	-0.06	-0.01	0.00
12	6	-0.01	0.01	0.00	0.02	-0.01	-0.01	-0.02	0.02	0.00
13	7	-0.01	0.00	-0.01	0.02	0.01	0.01	-0.02	0.00	-0.02
14	8	-0.01	0.06	0.01	0.00	0.01	0.00	-0.01	0.06	0.01
15	8	0.00	0.00	0.00	0.00	0.01	-0.02	0.00	-0.01	0.02
16	8	-0.01	0.01	0.00	0.00	0.00	0.00	-0.02	-0.01	0.00
17	1	-0.03	-0.19	-0.26	-0.11	-0.01	0.20	-0.03	-0.06	0.26
18	1	0.14	0.12	0.16	0.05	0.05	-0.04	-0.23	0.40	-0.39
19	1	-0.22	0.24	-0.14	-0.14	-0.01	0.05	0.10	0.16	-0.04
20	1	-0.21	0.17	0.16	0.10	-0.08	-0.05	0.06	0.12	0.00
21	1	0.21	-0.20	-0.15	0.41	0.12	0.40	0.04	-0.24	-0.11
22	1	-0.32	0.12	0.12	0.13	0.00	-0.12	0.15	0.06	-0.10

23	1	-0.02	0.07	-0.06	-0.07	-0.10	0.07	-0.30	-0.24	0.05
24	1	-0.19	-0.15	0.11	-0.25	-0.21	-0.04	0.01	-0.11	-0.03
25	1	-0.11	-0.24	-0.01	-0.37	0.16	-0.04	0.01	0.20	-0.01
26	1	0.13	0.17	0.18	0.23	-0.12	0.23	-0.06	-0.18	-0.08
27	1	0.01	-0.05	-0.02	0.02	0.01	0.04	0.00	-0.07	-0.07
28	1	-0.04	-0.09	-0.02	0.02	0.12	0.01	-0.07	-0.20	-0.04
29	1	-0.03	0.01	0.01	0.01	0.02	-0.02	-0.02	0.00	0.00

	37	38	39
	?A	?A	?A
Frequencies --	1050.8278	1068.4505	1102.6114
Red. masses --	4.3397	1.6967	1.9885
Frc consts --	2.8234	1.1412	1.4244
IR Inten --	13.3778	1.3469	60.2008
Raman Activ --	1.5525	4.9724	8.2226
Depolar --	0.6944	0.7489	0.6892

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.03	-0.02	-0.06	-0.04	-0.11	-0.04	-0.01	0.03	-0.01
2	6	0.13	-0.06	0.05	0.01	0.01	0.05	0.02	-0.03	0.00
3	6	-0.03	0.09	0.18	-0.01	-0.02	-0.01	0.00	-0.05	0.01
4	6	-0.15	0.00	-0.13	0.01	0.01	-0.02	0.01	-0.06	-0.01
5	6	0.14	-0.11	0.00	0.01	-0.01	0.01	-0.03	0.02	0.00
6	6	-0.18	-0.05	0.00	-0.01	0.01	-0.05	-0.01	0.02	0.06
7	6	-0.06	0.02	0.04	0.09	-0.09	0.04	-0.02	-0.02	-0.04
8	6	0.11	0.05	0.14	-0.04	0.01	0.01	-0.05	0.06	-0.08
9	6	0.14	0.08	-0.03	0.03	0.01	-0.02	0.19	-0.08	-0.01
10	6	0.00	0.09	-0.18	0.00	0.02	0.02	-0.03	0.04	0.05
11	6	0.06	0.02	-0.04	-0.02	0.13	-0.01	0.03	-0.02	0.01
12	6	-0.03	0.01	0.01	-0.01	0.01	0.00	-0.03	0.03	0.01
13	7	-0.04	-0.01	-0.04	0.00	0.00	0.00	-0.04	-0.01	-0.03
14	8	0.01	-0.05	0.00	0.00	0.00	0.00	0.01	0.07	0.02
15	8	-0.01	-0.02	0.04	0.00	-0.01	0.01	0.00	-0.01	0.02

16	8	-0.02	0.01	0.02	0.01	0.00	0.00	0.02	0.01	-0.01
17	1	-0.18	-0.09	0.06	-0.28	-0.28	-0.23	0.04	0.06	-0.01
18	1	0.13	-0.03	0.04	0.12	-0.01	0.17	0.03	-0.09	0.04
19	1	-0.16	0.12	0.21	-0.03	-0.01	-0.01	0.01	-0.09	0.03
20	1	-0.23	-0.05	-0.17	0.11	0.00	-0.01	0.03	-0.06	-0.01
21	1	-0.09	0.03	0.15	-0.09	-0.04	-0.15	0.00	0.20	0.25
22	1	-0.14	0.07	-0.13	0.41	-0.16	0.20	-0.06	0.02	-0.23
23	1	0.09	-0.16	0.20	-0.22	-0.04	-0.02	-0.42	0.16	-0.21
24	1	0.06	-0.08	-0.30	-0.05	0.04	0.06	-0.33	0.10	0.27
25	1	-0.18	-0.09	-0.01	-0.13	0.39	0.01	0.01	-0.02	0.01
26	1	0.18	0.02	0.18	-0.06	0.41	0.03	0.04	-0.08	0.01
27	1	-0.05	-0.03	-0.11	-0.01	-0.01	-0.02	-0.01	-0.10	-0.09
28	1	-0.03	-0.25	-0.03	-0.01	-0.05	-0.01	-0.12	-0.48	-0.09
29	1	0.09	0.13	-0.12	0.02	0.05	-0.03	-0.01	-0.04	0.04

	40	41	42
	?A	?A	?A
Frequencies --	1128.9327	1163.8970	1193.4603
Red. masses --	2.0163	1.8916	2.0682
Frc consts --	1.5140	1.5098	1.7356
IR Inten --	48.7097	49.1696	50.8429
Raman Activ --	2.6479	2.3216	3.2553
Depolar --	0.6458	0.6201	0.6529

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.04	-0.02	0.01	0.03	-0.01	-0.07	0.01	-0.02	0.02
2	6	0.03	0.00	-0.05	0.05	-0.01	0.02	-0.06	0.01	-0.02
3	6	0.06	-0.07	0.10	-0.04	0.01	0.04	0.06	-0.05	-0.05
4	6	0.05	0.02	0.10	-0.02	0.07	0.06	0.06	-0.01	0.02
5	6	-0.04	0.01	-0.12	0.03	-0.03	-0.06	-0.03	0.04	0.02
6	6	-0.02	-0.05	0.00	0.00	0.00	0.05	-0.01	-0.01	0.00
7	6	0.00	0.02	0.05	0.05	0.05	-0.06	0.00	0.01	0.00
8	6	0.06	-0.03	-0.01	0.01	-0.08	0.05	-0.01	-0.02	0.00

```
    9   6     0.00   0.02  -0.07    -0.03  -0.08   0.01     0.04   0.21
0.01
   10   6    -0.04   0.11   0.03    -0.04   0.02  -0.05    -0.01   0.01
0.02
   11   6    -0.01   0.02  -0.03    -0.08  -0.01   0.10    -0.01   0.00
0.01
   12   6     0.00   0.00   0.00     0.00   0.00   0.00     0.04  -0.01  -
0.02
   13   7     0.00   0.00   0.00     0.01   0.00   0.01    -0.04   0.00  -
0.06
   14   8     0.00  -0.02  -0.01     0.00   0.04   0.00     0.01  -0.09
0.00
   15   8     0.00  -0.01   0.00     0.01   0.01  -0.02    -0.02  -0.02
0.07
   16   8     0.01   0.03  -0.05     0.00   0.02  -0.02     0.01  -0.01
0.00
   17   1    -0.11  -0.05   0.10     0.09  -0.03  -0.38     0.20   0.04  -
0.30
   18   1     0.05   0.14  -0.10    -0.06  -0.31   0.08     0.15  -0.13
0.24
   19   1    -0.29   0.20   0.08     0.01  -0.02   0.05    -0.25   0.24  -
0.11
   20   1     0.20  -0.18   0.02    -0.07   0.11   0.07    -0.21   0.30
0.14
   21   1     0.03  -0.14  -0.06    -0.11   0.20   0.15     0.05   0.16
0.20
   22   1    -0.11   0.02   0.11     0.25   0.10  -0.39     0.03   0.06  -
0.25
   23   1    -0.04   0.26  -0.13    -0.05  -0.08   0.03    -0.19  -0.36
0.06
   24   1    -0.09  -0.23  -0.08     0.11   0.00  -0.16    -0.06  -0.23  -
0.06
   25   1    -0.08  -0.04  -0.02     0.28   0.09   0.04     0.00   0.07
0.01
   26   1     0.03   0.04   0.05    -0.25  -0.01  -0.24     0.01  -0.13  -
0.01
   27   1    -0.01   0.01  -0.03     0.02  -0.01   0.01    -0.03   0.04
0.11
   28   1     0.03   0.08   0.01    -0.02  -0.03  -0.02     0.02  -0.04
0.01
   29   1    -0.25  -0.47   0.38    -0.11  -0.21   0.17     0.00   0.01
0.00
                     43                     44                     45
                     ?A                     ?A                     ?A
 Frequencies --  1210.6932              1223.8810              1234.6400
 Red. masses --     1.9715                 2.0039                 2.0485
 Frc consts  --     1.7026                 1.7685                 1.8398
 IR Inten    --    50.7414                 7.0211                95.5183
 Raman Activ --     7.4566                 3.3775                 4.7415
 Depolar     --     0.6650                 0.4965                 0.3864
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.03  -0.01   0.00    -0.04  -0.02   0.08    -0.01   0.03
0.02
```

2	6	0.07	0.03	-0.02	0.02	0.11	-0.06	-0.05	-0.03	-0.02
3	6	-0.09	0.06	0.01	-0.02	0.02	0.03	0.07	0.01	0.01
4	6	0.01	-0.03	0.06	0.07	-0.02	-0.02	0.02	-0.04	-0.01
5	6	0.02	-0.03	-0.04	-0.01	0.01	-0.01	-0.01	0.02	0.01
6	6	0.04	-0.02	0.01	0.04	-0.10	-0.05	-0.04	0.01	0.00
7	6	0.00	0.01	0.01	-0.03	0.00	0.09	-0.02	0.00	0.00
8	6	-0.05	0.00	-0.06	0.07	0.05	0.01	-0.06	0.04	-0.06
9	6	0.01	0.14	0.11	-0.02	-0.09	-0.03	-0.03	-0.02	0.16
10	6	-0.03	-0.07	-0.02	0.00	0.00	0.02	0.02	-0.01	-0.08
11	6	0.01	0.01	-0.03	0.02	0.01	-0.09	0.03	-0.01	0.00
12	6	0.03	-0.01	-0.02	-0.03	0.00	0.01	-0.04	-0.05	0.03
13	7	-0.03	0.00	-0.06	0.02	0.00	0.05	0.02	-0.01	0.09
14	8	0.02	-0.04	0.00	-0.02	0.02	0.00	0.04	0.03	0.00
15	8	0.00	-0.01	0.04	0.01	0.02	-0.05	0.02	0.05	-0.10
16	8	0.00	0.04	-0.03	-0.01	-0.01	-0.01	0.00	0.00	-0.02
17	1	-0.13	-0.05	0.08	-0.01	-0.05	-0.20	-0.04	0.00	-0.02
18	1	-0.11	-0.06	-0.14	0.00	-0.32	0.14	0.13	0.11	0.08
19	1	0.45	-0.45	0.11	0.17	-0.16	0.07	-0.37	0.13	0.10
20	1	0.13	0.07	0.12	-0.41	0.31	0.09	-0.08	0.19	0.09
21	1	-0.08	0.04	-0.02	-0.09	0.21	0.16	0.13	-0.08	0.03
22	1	-0.01	0.00	0.08	-0.05	0.05	-0.12	0.25	-0.04	0.09
23	1	0.00	-0.01	-0.05	-0.16	-0.26	0.04	0.09	-0.13	0.03
24	1	0.22	0.16	-0.07	0.00	0.14	0.08	0.21	-0.10	-0.23
25	1	-0.07	-0.04	-0.02	-0.25	-0.03	-0.05	0.00	-0.03	0.01
26	1	0.04	0.06	0.05	0.13	0.01	0.15	0.02	0.15	0.05
27	1	-0.01	0.03	0.15	-0.01	0.00	-0.15	-0.06	0.03	-0.32
28	1	-0.04	-0.29	-0.03	0.04	0.23	0.02	-0.10	-0.49	-0.05

```
  29   1    -0.10  -0.34   0.22    -0.02  -0.10   0.04    -0.07  -0.17
0.12
                     46                     47                     48
                     ?A                     ?A                     ?A
 Frequencies --  1247.2374              1266.9684              1272.5276
 Red. masses --     2.0970                 1.0686                 1.4052
 Frc consts  --     1.9220                 1.0107                 1.3407
 IR Inten    --    35.4007                 8.9788                35.1760
 Raman Activ --     4.9019                12.9823                 1.4381
 Depolar     --     0.3793                 0.7455                 0.5275
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01  -0.03  -0.02     0.00   0.01  -0.02    -0.03   0.00  -
0.04
   2   6     0.03   0.01   0.02     0.02  -0.03  -0.01    -0.02  -0.06
0.02
   3   6    -0.05  -0.01  -0.03     0.00   0.01   0.01    -0.02   0.03  -
0.01
   4   6    -0.01   0.03   0.03    -0.01   0.01  -0.02    -0.01  -0.02
0.00
   5   6     0.00   0.00  -0.01     0.01  -0.01   0.00     0.01  -0.03
0.02
   6   6     0.02   0.00   0.01    -0.02  -0.01   0.02    -0.05   0.05  -
0.02
   7   6     0.02   0.00   0.00    -0.01  -0.01   0.01     0.01  -0.03  -
0.02
   8   6     0.01  -0.04   0.02    -0.02   0.03   0.01    -0.01   0.01
0.01
   9   6     0.04   0.15  -0.07     0.00  -0.01   0.01     0.02   0.02  -
0.04
  10   6    -0.03  -0.01   0.05     0.00  -0.01  -0.01     0.09  -0.02
0.00
  11   6    -0.03   0.01   0.00     0.00   0.00   0.01     0.01   0.02
0.03
  12   6    -0.05  -0.07   0.04     0.00   0.00   0.00    -0.01   0.00
0.00
  13   7     0.02  -0.03   0.15     0.00   0.00   0.00     0.00  -0.01
0.04
  14   8     0.01  -0.04   0.01     0.00   0.00   0.00    -0.02  -0.02
0.00
  15   8     0.00   0.04  -0.10     0.00   0.00   0.00     0.00   0.00  -
0.01
  16   8     0.00  -0.01   0.02     0.00   0.01  -0.01     0.01   0.04  -
0.04
  17   1     0.08   0.02  -0.01     0.19   0.07  -0.34     0.08   0.09
0.15
  18   1    -0.09  -0.08  -0.05     0.00  -0.05  -0.02     0.14   0.32  -
0.03
  19   1     0.26  -0.03  -0.14    -0.03  -0.04   0.05     0.05  -0.20
0.11
  20   1     0.14  -0.16  -0.04    -0.02   0.14   0.04     0.04   0.29
0.16
  21   1    -0.08   0.06   0.00     0.09  -0.16  -0.05     0.09  -0.01
0.03
```

```
  22   1    -0.21   0.04  -0.04    -0.17  -0.07   0.41     0.05  -0.01  -
0.15
  23   1    -0.07   0.09  -0.04     0.03   0.10   0.00     0.06  -0.26
0.11
  24   1    -0.03  -0.09   0.01    -0.01   0.09   0.04    -0.33   0.06
0.28
  25   1     0.01   0.06   0.00    -0.08   0.52   0.02     0.09  -0.08
0.02
  26   1    -0.01  -0.19  -0.04     0.10  -0.50  -0.03    -0.01   0.00  -
0.02
  27   1    -0.17   0.09  -0.72     0.01  -0.01   0.01    -0.04   0.02  -
0.19
  28   1    -0.01  -0.15  -0.01     0.00   0.01   0.00     0.07   0.33
0.04
  29   1     0.06   0.18  -0.12    -0.04  -0.09   0.07    -0.12  -0.31
0.22
                     49                     50                     51
                     ?A                     ?A                     ?A
 Frequencies --  1301.5673              1312.0290              1333.9540
 Red. masses --     1.6715                 2.0446                 1.5069
 Frc consts  --     1.6684                 2.0737                 1.5799
 IR Inten    --    28.6029                 7.2435                10.1697
 Raman Activ --     1.1930                 1.7807                 0.8801
 Depolar     --     0.6870                 0.6950                 0.7044
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.02   0.07   0.01    -0.08  -0.09  -0.06     0.04  -0.01  -
0.01
   2   6     0.06  -0.01   0.00     0.03   0.02   0.05     0.00   0.04
0.05
   3   6    -0.03  -0.02  -0.01    -0.04  -0.02   0.00     0.04  -0.03  -
0.03
   4   6    -0.01  -0.03   0.06     0.01   0.00   0.02    -0.10   0.00
0.00
   5   6    -0.01   0.01  -0.02    -0.01   0.00  -0.03     0.00  -0.02
0.03
   6   6    -0.09  -0.05  -0.01    -0.06  -0.01  -0.06    -0.02   0.02  -
0.07
   7   6    -0.05   0.07   0.02     0.10  -0.06   0.07    -0.02  -0.01
0.01
   8   6     0.02  -0.03  -0.08    -0.01   0.02  -0.04     0.09   0.03  -
0.02
   9   6    -0.01   0.02   0.05    -0.06  -0.05   0.13     0.01   0.00
0.04
  10   6     0.11   0.02  -0.02     0.07   0.04  -0.04    -0.04  -0.06
0.02
  11   6     0.01  -0.05   0.00    -0.01   0.10   0.00     0.00  -0.02
0.00
  12   6     0.00   0.00   0.00    -0.01  -0.01   0.00    -0.01  -0.01
0.01
  13   7     0.00   0.00   0.00     0.01   0.01  -0.02     0.00   0.00
0.00
  14   8    -0.01  -0.01  -0.01     0.00   0.01  -0.01    -0.01  -0.01  -
0.01
```

15	8	0.00	0.00	0.00	0.01	0.01	-0.01	0.00	0.01	-0.01
16	8	0.00	-0.01	0.02	0.01	0.00	0.02	0.01	0.03	-0.02
17	1	-0.30	-0.14	-0.17	0.36	0.20	0.18	-0.01	-0.02	0.13
18	1	-0.26	-0.10	-0.25	-0.10	0.10	-0.11	-0.18	-0.15	-0.02
19	1	0.15	0.11	-0.16	0.12	0.14	-0.15	-0.24	0.13	-0.02
20	1	0.05	-0.09	0.04	0.10	0.12	0.09	0.42	-0.10	0.01
21	1	0.22	-0.01	0.27	0.05	0.13	0.14	0.28	0.02	0.15
22	1	0.42	0.01	0.06	-0.28	0.04	-0.20	-0.05	0.01	-0.07
23	1	0.05	-0.04	-0.07	-0.23	0.12	-0.13	-0.38	-0.24	-0.06
24	1	-0.31	-0.17	0.15	-0.04	-0.35	-0.15	0.31	0.39	0.01
25	1	-0.05	0.22	0.01	0.02	-0.13	0.00	-0.02	0.10	0.00
26	1	0.00	0.04	0.01	0.08	-0.31	0.01	0.00	-0.03	0.00
27	1	-0.01	0.01	0.00	0.05	-0.01	0.18	-0.01	0.00	-0.02
28	1	0.03	0.17	0.02	0.00	0.02	0.01	0.03	0.17	0.02
29	1	0.07	0.16	-0.11	0.06	0.17	-0.10	-0.06	-0.09	0.09

	52	53	54
	?A	?A	?A
Frequencies --	1346.4508	1354.1387	1370.7487
Red. masses --	1.4730	1.5493	1.5747
Frc consts --	1.5733	1.6739	1.7432
IR Inten --	6.5488	7.8033	16.4767
Raman Activ --	2.1826	1.6021	3.2293
Depolar --	0.7383	0.2811	0.1558

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	-0.03	0.02	-0.08	0.01	-0.04	0.00	-0.02	0.01
2	6	0.00	0.08	0.04	0.10	0.02	0.04	0.01	0.05	-0.02
3	6	0.04	-0.02	-0.03	0.01	-0.06	0.00	0.06	0.05	-0.01
4	6	-0.06	-0.01	-0.02	0.06	-0.06	0.01	0.05	0.04	-0.01
5	6	0.00	-0.01	0.02	-0.02	0.00	-0.01	0.04	0.04	-0.03
6	6	0.04	-0.07	0.03	-0.02	0.06	0.02	-0.08	0.04	0.04
7	6	0.03	0.02	0.04	-0.01	-0.03	-0.03	0.07	-0.02	0.00

8	6	-0.09	0.00	-0.02	-0.02	0.01	0.05	-0.03	-0.04	-0.02
9	6	0.01	0.00	-0.01	0.02	0.00	-0.06	0.02	0.04	0.05
10	6	0.03	0.00	-0.07	-0.06	-0.01	0.02	0.05	-0.05	-0.03
11	6	0.00	0.02	-0.03	0.02	0.03	0.01	-0.03	0.02	0.00
12	6	0.00	0.00	0.00	0.01	0.01	-0.01	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00
14	8	0.00	0.00	0.01	0.01	0.00	0.01	-0.02	-0.01	-0.01
15	8	0.00	0.00	0.00	-0.01	-0.01	0.01	0.00	0.00	0.00
16	8	0.01	0.02	-0.01	0.01	0.01	0.00	-0.04	-0.05	0.01
17	1	0.07	-0.01	0.01	-0.03	0.07	0.12	-0.02	-0.04	-0.04
18	1	-0.28	-0.27	-0.04	-0.41	-0.17	-0.34	-0.13	-0.34	0.05
19	1	-0.29	0.12	0.01	-0.05	0.22	-0.15	-0.30	-0.28	0.31
20	1	0.36	0.07	0.07	-0.26	0.39	0.20	-0.24	-0.20	-0.16
21	1	-0.37	0.17	-0.04	0.19	-0.29	-0.15	0.23	-0.30	-0.05
22	1	-0.05	0.04	-0.04	0.07	-0.06	0.02	-0.17	0.03	-0.12
23	1	0.47	-0.01	0.13	0.12	-0.05	0.10	-0.10	0.25	-0.12
24	1	-0.31	0.12	0.17	0.14	0.19	-0.01	-0.12	0.16	0.16
25	1	-0.04	-0.04	-0.03	0.05	-0.15	0.01	0.03	-0.17	-0.01
26	1	0.05	-0.04	0.04	0.00	0.03	-0.01	-0.05	0.04	-0.03
27	1	0.00	0.00	-0.02	-0.01	0.00	-0.04	-0.02	0.01	-0.05
28	1	0.00	-0.04	-0.01	-0.02	-0.09	-0.01	0.04	0.19	0.02
29	1	-0.03	-0.05	0.05	0.04	0.06	-0.04	0.00	-0.03	-0.04

	55	56	57
	?A	?A	?A
Frequencies --	1381.9387	1392.1221	1405.0211
Red. masses --	1.4844	1.3429	1.6144
Frc consts --	1.6702	1.5333	1.8777
IR Inten --	44.8829	1.2708	11.3449
Raman Activ --	2.5799	1.5335	2.7194
Depolar --	0.6697	0.7461	0.6625

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z

1	6	0.00	0.06	0.00	0.00	-0.01	0.00	0.08	0.03	-0.01
2	6	0.02	-0.06	0.07	-0.01	-0.04	0.04	-0.02	0.02	-0.05
3	6	0.03	0.00	0.00	0.02	-0.01	0.03	-0.03	-0.04	0.03
4	6	0.03	-0.02	0.01	0.05	0.02	-0.01	0.00	-0.06	-0.04
5	6	0.01	0.02	-0.03	0.00	-0.01	0.01	-0.04	-0.04	0.04
6	6	0.09	-0.01	0.04	0.00	-0.04	-0.09	-0.03	0.00	0.02
7	6	0.01	-0.03	-0.04	0.02	0.03	0.00	0.09	0.02	-0.02
8	6	0.03	0.02	0.00	-0.04	-0.04	0.00	-0.04	-0.02	0.03
9	6	0.03	0.01	0.09	0.00	0.02	-0.01	0.05	-0.01	0.05
10	6	-0.02	0.00	-0.06	-0.02	-0.05	0.00	0.00	0.00	-0.04
11	6	-0.01	-0.02	0.00	-0.02	0.07	0.00	-0.04	-0.03	0.00
12	6	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.00
13	7	-0.01	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.01
14	8	-0.02	-0.02	-0.02	0.00	0.00	0.00	-0.02	-0.01	-0.01
15	8	0.00	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
16	8	-0.01	-0.02	0.01	0.00	0.00	0.00	0.03	0.04	-0.02
17	1	-0.19	-0.07	-0.14	-0.08	-0.07	-0.11	-0.36	-0.20	0.19
18	1	-0.21	0.28	-0.31	0.01	0.31	-0.11	0.20	-0.13	0.23
19	1	-0.20	0.03	0.06	-0.06	0.13	-0.02	0.21	0.28	-0.25
20	1	-0.15	0.07	0.04	-0.23	-0.10	-0.10	-0.06	0.28	0.12
21	1	-0.46	0.18	-0.19	0.09	0.39	0.38	0.07	-0.03	0.07
22	1	-0.21	-0.04	0.11	0.14	-0.01	0.14	-0.35	0.05	0.08
23	1	-0.38	-0.08	-0.07	0.16	0.25	-0.04	-0.01	0.32	-0.07
24	1	-0.08	0.01	-0.03	0.12	0.42	0.12	0.05	0.03	-0.06
25	1	-0.04	0.00	0.00	0.07	-0.22	-0.01	0.01	0.04	-0.02
26	1	-0.06	0.06	-0.06	0.05	-0.23	0.00	-0.09	0.08	-0.04
27	1	-0.02	0.00	-0.07	-0.01	0.00	-0.03	-0.03	0.00	-0.10

```
  28   1     0.06   0.29   0.04     0.00   0.00  -0.01     0.05   0.25
0.03
  29   1     0.03   0.03  -0.05    -0.01  -0.01   0.00    -0.01  -0.03
0.06
                     58                     59                     60
                     ?A                     ?A                     ?A
 Frequencies --  1410.6109              1423.6718              1433.5232
 Red. masses --     1.6210                 1.4587                 1.4298
 Frc consts  --     1.9004                 1.7419                 1.7312
 IR Inten    --     7.8333                 2.6593                 2.0459
 Raman Activ --     6.9569                 1.1076                 1.2464
 Depolar     --     0.6298                 0.7330                 0.7474
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.08  -0.06   0.00    -0.05  -0.01   0.13     0.03   0.03
0.06
   2   6    -0.01   0.04  -0.04     0.03  -0.04  -0.04     0.00  -0.04
0.02
   3   6     0.00   0.00   0.04    -0.01  -0.01   0.02     0.02   0.04  -
0.05
   4   6    -0.01   0.00  -0.03    -0.03   0.02  -0.01    -0.05  -0.06  -
0.06
   5   6    -0.03  -0.03  -0.02    -0.03  -0.02  -0.01    -0.02  -0.02  -
0.02
   6   6     0.03  -0.03   0.03    -0.04   0.01   0.01     0.00   0.03  -
0.03
   7   6    -0.10   0.03  -0.05     0.08   0.01  -0.06    -0.02   0.00
0.06
   8   6     0.01  -0.06   0.01    -0.02   0.02   0.01     0.02  -0.06
0.04
   9   6     0.06   0.01   0.07     0.01  -0.01   0.00     0.01   0.00  -
0.01
  10   6    -0.01  -0.01  -0.04     0.00   0.00   0.00    -0.02   0.01
0.05
  11   6     0.06   0.00   0.02     0.00  -0.02  -0.02    -0.01   0.02  -
0.03
  12   6     0.02   0.01   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   7    -0.02  -0.01   0.01     0.00   0.00   0.00     0.00   0.00
0.00
  14   8    -0.03  -0.01  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   8     0.02   0.02   0.01     0.01   0.01   0.00     0.01   0.01
0.01
  17   1     0.43   0.26   0.12     0.26   0.05  -0.57    -0.10  -0.11  -
0.28
  18   1     0.09  -0.09   0.13     0.00   0.08  -0.13    -0.05   0.10  -
0.10
  19   1     0.02   0.06   0.00     0.12   0.05  -0.06    -0.12  -0.27
0.19
  20   1     0.11   0.09   0.03     0.28  -0.02   0.00     0.26   0.41
0.19
```

```
  21   1    -0.12   0.00  -0.04     0.17  -0.04   0.12     0.05  -0.02  -
0.04
  22   1     0.44  -0.07   0.20    -0.28   0.00   0.20     0.14   0.06  -
0.30
  23   1    -0.14   0.33  -0.15     0.01  -0.16   0.07     0.01   0.46  -
0.12
  24   1     0.02   0.10  -0.01     0.03   0.04   0.00     0.13  -0.17  -
0.11
  25   1     0.06  -0.04   0.03     0.02  -0.28  -0.02    -0.04  -0.08  -
0.02
  26   1     0.05   0.15   0.06    -0.07   0.40   0.04     0.04  -0.09
0.03
  27   1    -0.05   0.00  -0.16     0.00   0.00  -0.02     0.00   0.00  -
0.02
  28   1     0.06   0.34   0.04     0.00   0.02   0.00     0.00   0.02
0.01
  29   1     0.05   0.12  -0.06     0.03   0.06  -0.03     0.05   0.09  -
0.06
                      61                    62                    63
                      ?A                    ?A                    ?A
 Frequencies --  1436.5842             1455.8176             1477.8937
 Red. masses --     1.4989                1.4812                2.0407
 Frc consts  --     1.8226                1.8497                2.6261
 IR Inten    --     5.3767               13.7526              100.6098
 Raman Activ --     3.4665                1.3776                4.5742
 Depolar     --     0.7407                0.6763                0.1574
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.02  -0.01  -0.02     0.05   0.00   0.05     0.01  -0.01  -
0.03
   2   6     0.00   0.04   0.03     0.00   0.00  -0.04     0.00  -0.01
0.00
   3   6     0.01   0.03  -0.07    -0.02  -0.02   0.01     0.00   0.01
0.01
   4   6    -0.02  -0.03  -0.01    -0.02   0.01   0.01     0.01   0.01
0.07
   5   6     0.02   0.03   0.01     0.00  -0.01   0.03     0.00   0.04  -
0.09
   6   6    -0.02  -0.08  -0.01     0.01   0.04   0.05    -0.01   0.01  -
0.03
   7   6     0.01   0.03  -0.12    -0.06  -0.05  -0.02     0.01   0.00
0.04
   8   6     0.01   0.01   0.03     0.02   0.03  -0.02    -0.12   0.04  -
0.07
   9   6     0.01  -0.01  -0.03     0.02  -0.01   0.03     0.16  -0.07
0.04
  10   6     0.00   0.05   0.06     0.00   0.01  -0.02    -0.08   0.02
0.04
  11   6    -0.01   0.04   0.03    -0.03   0.13  -0.01     0.00   0.00  -
0.01
  12   6     0.00   0.01   0.00     0.00   0.00   0.00     0.05   0.04
0.00
  13   7     0.00   0.00   0.00     0.00   0.00   0.00    -0.04  -0.01
0.00
```

14	8	0.00	0.00	0.00	-0.01	0.00	0.00	-0.04	0.00	-0.01
15	8	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	-0.01	0.01
16	8	-0.01	-0.02	0.00	0.01	0.01	-0.01	-0.01	-0.03	0.03
17	1	-0.10	-0.05	0.19	-0.16	-0.18	-0.21	-0.02	-0.01	0.06
18	1	-0.11	-0.17	0.04	0.08	-0.09	0.06	0.06	0.05	0.03
19	1	-0.11	-0.25	0.14	0.14	0.12	-0.13	-0.02	-0.12	0.10
20	1	0.05	0.15	0.08	0.08	-0.14	-0.06	0.08	-0.09	0.03
21	1	0.05	0.16	0.28	-0.06	-0.21	-0.22	0.09	0.02	0.05
22	1	-0.01	-0.12	0.59	0.24	-0.09	0.01	-0.01	0.03	-0.09
23	1	-0.11	-0.06	0.03	-0.07	-0.18	0.01	0.43	-0.31	0.16
24	1	0.01	-0.37	-0.12	-0.03	-0.05	-0.03	0.35	-0.14	-0.27
25	1	0.14	-0.27	0.00	0.09	-0.51	-0.03	0.00	0.12	0.00
26	1	-0.01	-0.05	-0.03	0.12	-0.51	0.01	0.04	-0.10	0.03
27	1	0.00	0.00	0.00	-0.01	0.00	-0.02	-0.07	-0.02	-0.23
28	1	0.00	0.00	0.01	0.02	0.10	0.01	0.08	0.44	0.06
29	1	-0.01	-0.05	0.02	-0.03	-0.05	0.05	0.07	0.13	-0.12

	64			65			66		
	?A			?A			?A		
Frequencies --	1497.4320			1514.1023			1632.2094		
Red. masses --	2.2394			2.7307			8.2172		
Frc consts --	2.9585			3.6884			12.8981		
IR Inten --	43.7213			113.5306			489.6404		
Raman Activ --	3.6014			13.2523			13.2670		
Depolar --	0.6102			0.4528			0.2147		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.03	0.00	0.02	0.03	0.00	-0.01	0.00	0.00	0.00
2 6	0.04	0.00	0.04	-0.02	0.00	-0.02	0.01	0.01	0.00
3 6	-0.01	0.00	-0.10	0.01	0.00	0.06	0.01	0.02	-0.03
4 6	0.01	0.03	-0.06	-0.01	-0.02	0.04	0.03	0.03	0.01
5 6	0.02	-0.04	0.20	-0.03	0.00	-0.13	-0.11	-0.12	0.04
6 6	0.00	0.00	-0.01	0.00	0.00	0.00	-0.01	-0.01	-0.01

7	6	0.00	0.00	0.03	0.02	-0.01	-0.01	0.00	0.00	-0.01
8	6	0.00	-0.01	-0.01	0.05	0.03	0.01	-0.01	0.00	0.01
9	6	-0.01	-0.04	0.05	-0.16	-0.03	0.01	-0.07	-0.02	-0.06
10	6	-0.01	0.05	0.03	0.04	-0.03	-0.03	0.03	0.03	0.01
11	6	0.02	-0.02	-0.01	-0.02	0.02	0.00	0.03	0.01	0.02
12	6	0.12	0.08	-0.08	0.22	0.12	-0.10	0.28	-0.05	0.59
13	7	-0.04	-0.03	0.03	-0.08	-0.04	0.02	-0.20	-0.01	-0.25
14	8	0.00	0.00	-0.01	0.03	0.02	0.01	0.01	0.01	0.00
15	8	-0.02	-0.03	0.06	-0.04	-0.04	0.08	0.01	0.06	-0.18
16	8	0.00	0.03	-0.06	0.00	-0.01	0.04	0.05	0.06	-0.01
17	1	0.11	0.07	-0.11	-0.09	-0.06	0.07	0.00	0.00	0.01
18	1	-0.21	-0.02	-0.18	0.12	0.01	0.11	-0.03	-0.02	-0.02
19	1	0.02	0.02	-0.13	-0.04	-0.03	0.11	-0.05	-0.12	0.07
20	1	-0.26	-0.28	-0.25	0.16	0.14	0.14	-0.17	-0.09	-0.06
21	1	0.00	0.00	-0.01	0.01	0.00	0.00	0.03	0.00	0.02
22	1	0.03	0.03	-0.10	-0.08	-0.02	0.06	-0.01	0.00	0.02
23	1	0.02	0.14	-0.06	-0.13	-0.11	0.01	-0.01	-0.06	0.04
24	1	0.08	-0.32	-0.18	-0.12	0.19	0.15	-0.01	-0.06	0.01
25	1	-0.07	0.05	0.00	0.03	-0.04	0.00	-0.32	-0.08	0.06
26	1	0.00	0.08	0.00	0.00	-0.09	-0.01	-0.14	-0.03	-0.30
27	1	-0.13	0.04	-0.43	-0.20	0.06	-0.62	-0.19	-0.12	-0.15
28	1	0.00	0.06	0.01	-0.06	-0.30	-0.04	-0.01	0.01	0.02
29	1	-0.14	-0.31	0.22	0.11	0.22	-0.16	0.03	0.05	0.00

	67	68	69
	?A	?A	?A
Frequencies --	1636.6225	1646.9473	3215.8736
Red. masses --	1.1570	3.9709	1.0588
Frc consts --	1.8258	6.3460	6.4518
IR Inten --	61.0420	283.9217	31.4925
Raman Activ --	14.9995	7.2314	139.2899
Depolar --	0.4753	0.0578	0.1920

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.01	0.00	-0.02	-0.01	0.02	0.01	-0.01	0.00
2	6	0.00	0.00	0.00	-0.01	-0.02	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	-0.06	-0.06	0.04	0.00	0.00	0.00
4	6	0.00	0.00	-0.01	-0.07	-0.06	-0.06	0.00	0.00	0.00
5	6	0.02	0.02	0.01	0.27	0.32	0.02	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
7	6	0.00	-0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00
8	6	0.01	0.00	0.00	0.00	-0.03	0.02	0.00	0.00	0.00
9	6	-0.01	0.00	0.00	-0.01	-0.01	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	-0.02	-0.01	0.00	0.00	0.00
11	6	-0.08	-0.02	-0.04	0.04	0.00	0.01	-0.06	-0.01	-0.02
12	6	0.03	0.00	0.05	0.07	0.01	0.08	0.00	0.00	0.00
13	7	-0.02	0.00	-0.02	-0.04	-0.01	-0.04	0.00	0.00	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	-0.01	0.00	0.00	-0.02	0.00	0.00	0.00
16	8	-0.01	-0.01	0.00	-0.12	-0.14	0.00	0.00	0.00	0.00
17	1	-0.01	0.01	-0.01	0.08	0.03	-0.05	-0.06	0.10	-0.02
18	1	-0.02	0.00	-0.02	0.04	0.04	0.02	0.00	0.00	0.00
19	1	0.02	0.02	-0.03	0.26	0.31	-0.27	0.00	0.00	0.00
20	1	-0.01	0.01	0.00	0.28	0.26	0.11	0.00	0.00	0.00
21	1	-0.01	0.00	-0.02	0.01	0.01	0.00	-0.01	-0.01	0.01
22	1	-0.01	-0.01	-0.01	0.05	0.02	-0.03	-0.01	-0.05	-0.01
23	1	-0.03	0.01	-0.01	0.01	0.17	-0.04	0.00	0.00	-0.01
24	1	0.00	0.00	0.00	0.02	0.10	0.03	0.00	0.00	0.00
25	1	0.67	0.16	-0.13	-0.23	-0.07	0.04	0.07	-0.01	0.62
26	1	0.28	0.07	0.64	-0.09	0.04	-0.19	0.66	0.15	-0.36

```
  27   1    -0.02  -0.01  -0.02    -0.05   0.00  -0.07     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.03   0.00     0.00   0.00
0.00
  29   1    -0.02  -0.04   0.02    -0.16  -0.37   0.12     0.00   0.00
0.00
                     70                     71                     72
                     ?A                     ?A                     ?A
 Frequencies --  3263.0912              3275.4162              3299.1238
 Red. masses --     1.1063                 1.0881                 1.0892
 Frc consts  --     6.9405                 6.8776                 6.9846
 IR Inten    --    18.0290                23.7544                12.1435
 Raman Activ --    89.7682               107.5007                67.4142
 Depolar     --     0.7494                 0.3496                 0.7302
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.04  -0.07   0.01     0.01  -0.01
0.00
   2   6     0.00   0.00   0.00    -0.01   0.01   0.01     0.03  -0.02  -
0.04
   3   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.01
0.01
   4   6     0.00   0.00   0.00     0.00   0.00  -0.01     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00     0.00   0.00   0.00    -0.03  -0.04
0.04
   7   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.01
0.00
   8   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00  -
0.01
  11   6    -0.04  -0.01   0.09     0.01   0.00   0.01     0.00   0.00
0.00
  12   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  17   1     0.03  -0.04   0.01    -0.48   0.82  -0.13    -0.09   0.15  -
0.03
  18   1    -0.01   0.00   0.01     0.15  -0.08  -0.15    -0.39   0.21
0.42
  19   1     0.00   0.00   0.00     0.00   0.01   0.01    -0.04  -0.07  -
0.12
```

20	1	0.00	0.00	0.00	0.00	-0.03	0.06	0.00	-0.01	0.02
21	1	0.00	0.00	0.00	-0.01	-0.02	0.02	0.34	0.44	-0.47
22	1	0.00	0.01	0.00	0.01	0.05	0.01	-0.01	-0.14	-0.03
23	1	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.01
24	1	0.00	0.00	0.00	0.00	0.00	0.00	0.03	-0.03	0.06
25	1	-0.11	0.00	-0.76	-0.01	0.00	-0.10	0.00	0.00	-0.02
26	1	0.55	0.12	-0.28	-0.05	-0.01	0.03	-0.01	0.00	0.01
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

		73			74			75		
		?A			?A			?A		
Frequencies --		3310.2970			3323.5914			3327.1647		
Red. masses --		1.0892			1.0891			1.0900		
Frc consts --		7.0323			7.0885			7.1090		
IR Inten --		25.9264			12.8686			10.4356		
Raman Activ --		121.0822			73.4652			178.5886		
Depolar --		0.4323			0.3191			0.1279		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.00
2	6	0.04	-0.02	-0.04	0.02	-0.01	-0.02	-0.01	0.01	0.01
3	6	0.01	0.01	0.03	-0.02	-0.04	-0.06	0.01	0.01	0.02
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.02	0.03	-0.03	0.00	0.00	0.00	-0.01	-0.02	0.02
7	6	0.00	-0.02	0.00	0.00	-0.03	-0.01	-0.01	-0.07	-0.02
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	-0.01
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

13	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	1	-0.06	0.11	-0.02	-0.02	0.03	-0.01	0.04	-0.06	0.01
18	1	-0.42	0.23	0.45	-0.19	0.10	0.20	0.14	-0.08	-0.15
19	1	-0.10	-0.17	-0.29	0.27	0.42	0.73	-0.07	-0.11	-0.19
20	1	0.00	-0.01	0.02	-0.01	-0.02	0.04	0.00	0.00	0.00
21	1	-0.27	-0.35	0.37	0.00	-0.01	0.00	0.15	0.19	-0.21
22	1	0.03	0.29	0.06	0.03	0.31	0.06	0.09	0.83	0.17
23	1	0.01	-0.01	-0.03	0.01	-0.02	-0.06	0.05	-0.06	-0.21
24	1	-0.02	0.02	-0.03	-0.06	0.04	-0.09	0.04	-0.03	0.07
25	1	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.04
26	1	-0.01	0.00	0.01	0.01	0.00	0.00	0.04	0.01	-0.02
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	1	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00

	76			77			78		
	?A			?A			?A		
Frequencies --	3343.9236			3355.5483			3367.5138		
Red. masses --	1.0888			1.0890			1.0903		
Frc consts --	7.1729			7.2243			7.2846		
IR Inten --	2.6123			0.6543			1.4181		
Raman Activ --	36.6432			133.9596			127.4456		
Depolar --	0.7257			0.1147			0.1229		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	-0.01
4 6	0.01	0.02	-0.05	0.01	0.03	-0.05	0.00	0.00	0.01
5 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
   6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.01  -
0.01
   7   6     0.00   0.01   0.00     0.00  -0.01   0.00     0.00   0.00
0.00
   8   6    -0.01   0.02   0.06     0.01  -0.02  -0.05     0.00   0.00
0.01
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00    -0.01   0.00  -0.01    -0.04   0.03  -
0.07
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  17   1     0.02  -0.04   0.00     0.03  -0.05   0.01    -0.01   0.01
0.00
  18   1     0.00   0.00   0.00     0.02  -0.01  -0.02    -0.03   0.01
0.03
  19   1    -0.01  -0.01  -0.02     0.00   0.00  -0.01     0.04   0.06
0.10
  20   1    -0.07  -0.30   0.63    -0.07  -0.30   0.63     0.01   0.03  -
0.06
  21   1    -0.01  -0.02   0.02     0.01   0.01  -0.01    -0.06  -0.07
0.07
  22   1    -0.02  -0.17  -0.03     0.02   0.13   0.03     0.00  -0.04  -
0.01
  23   1     0.16  -0.19  -0.64    -0.16   0.19   0.63     0.02  -0.03  -
0.09
  24   1    -0.01   0.01  -0.02     0.06  -0.05   0.11     0.46  -0.34
0.79
  25   1     0.00   0.00  -0.01     0.00   0.00   0.02     0.00   0.00
0.00
  26   1     0.00   0.00   0.00     0.01   0.00   0.00     0.00   0.00
0.00
  27   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  29   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                      79                     80                     81
                      ?A                     ?A                     ?A
 Frequencies --   3609.1732              3775.7696              3847.4891
 Red. masses --      1.0729                 1.0670                 1.0669
 Frc consts  --      8.2342                 8.9622                 9.3051
 IR Inten    --      6.3270               281.9547                91.5877
```

Raman Activ --		211.7675			92.3217			87.1302		
Depolar --		0.3376			0.2712			0.2336		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
13	7	-0.06	-0.03	0.01	0.00	0.00	0.00	0.00	0.00	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	-0.06	0.02	-0.02
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.04	0.02	0.04	0.00	0.00	0.00
17	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
18	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
22	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
23	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
25	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  27   1     0.91   0.39  -0.14     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.01   0.00   0.00     0.88  -0.28
0.37
  29   1     0.00   0.00   0.00    -0.63  -0.30  -0.71     0.01   0.00
0.01

 -------------------
 - Thermochemistry -
 -------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Atom  1 has atomic number  6 and mass  12.00000
 Atom  2 has atomic number  6 and mass  12.00000
 Atom  3 has atomic number  6 and mass  12.00000
 Atom  4 has atomic number  6 and mass  12.00000
 Atom  5 has atomic number  6 and mass  12.00000
 Atom  6 has atomic number  6 and mass  12.00000
 Atom  7 has atomic number  6 and mass  12.00000
 Atom  8 has atomic number  6 and mass  12.00000
 Atom  9 has atomic number  6 and mass  12.00000
 Atom 10 has atomic number  6 and mass  12.00000
 Atom 11 has atomic number  6 and mass  12.00000
 Atom 12 has atomic number  6 and mass  12.00000
 Atom 13 has atomic number  7 and mass  14.00307
 Atom 14 has atomic number  8 and mass  15.99491
 Atom 15 has atomic number  8 and mass  15.99491
 Atom 16 has atomic number  8 and mass  15.99491
 Atom 17 has atomic number  1 and mass   1.00783
 Atom 18 has atomic number  1 and mass   1.00783
 Atom 19 has atomic number  1 and mass   1.00783
 Atom 20 has atomic number  1 and mass   1.00783
 Atom 21 has atomic number  1 and mass   1.00783
 Atom 22 has atomic number  1 and mass   1.00783
 Atom 23 has atomic number  1 and mass   1.00783
 Atom 24 has atomic number  1 and mass   1.00783
 Atom 25 has atomic number  1 and mass   1.00783
 Atom 26 has atomic number  1 and mass   1.00783
 Atom 27 has atomic number  1 and mass   1.00783
 Atom 28 has atomic number  1 and mass   1.00783
 Atom 29 has atomic number  1 and mass   1.00783
 Molecular mass:   219.08954 amu.
 Principal axes and moments of inertia in atomic units:
                           1         2         3
     EIGENVALUES --  1908.97467 2746.56694 3352.76535
           X            0.99978   0.00784   0.01954
           Y           -0.00804   0.99992   0.01003
           Z           -0.01946  -0.01019   0.99976
 THIS MOLECULE IS AN ASYMMETRIC TOP.
 ROTATIONAL SYMMETRY NUMBER  1.
 WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
           MAY CAUSE SIGNIFICANT ERROR
 ROTATIONAL TEMPERATURES (KELVIN)      0.04537     0.03154     0.02583
```

ROTATIONAL CONSTANTS (GHZ) 0.94540 0.65709 0.53828

1 IMAGINARY FREQUENCIES IGNORED.

Zero-point vibrational energy 662428.5 (Joules/Mol)

158.32421 (Kcal/Mol)

WARNING-- EXPLICIT CONSIDERATION OF 14 DEGREES OF FREEDOM AS VIBRATIONS MAY CAUSE SIGNIFICANT ERROR

VIBRATIONAL TEMPERATURES: (KELVIN)					
	184.42	210.24	239.96	385.67	439.37
	473.80	536.29	555.12	596.25	648.99
	688.40	753.42	782.18	860.28	910.79
	970.55	996.53	1024.93	1143.13	1175.21
	1186.16	1192.83	1222.91	1255.70	1272.55
	1304.33	1313.22	1351.04	1395.12	1418.78
	1437.59	1456.31	1457.66	1484.75	1497.92
	1511.90	1537.25	1586.40	1624.27	1674.58
	1717.11	1741.91	1760.88	1776.36	1794.49
	1822.87	1830.87	1872.65	1887.71	1919.25
	1937.23	1948.29	1972.19	1988.29	2002.94
	2021.50	2029.54	2048.33	2062.51	2066.91
	2094.58	2126.35	2154.46	2178.44	2348.37
	2354.72	2369.58	4626.90	4694.83	4712.57
	4746.68	4762.75	4781.88	4787.02	4811.13
	4827.86	4845.07	5192.77	5432.46	5535.65

Zero-point correction=	0.252306
(Hartree/Particle)	
Thermal correction to Energy=	0.262100
Thermal correction to Enthalpy=	0.263044
Thermal correction to Gibbs Free Energy=	0.217263
Sum of electronic and zero-point Energies=	-736.635022
Sum of electronic and thermal Energies=	-736.625227
Sum of electronic and thermal Enthalpies=	-736.624283
Sum of electronic and thermal Free Energies=	-736.670064

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	164.470	43.466	96.354
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	42.056
ROTATIONAL	0.889	2.981	31.242
VIBRATIONAL	162.693	37.505	23.056
VIBRATION 1	0.611	1.925	2.973
VIBRATION 2	0.617	1.907	2.722
VIBRATION 3	0.624	1.883	2.471
VIBRATION 4	0.673	1.732	1.609
VIBRATION 5	0.696	1.664	1.387
VIBRATION 6	0.712	1.617	1.263
VIBRATION 7	0.744	1.528	1.068
VIBRATION 8	0.755	1.500	1.016
VIBRATION 9	0.778	1.439	0.911
VIBRATION 10	0.810	1.359	0.793
VIBRATION 11	0.835	1.298	0.714
VIBRATION 12	0.879	1.198	0.602
VIBRATION 13	0.899	1.154	0.558
VIBRATION 14	0.956	1.036	0.453

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.116573D-99	-99.933400	-230.105158
TOTAL V=0	0.131333D+17	16.118374	37.113927
VIB (BOT)	0.609341-114	-114.215139	-262.990077
VIB (BOT) 1	0.159116D+01	0.201714	0.464464
VIB (BOT) 2	0.138916D+01	0.142751	0.328696
VIB (BOT) 3	0.120957D+01	0.082631	0.190266
VIB (BOT) 4	0.721689D+00	-0.141650	-0.326160
VIB (BOT) 5	0.620866D+00	-0.207002	-0.476639
VIB (BOT) 6	0.567632D+00	-0.245933	-0.566282
VIB (BOT) 7	0.487516D+00	-0.312011	-0.718431
VIB (BOT) 8	0.466695D+00	-0.330967	-0.762079
VIB (BOT) 9	0.425505D+00	-0.371095	-0.854479
VIB (BOT) 10	0.379844D+00	-0.420395	-0.967994
VIB (BOT) 11	0.350010D+00	-0.455919	-1.049793
VIB (BOT) 12	0.307210D+00	-0.512565	-1.180223
VIB (BOT) 13	0.290428D+00	-0.536962	-1.236401
VIB (BOT) 14	0.250265D+00	-0.601600	-1.385236
VIB (V=0)	0.686491D+02	1.836635	4.229008
VIB (V=0) 1	0.216787D+01	0.336033	0.773746
VIB (V=0) 2	0.197640D+01	0.295875	0.681276
VIB (V=0) 3	0.180884D+01	0.257400	0.592686
VIB (V=0) 4	0.137797D+01	0.139241	0.320613
VIB (V=0) 5	0.129717D+01	0.112996	0.260183
VIB (V=0) 6	0.125644D+01	0.099143	0.228285
VIB (V=0) 7	0.119834D+01	0.078578	0.180933
VIB (V=0) 8	0.118396D+01	0.073338	0.168867
VIB (V=0) 9	0.115655D+01	0.063163	0.145439
VIB (V=0) 10	0.112792D+01	0.052278	0.120374
VIB (V=0) 11	0.111033D+01	0.045453	0.104661
VIB (V=0) 12	0.108684D+01	0.036165	0.083272
VIB (V=0) 13	0.107823D+01	0.032711	0.075319
VIB (V=0) 14	0.105914D+01	0.024951	0.057453
ELECTRONIC	0.100000D+01	0.000000	0.000000
TRANSLATIONAL	0.127466D+09	8.105393	18.663357
ROTATIONAL	0.150088D+07	6.176346	14.221563

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000009471	0.000008321	0.000015465
2	6	-0.000011674	0.000005709	0.000001508
3	6	0.000022131	-0.000011140	0.000006046
4	6	0.000005461	-0.000037577	-0.000022720
5	6	-0.000008678	0.000008473	0.000008108
6	6	0.000005855	-0.000005457	-0.000001938
7	6	0.000000331	-0.000016704	0.000000079
8	6	-0.000010797	0.000038846	-0.000003615
9	6	-0.000000931	-0.000021993	-0.000005983
10	6	-0.000010031	0.000018064	0.000008789
11	6	0.000007632	0.000001242	-0.000009467
12	6	0.000003851	-0.000010978	0.000025912
13	7	-0.000002124	0.000000705	-0.000006019

14	8	0.000002812	0.000010802	-0.000000084
15	8	-0.000003570	0.000007708	-0.000020172
16	8	0.000011246	-0.000001204	-0.000003460
17	1	0.000000638	0.000000185	0.000000158
18	1	0.000002702	0.000000305	0.000000717
19	1	-0.000001471	0.000004845	0.000000667
20	1	-0.000004108	0.000006459	0.000002084
21	1	-0.000000848	-0.000000356	0.000000096
22	1	0.000000299	-0.000000086	-0.000000904
23	1	0.000000468	-0.000004226	-0.000000919
24	1	0.000000079	-0.000001900	-0.000000134
25	1	-0.000000064	-0.000001924	-0.000000873
26	1	0.000001966	0.000000597	0.000000719
27	1	0.000004086	0.000001893	0.000002761
28	1	-0.000002597	-0.000002749	0.000001695
29	1	-0.000003194	0.000002141	0.000001482

Cartesian Forces: Max 0.000038846 RMS 0.000009788

Internal Coordinate Forces (Hartree/Bohr or radian)

Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	C		-0.000009(1)		0.000008(30)		0.000015(59)	
2	C		-0.000012(2)		0.000006(31)		0.000002(60)	
3	C		0.000022(3)		-0.000011(32)		0.000006(61)	
4	C		0.000005(4)		-0.000038(33)		-0.000023(62)	
5	C		-0.000009(5)		0.000008(34)		0.000008(63)	
6	C		0.000006(6)		-0.000005(35)		-0.000002(64)	
7	C		0.000000(7)		-0.000017(36)		0.000000(65)	
8	C		-0.000011(8)		0.000039(37)		-0.000004(66)	
9	C		-0.000001(9)		-0.000022(38)		-0.000006(67)	
10	C		-0.000010(10)		0.000018(39)		0.000009(68)	
11	C		0.000008(11)		0.000001(40)		-0.000009(69)	
12	C		0.000004(12)		-0.000011(41)		0.000026(70)	
13	N		-0.000002(13)		0.000001(42)		-0.000006(71)	
14	O		0.000003(14)		0.000011(43)		0.000000(72)	
15	O		-0.000004(15)		0.000008(44)		-0.000020(73)	
16	O		0.000011(16)		-0.000001(45)		-0.000003(74)	
17	H		0.000001(17)		0.000000(46)		0.000000(75)	
18	H		0.000003(18)		0.000000(47)		0.000001(76)	
19	H		-0.000001(19)		0.000005(48)		0.000001(77)	
20	H		-0.000004(20)		0.000006(49)		0.000002(78)	
21	H		-0.000001(21)		0.000000(50)		0.000000(79)	
22	H		0.000000(22)		0.000000(51)		-0.000001(80)	
23	H		0.000000(23)		-0.000004(52)		-0.000001(81)	
24	H		0.000000(24)		-0.000002(53)		0.000000(82)	
25	H		0.000000(25)		-0.000002(54)		-0.000001(83)	
26	H		0.000002(26)		0.000001(55)		0.000001(84)	
27	H		0.000004(27)		0.000002(56)		0.000003(85)	
28	H		-0.000003(28)		-0.000003(57)		0.000002(86)	
29	H		-0.000003(29)		0.000002(58)		0.000001(87)	

Internal Forces: Max 0.000038846 RMS 0.000009788

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GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   1 out of a maximum of  97
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
    Eigenvalues ---   -0.00326   0.00306   0.00491   0.00659   0.00685
    Eigenvalues ---    0.01155   0.01357   0.01769   0.02460   0.02598
    Eigenvalues ---    0.03373   0.04117   0.04273   0.04564   0.04642
    Eigenvalues ---    0.04704   0.04905   0.04983   0.05018   0.05132
    Eigenvalues ---    0.05186   0.05358   0.05500   0.05778   0.05866
    Eigenvalues ---    0.05942   0.06079   0.06902   0.06947   0.07848
    Eigenvalues ---    0.08364   0.10079   0.10609   0.11123   0.13710
    Eigenvalues ---    0.14865   0.15958   0.16997   0.18758   0.19107
    Eigenvalues ---    0.20107   0.21132   0.25015   0.26483   0.28550
    Eigenvalues ---    0.31666   0.33418   0.34518   0.37634   0.39098
    Eigenvalues ---    0.40273   0.43299   0.43565   0.48920   0.50580
    Eigenvalues ---    0.50626   0.53155   0.55880   0.57502   0.58163
    Eigenvalues ---    0.63429   0.66389   0.69040   0.71827   0.73687
    Eigenvalues ---    0.84205   0.88047   0.90148   0.95162   0.96469
    Eigenvalues ---    0.97581   0.99811   1.02884   1.03393   1.06091
    Eigenvalues ---    1.07120   1.09078   1.12354   1.13660   1.36808
    Eigenvalues ---    1.39965
Eigenvalue   1 out of range, new value =    0.003263 Eigenvector:
                          1
          X1          -0.01168
          Y1           0.00444
          Z1           0.03878
          X2          -0.02275
          Y2          -0.02956
          Z2           0.03298
          X3          -0.04023
          Y3          -0.01274
          Z3           0.05748
          X4          -0.00648
          Y4           0.03538
          Z4           0.04977
          X5           0.01127
          Y5          -0.02136
          Z5           0.06981
          X6          -0.00774
          Y6          -0.02292
          Z6          -0.00893
          X7          -0.00600
          Y7           0.01180
          Z7          -0.01614
          X8          -0.00944
          Y8           0.03153
          Z8           0.00113
          X9          -0.00661
          Y9           0.03322
          Z9          -0.00681
          X10         -0.00729
          Y10         -0.00734
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Z10	0.00283
X11	-0.00641
Y11	0.01440
Z11	0.00094
X12	-0.01023
Y12	0.02196
Z12	-0.06485
X13	-0.19287
Y13	0.48967
Z13	0.10291
X14	-0.02316
Y14	0.02745
Z14	-0.03424
X15	0.17637
Y15	-0.46560
Z15	-0.26758
X16	0.16649
Y16	-0.13678
Z16	0.02150
X17	-0.01479
Y17	0.00318
Z17	0.05683
X18	-0.04132
Y18	-0.06092
Z18	0.03257
X19	-0.03419
Y19	-0.03823
Z19	0.06820
X20	0.00109
Y20	0.06208
Z20	0.06232
X21	0.00036
Y21	-0.04603
Z21	-0.02619
X22	-0.00198
Y22	0.01739
Z22	-0.04285
X23	0.00315
Y23	0.05918
Z23	-0.00423
X24	-0.00706
Y24	-0.01437
Z24	-0.00202
X25	-0.00190
Y25	0.03673
Z25	0.00027
X26	-0.00824
Y26	-0.00217
Z26	-0.00817
X27	-0.15849
Y27	0.39833
Z27	0.06567
X28	-0.02357
Y28	-0.01553

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          Z28         -0.09063
          X29          0.19575
          Y29         -0.21308
          Z29          0.02428
Angle between quadratic step and forces=  71.32 degrees.
Linear search not attempted -- first point.
TrRot=  0.000002 -0.000003 -0.000010 -0.000001  0.000002 -0.000001
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   X1       -4.01125  -0.00001   0.00000   0.00000   0.00000  -4.01124
   Y1        1.70345   0.00001   0.00000   0.00000   0.00000   1.70346
   Z1       -0.00063   0.00002   0.00000   0.00004   0.00004  -0.00059
   X2       -2.92801  -0.00001   0.00000   0.00001   0.00002  -2.92799
   Y2        0.97681   0.00001   0.00000   0.00001   0.00001   0.97682
   Z2        2.65211   0.00000   0.00000   0.00002   0.00002   2.65213
   X3       -0.00211   0.00002   0.00000   0.00008   0.00009  -0.00202
   Y3        1.65705  -0.00001   0.00000  -0.00001  -0.00001   1.65704
   Z3        2.64289   0.00001   0.00000   0.00001   0.00000   2.64290
   X4       -1.54529   0.00001   0.00000   0.00002   0.00002  -1.54527
   Y4        1.76082  -0.00004   0.00000  -0.00008  -0.00008   1.76074
   Z4       -1.63266  -0.00002   0.00000  -0.00005  -0.00005  -1.63271
   X5        0.25577  -0.00001   0.00000   0.00000   0.00001   0.25578
   Y5        2.90860   0.00001   0.00000   0.00001   0.00000   2.90861
   Z5        0.16379   0.00001   0.00000  -0.00001  -0.00002   0.16377
   X6       -2.27838   0.00001   0.00000   0.00004   0.00004  -2.27833
   Y6       -1.89887  -0.00001   0.00000  -0.00001  -0.00001  -1.89889
   Z6        2.36312   0.00000   0.00000  -0.00001  -0.00002   2.36310
   X7       -3.04537   0.00000   0.00000   0.00004   0.00004  -3.04533
   Y7       -2.46637  -0.00002   0.00000  -0.00002  -0.00002  -2.46639
   Z7       -0.41565   0.00000   0.00000  -0.00003  -0.00003  -0.41568
   X8       -0.86645  -0.00001   0.00000   0.00000  -0.00001  -0.86645
   Y8       -1.18224   0.00004   0.00000   0.00008   0.00008  -1.18216
   Z8       -1.88492   0.00000   0.00000  -0.00004  -0.00005  -1.88497
   X9        1.48262   0.00000   0.00000   0.00000   0.00000   1.48262
   Y9       -1.81146  -0.00002   0.00000  -0.00003  -0.00003  -1.81150
   Z9       -0.33931  -0.00001   0.00000  -0.00002  -0.00003  -0.33934
  X10        0.60467  -0.00001   0.00000   0.00000   0.00001   0.60468
  Y10       -1.26289   0.00002   0.00000   0.00004   0.00003  -1.26286
  Z10        2.34535   0.00001   0.00000   0.00001   0.00000   2.34535
  X11       -5.33196   0.00001   0.00000   0.00004   0.00004  -5.33191
  Y11       -0.73530   0.00000   0.00000  -0.00001  -0.00001  -0.73531
  Z11       -0.85505  -0.00001   0.00000  -0.00003  -0.00002  -0.85507
  X12        3.87195   0.00000   0.00000   0.00002   0.00002   3.87198
  Y12       -0.35866  -0.00001   0.00000  -0.00005  -0.00006  -0.35871
  Z12       -1.12680   0.00003   0.00000   0.00001  -0.00001  -1.12681
  X13        5.57198   0.00000   0.00000   0.00003   0.00003   5.57201
  Y13       -0.27066   0.00000   0.00000  -0.00003  -0.00004  -0.27070
  Z13        0.65024  -0.00001   0.00000  -0.00002  -0.00004   0.65020
  X14        1.84585   0.00000   0.00000  -0.00011  -0.00011   1.84574
  Y14       -4.51708   0.00001   0.00000   0.00001   0.00000  -4.51708
  Z14       -0.57402   0.00000   0.00000  -0.00002  -0.00004  -0.57406
  X15        3.85159   0.00000   0.00000  -0.00003  -0.00004   3.85155
  Y15        0.61579   0.00001   0.00000   0.00000  -0.00001   0.61578
  Z15       -3.33658  -0.00002   0.00000  -0.00002  -0.00004  -3.33662
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X16	1.54701	0.00001	0.00000	-0.00004	-0.00003	1.54697
Y16	4.90162	0.00000	0.00000	0.00004	0.00003	4.90165
Z16	-0.35213	0.00000	0.00000	-0.00001	-0.00002	-0.35215
X17	-5.09974	0.00000	0.00000	0.00002	0.00003	-5.09971
Y17	3.43028	0.00000	0.00000	0.00001	0.00002	3.43029
Z17	-0.05443	0.00000	0.00000	0.00001	0.00001	-0.05442
X18	-4.01274	0.00000	0.00000	0.00007	0.00009	-4.01266
Y18	1.60379	0.00000	0.00000	0.00000	0.00000	1.60379
Z18	4.25786	0.00000	0.00000	0.00007	0.00007	4.25792
X19	0.84791	0.00000	0.00000	0.00004	0.00006	0.84797
Y19	2.61611	0.00000	0.00000	0.00007	0.00007	2.61618
Z19	4.22322	0.00000	0.00000	-0.00001	-0.00002	4.22320
X20	-1.63242	0.00000	0.00000	-0.00010	-0.00010	-1.63252
Y20	2.71328	0.00001	0.00000	0.00007	0.00007	2.71335
Z20	-3.42572	0.00000	0.00000	0.00003	0.00003	-3.42569
X21	-2.99071	0.00000	0.00000	0.00003	0.00004	-2.99067
Y21	-3.19535	0.00000	0.00000	-0.00002	-0.00002	-3.19536
Z21	3.76276	0.00000	0.00000	-0.00002	-0.00002	3.76273
X22	-3.26360	0.00000	0.00000	0.00007	0.00006	-3.26353
Y22	-4.44048	0.00000	0.00000	-0.00001	-0.00001	-4.44049
Z22	-0.86125	0.00000	0.00000	-0.00006	-0.00006	-0.86131
X23	-0.66805	0.00000	0.00000	0.00002	0.00001	-0.66804
Y23	-1.69367	0.00000	0.00000	-0.00003	-0.00004	-1.69371
Z23	-3.84237	0.00000	0.00000	-0.00001	-0.00002	-3.84239
X24	1.83335	0.00000	0.00000	0.00000	0.00001	1.83336
Y24	-1.99514	0.00000	0.00000	-0.00002	-0.00002	-1.99516
Z24	3.78457	0.00000	0.00000	-0.00001	-0.00003	3.78455
X25	-5.93186	0.00000	0.00000	0.00006	0.00006	-5.93180
Y25	-0.67454	0.00000	0.00000	-0.00001	0.00000	-0.67454
Z25	-2.81222	0.00000	0.00000	-0.00003	-0.00003	-2.81225
X26	-6.93636	0.00000	0.00000	0.00004	0.00004	-6.93632
Y26	-1.19863	0.00000	0.00000	-0.00004	-0.00003	-1.19866
Z26	0.33286	0.00000	0.00000	-0.00004	-0.00004	0.33282
X27	7.19899	0.00000	0.00000	0.00003	0.00003	7.19902
Y27	0.55181	0.00000	0.00000	0.00003	0.00002	0.55183
Z27	0.06497	0.00000	0.00000	0.00005	0.00002	0.06500
X28	3.56954	0.00000	0.00000	-0.00023	-0.00024	3.56930
Y28	-4.97384	0.00000	0.00000	-0.00016	-0.00017	-4.97401
Z28	-0.15760	0.00000	0.00000	0.00030	0.00028	-0.15733
X29	2.88905	0.00000	0.00000	-0.00023	-0.00022	2.88883
Y29	5.40284	0.00000	0.00000	0.00022	0.00022	5.40306
Z29	0.80406	0.00000	0.00000	0.00013	0.00012	0.80417

Item	Value	Threshold	Converged?
Maximum Force	0.000039	0.000450	YES
RMS Force	0.000010	0.000300	YES
Maximum Displacement	0.000279	0.001800	YES
RMS Displacement	0.000068	0.001200	YES

Predicted change in Energy=-9.301512D-09
Optimization completed.
   -- Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1\1\GINC-PELICAN\Freq\RHF\3-21+G*\C12H13N1O3\SINGH\11-Oct-2001\0\\#N R
HF/3-21+G* FREQ\\Freq calc of output str of TS1\\0,1\C,-2.1226605153,0

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\C,-0.4585043547,-0.6256158832,-0.997458014\C,0.7845689462,-0.95858571
24,-0.1795543497\C,0.3199775361,-0.6682952085,1.2411066527\C,-2.821550
2953,-0.3891052777,-0.4524721155\C,2.0489501932,-0.1897927609,-0.59627
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374787,-0.3037581556\O,2.0381712766,0.3258616691,-1.765644536\O,0.8186
399006,2.5938236117,-0.186337319\H,-2.6986685616,1.8152237141,-0.02880
3898\H,-2.1234524161,0.8486891898,2.2531618499\H,0.4486934439,1.384387
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SIGN SEEN IN A RESTAURANT-
WE RESERVE THE RIGHT TO SERVE REFUSE TO ANYONE.
Job cpu time: 0 days 3 hours 27 minutes 1.5 seconds.
File lengths (MBytes): RWF= 322 Int=   0 D2E=   0 Chk=   7 Scr=
1
Normal termination of Gaussian 98.

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%chk=mech1s13ts1
%nosave
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TS1

0  1
 C
 C                  1             B1
 C                  2             B2    1             A1
 C                  1             B3    2             A2    3
D1
 C                  3             B4    2             A3    1
D2
 C                  2             B5    1             A4    4
D3
 C                  6             B6    2             A5    1
D4
 C                  4             B7    1             A6    2
D5
 C                  8             B8    4             A7    1
D6
 C                  6             B9    2             A8    1
D7
 C                  7            B10    6             A9    2
D8
 C                  9            B11    8            A10    4
D9
 N                 12            B12    9            A11    8
D10
 O                  9            B13    8            A12    4
D11
 O                 12            B14    9            A13    8
D12
 O                  5            B15    3            A14    2
D13
 H                  1            B16    2            A15    6
D14
 H                  2            B17    1            A16    4
D15
 H                  3            B18    2            A17    1
D16
 H                  4            B19    1            A18    2
D17
 H                  6            B20    2            A19    1
D18
 H                  7            B21    6            A20    2
D19
 H                  8            B22    4            A21    1
D20
 H                 10            B23    6            A22    2
D21
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 H                11            B24    7             A23    6
D22
 H                11            B25    7             A24    6
D23
 H                13            B26   12             A25    9
D24
 H                14            B27    9             A26    8
D25
 H                16            B28    5             A27    3
D26
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B26	1.000001
B27	0.960000
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A1	109.288535
A2	102.169527
A3	100.119653
A4	109.231843
A5	96.449998
A6	96.210351
A7	109.398909
A8	92.656791
A9	108.626865
A10	114.219590
A11	119.999956
A12	110.163988
A13	120.000012
A14	128.325451
A15	114.846957

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  A16          102.301859
  A17          115.817974
  A18          125.745245
  A19          114.637186
  A20          111.448833
  A21          108.896869
  A22          122.369430
  A23          115.064287
  A24          114.809742
  A25          119.999911
  A26          109.471273
  A27          120.000022
  D1            20.142732
  D2            12.568187
  D3           -75.017787
  D4            -5.394427
  D5            77.086014
  D6          -119.288580
  D7            97.118548
  D8           -32.329353
  D9           -56.966678
  D10          151.629711
  D11         -178.566253
  D12          -28.370220
  D13          140.621661
  D14          166.653104
  D15          155.279442
  D16          145.455313
  D17         -164.505656
  D18         -140.954818
  D19         -164.430856
  D20          110.525526
  D21          132.304222
  D22          172.734799
  D23          -63.153711
  D24         -179.999974
  D25         -174.788573
  D26            0.453233

1  2 1.0  4 1.0  11 1.0  17 1.0
2  3 1.0  6 1.0  18 1.0
3  5 1.0  10 1.0  19 1.0
4  5 1.0  8 1.0  20 1.0
5  16 2.0
6  7 1.0  10 1.0  21 1.0
7  8 1.0  11 1.0  22 1.0
8  9 1.0  23 1.0
9  10 1.0  12 1.0  14 1.0
10  24 1.0
11  25 1.0  26 1.0
12  13 2.0  15 2.0
13  27 1.0
14  28 1.0
15
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16 29 1.0
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1 2 1.0 4 1.0 11 1.0 17 1.0
2 3 1.0 6 1.0 18 1.0
3 5 1.0 10 1.0 19 1.0
4 5 1.0 8 1.0 20 1.0
5 16 2.0
6 7 1.0 10 1.0 21 1.0
7 8 1.0 11 1.0 22 1.0
8 9 1.0 23 1.0
9 10 1.0 12 1.0 14 1.0
10 24 1.0
11 25 1.0 26 1.0
12 13 2.0 15 2.0
13 27 1.0
14 28 1.0
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16 29 1.0
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```
%mem=6MW
%nproc=1
%chk=512TS2end.chk
# opt=(gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity optcyc=200

Std input@99.9899degrees-optcyc=200-ts search

0  1
 C                  0.000000    0.000000    0.000000
 C                  0.000000    0.000000    1.564288
 C                  1.517176    0.000000    2.038813
 C                  1.436901   -0.540756   -0.304299
 C                  2.221280    0.135172    0.748771
 C                 -0.123182   -1.520040    1.927083
 C                 -0.167765   -2.206064    0.532599
 C                  1.311016   -2.090112    0.090348
 C                  2.100329   -2.382905    1.361722
 C                  1.367335   -1.538209    2.394985
 C                 -0.910179   -1.187929   -0.344634
 C                  3.605626   -2.087014    1.262129
 N                  4.168186   -1.916914    2.424194
 O                  1.859813   -3.778526    1.672588
 O                  4.089931   -2.007519    0.082061
 O                  3.249267    0.864915    0.494906
 H                 -0.226663    0.950517   -0.461254
 H                 -0.657002    0.713050    2.034942
 H                  1.846703    0.652492    2.829331
 H                  1.822817   -0.389193   -1.296554
 H                 -0.890466   -1.819012    2.622236
 H                 -0.533581   -3.219179    0.535462
 H                  1.615171   -2.710525   -0.734159
 H                  1.618410   -1.774175    3.411948
 H                 -0.893648   -1.440969   -1.398279
 H                 -1.934813   -1.020327   -0.031380
 H                  5.172838   -1.805138    2.354820
 H                  2.547558   -4.119327    2.264042
 H                  3.802302    1.164094    1.239009

 1  2 1.0  4 1.0  11 1.0  17 1.0
 2  3 1.0  6 1.0  18 1.0
 3  5 1.0  10 1.0  19 1.0
 4  5 1.0  8 1.0  20 1.0
 5  16 2.0
 6  7 1.0  10 1.0  21 1.0
 7  8 1.0  11 1.0  22 1.0
 8  9 1.0  23 1.0
 9  10 1.0  12 1.0  14 1.0
 10  24 1.0
 11  25 1.0  26 1.0
 12  13 2.0  15 2.0
 13  27 1.0
 14  28 1.0
 15
 16  29 1.0
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Entering Link 1 = C:\G98W\l1.exe PID=   136.

Gaussian, Inc. access to this program. By using this program,
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Cite this work as:
Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

****
Gaussian 98: x86-Win32-G98RevA.7 11-Apr-1999
13-Mar-2002
****
%chk=m1s13Nbotts2F
Default route: MaxDisk=2000MB

#N RHF/3-21+G* FREQ

1/10=4,30=1,38=1/1,3;
2/17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11,27=262144000/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Freq calc of output str of m1s13Nbotts2

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C -2.08161 0.91435 -0.38648

C	-1.75152	0.5868	1.10709
C	-0.21862	0.9362	1.34193
C	-0.65243	0.89909	-1.02439
C	0.13999	1.54057	0.04409
C	-1.40779	-0.94231	1.07576
C	-1.57107	-1.30289	-0.42775
C	-0.29714	-0.66482	-1.03255
C	0.79041	-0.97045	-0.00836
C	0.10312	-0.61634	1.30338
C	-2.71416	-0.38988	-0.89366
C	2.11629	-0.22857	-0.243
N	2.84984	-0.14697	0.82986
O	0.98098	-2.40744	-0.04003
O	2.30457	0.23586	-1.4187
O	0.8731	2.57793	-0.15632
H	-2.6328	1.82979	-0.54699
H	-2.45255	0.9585	1.83648
H	0.09476	1.47628	2.21906
H	-0.53561	1.36227	-1.98787
H	-1.91027	-1.59347	1.77207
H	-1.66032	-2.35594	-0.63596
H	-0.02736	-0.98045	-2.02494
H	0.61435	-0.97495	2.17686
H	-2.85704	-0.40021	-1.96788
H	-3.65797	-0.60234	-0.40358
H	3.75576	0.2689	0.64819
H	1.84125	-2.64549	0.33709
H	1.4769	2.86455	0.55243

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 97 maximum allowed number of steps= 174.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C	0	-2.081605		0.914350		-0.386478	
2	2	C	0	-1.751517		0.586802		1.107092	
3	3	C	0	-0.218621		0.936202		1.341930	
4	4	C	0	-0.652432		0.899087		-1.024389	
5	5	C	0	0.139986		1.540574		0.044094	
6	6	C	0	-1.407789		-0.942311		1.075756	
7	7	C	0	-1.571069		-1.302895		-0.427748	
8	8	C	0	-0.297140		-0.664817		-1.032551	
9	9	C	0	0.790407		-0.970453		-0.008362	
10	10	C	0	0.103116		-0.616343		1.303378	
11	11	C	0	-2.714157		-0.389883		-0.893657	
12	12	C	0	2.116285		-0.228574		-0.243000	
13	13	N	0	2.849843		-0.146965		0.829863	
14	14	O	0	0.980979		-2.407436		-0.040033	

15	15	O	0	2.304575	0.235864	-1.418703
16	16	O	0	0.873098	2.577933	-0.156316
17	17	H	0	-2.632801	1.829791	-0.546992
18	18	H	0	-2.452549	0.958497	1.836478
19	19	H	0	0.094761	1.476281	2.219061
20	20	H	0	-0.535607	1.362266	-1.987867
21	21	H	0	-1.910266	-1.593471	1.772072
22	22	H	0	-1.660322	-2.355944	-0.635963
23	23	H	0	-0.027363	-0.980446	-2.024938
24	24	H	0	0.614350	-0.974947	2.176863
25	25	H	0	-2.857040	-0.400208	-1.967877
26	26	H	0	-3.657966	-0.602340	-0.403576
27	27	H	0	3.755758	0.268902	0.648193
28	28	H	0	1.841248	-2.645489	0.337094
29	29	H	0	1.476898	2.864546	0.552432

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.081605	0.914350	-0.386478
2	6	0	-1.751517	0.586802	1.107092
3	6	0	-0.218621	0.936202	1.341930
4	6	0	-0.652432	0.899087	-1.024389
5	6	0	0.139986	1.540574	0.044094
6	6	0	-1.407789	-0.942311	1.075756
7	6	0	-1.571069	-1.302895	-0.427748
8	6	0	-0.297140	-0.664817	-1.032551
9	6	0	0.790407	-0.970453	-0.008362
10	6	0	0.103116	-0.616343	1.303378
11	6	0	-2.714157	-0.389883	-0.893657
12	6	0	2.116285	-0.228574	-0.243000
13	7	0	2.849843	-0.146965	0.829863
14	8	0	0.980979	-2.407436	-0.040033
15	8	0	2.304575	0.235864	-1.418703
16	8	0	0.873098	2.577933	-0.156316
17	1	0	-2.632801	1.829791	-0.546992
18	1	0	-2.452549	0.958497	1.836478
19	1	0	0.094761	1.476281	2.219061
20	1	0	-0.535607	1.362266	-1.987867
21	1	0	-1.910266	-1.593471	1.772072
22	1	0	-1.660322	-2.355944	-0.635963
23	1	0	-0.027363	-0.980446	-2.024938
24	1	0	0.614350	-0.974947	2.176863
25	1	0	-2.857040	-0.400208	-1.967877
26	1	0	-3.657966	-0.602340	-0.403576
27	1	0	3.755758	0.268902	0.648193
28	1	0	1.841248	-2.645489	0.337094
29	1	0	1.476898	2.864546	0.552432

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				

2	C	1.564288	0.000000			
3	C	2.541374	1.589654	0.000000		
4	C	1.565151	2.418413	2.406041	0.000000	
5	C	2.347981	2.370112	1.475887	1.476851	0.000000
6	C	2.457508	1.567583	2.239147	2.893427	3.102362
7	C	2.275637	2.441158	3.158232	2.459390	3.351964
8	C	2.468905	2.873993	2.864889	1.603775	2.492788
9	C	3.455996	3.182870	2.544948	2.570851	2.594428
10	C	3.157790	2.219403	1.586000	2.878520	2.497888
11	C	1.535701	2.425610	3.603339	2.435004	3.571019
12	C	4.353061	4.177018	3.052948	3.089981	2.667970
13	N	5.188936	4.667739	3.294076	4.098586	3.287635
14	O	4.531413	4.212825	3.811663	3.817078	4.037466
15	O	4.556798	4.791104	3.805008	3.056017	2.920186
16	O	3.398640	3.528372	2.476262	2.428851	1.285975
17	H	1.080562	2.248928	3.192929	2.239638	2.849803
18	H	2.254126	1.077779	2.288123	3.380608	3.205104
19	H	3.441100	2.331607	1.076686	3.378079	2.176387
20	H	2.270503	3.414462	3.371878	1.075394	2.148740
21	H	3.313286	2.284949	3.073423	3.951605	4.124522
22	H	3.306742	3.421449	4.102291	3.429569	4.345853
23	H	3.239554	3.903663	3.878907	2.219111	3.265646
24	H	4.172330	3.029983	2.245761	3.919790	3.331902
25	H	2.197768	3.413474	4.438701	2.727386	4.098393
26	H	2.187591	2.707531	4.152469	3.416566	4.383712
27	H	5.963384	5.535497	4.089285	4.756764	3.880192
28	H	5.346474	4.893727	4.252207	4.542697	4.528053
29	H	4.165064	3.989791	2.686373	3.299006	1.949011

		6	7	8	9	10
6	C	0.000000				
7	C	1.554736	0.000000			
8	C	2.399063	1.547845	0.000000		
9	C	2.451157	2.421357	1.524839	0.000000	
10	C	1.562338	2.504206	2.370468	1.522637	0.000000
11	C	2.427007	1.535354	2.436565	3.660980	3.579843
12	C	3.829835	3.845111	2.576494	1.537333	2.567976
13	N	4.338256	4.739433	3.693272	2.371082	2.826489
14	O	3.016254	2.807718	2.378109	1.449911	2.404872
15	O	4.625156	4.286069	2.780155	2.395197	3.603110
16	O	4.371792	4.594394	3.557060	3.552432	3.595411
17	H	3.437807	3.309866	3.451688	4.455316	4.110071
18	H	2.298541	3.319280	3.938561	4.200125	3.048892
19	H	3.068288	4.183827	3.912910	3.381101	2.284211
20	H	3.931611	3.257182	2.253566	3.334416	3.892962
21	H	1.077659	2.244704	3.366078	3.294197	2.286517
22	H	2.234304	1.077141	2.208044	2.884361	3.145945
23	H	3.394309	2.244553	1.075748	2.176103	3.350714
24	H	2.302726	3.415788	3.350721	2.192310	1.073747
25	H	3.414368	2.200128	2.738237	4.179563	4.417052
26	H	2.714277	2.201477	3.419746	4.481040	4.130330
27	H	5.320908	5.657144	4.485835	3.280301	3.815065
28	H	3.742015	3.745858	3.220511	2.007325	2.841169
29	H	4.804940	5.255323	4.256264	3.936112	3.816777

		11	12	13	14	15

11	C	0.000000				
12	C	4.876735	0.000000			
13	N	5.829891	1.302230	0.000000		
14	O	4.295722	2.465270	3.059265	0.000000	
15	O	5.084772	1.278058	2.345192	3.261851	0.000000
16	O	4.713810	3.070751	3.507868	4.987892	3.021264
17	H	2.248054	5.184891	5.988546	5.592004	5.261004
18	H	3.056175	5.158257	5.509145	5.161387	5.809357
19	H	4.589292	3.613147	3.486442	4.579536	4.433423
20	H	3.002233	3.550755	4.656034	4.506079	3.107952
21	H	3.033311	4.704952	5.063475	3.507928	5.593961
22	H	2.245522	4.352342	5.231618	2.708183	4.801100
23	H	2.974462	2.887186	4.137982	2.644410	2.699049
24	H	4.566109	2.944252	2.738137	2.664783	4.153435
25	H	1.083730	5.266747	6.360817	4.740879	5.229574
26	H	1.084478	5.788563	6.639301	4.991027	6.106141
27	H	6.683644	1.931212	1.013228	3.916100	2.525685
28	H	5.230126	2.500726	2.739107	0.968998	3.405832
29	H	5.499766	3.257134	3.321317	5.328297	3.388273

		16	17	18	19	20
16	O	0.000000				
17	H	3.606060	0.000000			
18	H	4.201634	2.544125	0.000000		
19	H	2.731641	3.900720	2.627405	0.000000	
20	H	2.610915	2.587068	4.296895	4.255421	0.000000
21	H	5.372747	4.197480	2.609743	3.693685	4.976265
22	H	5.566994	4.298140	4.210238	5.090916	4.113115
23	H	4.118815	4.107318	4.954953	4.905298	2.397496
24	H	4.258360	5.082316	3.641420	2.506047	4.912224
25	H	5.105390	2.653694	4.059903	5.455712	2.914750
26	H	5.541283	2.643254	2.984474	5.028106	4.014820
27	H	3.780025	6.684200	6.358509	4.162726	5.153646
28	H	5.335251	6.389589	5.802892	4.856028	5.207397
29	H	0.974189	4.378250	4.552181	2.572010	3.572134

		21	22	23	24	25
21	H	0.000000				
22	H	2.538202	0.000000			
23	H	4.282337	2.547116	0.000000		
24	H	2.630611	3.872115	4.250524	0.000000	
25	H	4.038252	2.651609	2.889118	5.436887	0.000000
26	H	2.961459	2.668279	3.994128	5.005016	1.769005
27	H	6.069215	6.154088	4.797760	3.708428	7.142873
28	H	4.152079	3.645774	3.441405	2.771415	5.694567
29	H	5.730124	6.205477	4.867196	4.257285	5.982775

		26	27	28	29
26	H	0.000000			
27	H	7.538474	0.000000		
28	H	5.913071	3.500829	0.000000	
29	H	6.268977	3.455393	5.526265	0.000000

Interatomic angles:

C1-C2-C3=107.368	C2-C1-C4=101.211	C1-C4-C3= 76.3284
C2-C3-C4= 71.1832	C2-C1-C5= 71.4036	C1-C5-C3= 79.755
C2-C3-C5=101.2097	C1-C4-C5=101.0015	C2-C5-C4= 73.8282
C3-C5-C4=109.1453	C1-C2-C6=103.3816	C1-C6-C3= 65.3245

C3-C2-C6= 90.3387 C4-C1-C6= 89.1276 C4-C2-C6= 90.4979
C4-C3-C6= 76.9615 C5-C1-C6= 80.3842 C5-C2-C6=102.0392
C5-C3-C6=111.5956 C5-C4-C6= 83.7639 C2-C1-C7= 76.4648
C3-C1-C7= 81.7351 C3-C2-C7=101.0547 C4-C1-C7= 77.1881
C4-C2-C7= 60.8056 C3-C4-C7= 80.942 C5-C1-C7= 92.9186
C5-C2-C7= 88.3112 C5-C4-C7=114.4438 C1-C7-C6= 77.2938
C2-C6-C7=102.8581 C3-C6-C7=111.4262 C4-C7-C6= 89.2966
C2-C1-C8= 87.9029 C3-C1-C8= 69.7348 C2-C3-C8= 74.2345
C1-C4-C8=102.3493 C2-C4-C8= 88.8109 C3-C4-C8= 88.86
C5-C1-C8= 62.271 C2-C5-C8= 72.4068 C3-C5-C8= 88.562
C5-C4-C8=107.9615 C1-C6-C8= 61.0958 C2-C6-C8= 90.3581
C3-C6-C8= 76.2057 C4-C8-C6= 90.33 C5-C8-C6= 78.6942
C1-C7-C8= 77.882 C2-C7-C8= 89.2779 C3-C8-C7= 85.9331
C4-C8-C7=102.5721 C5-C8-C7=109.8934 C6-C7-C8=101.2925
C1-C3-C9= 85.6042 C2-C3-C9= 98.0059 C1-C4-C9=111.0073
C2-C4-C9= 79.2127 C4-C3-C9= 62.491 C1-C5-C9= 88.5882
C2-C5-C9= 79.6106 C5-C3-C9= 75.1605 C5-C4-C9= 74.2648
C1-C6-C9= 89.5072 C2-C6-C9=102.5144 C3-C6-C9= 65.5396
C4-C9-C6= 70.3141 C5-C9-C6= 75.8252 C1-C7-C9= 94.697
C2-C7-C9= 81.7734 C3-C9-C7= 78.9352 C4-C7-C9= 63.5644
C5-C9-C7= 83.7933 C6-C7-C9= 72.4366 C1-C8-C9=117.9005
C2-C8-C9= 87.0288 C3-C9-C8= 85.6084 C4-C8-C9=110.4898
C5-C8-C9= 76.2412 C6-C8-C9= 73.5449 C7-C8-C9=104.0004
C1-C2-C10=111.9803 C1-C3-C10= 97.1092 C2-C3-C10= 88.6744
C1-C4-C10= 85.1365 C4-C2-C10= 76.5956 C4-C3-C10= 89.8607
C1-C5-C10= 81.2677 C5-C2-C10= 65.8528 C5-C3-C10=109.2805
C4-C5-C10= 88.9543 C1-C6-C10=101.1991 C2-C6-C10= 90.322
C3-C10-C6= 90.6646 C4-C10-C6= 74.8223 C5-C10-C6= 96.949
C1-C7-C10= 82.5493 C7-C2-C10= 64.7983 C3-C10-C7= 98.6013
C4-C7-C10= 70.8842 C5-C10-C7= 84.1513 C7-C6-C10=106.9086
C1-C8-C10= 81.4363 C2-C10-C8= 77.4574 C3-C10-C8= 90.5568
C4-C8-C10= 90.7134 C5-C8-C10= 61.7505 C6-C10-C8= 71.8727
C7-C8-C10= 76.2524 C2-C10-C9=115.2822 C3-C10-C9=109.887
C4-C9-C10= 85.2976 C5-C10-C9= 76.1042 C6-C10-C9=105.2176
C7-C9-C10= 74.9847 C8-C9-C10=102.1276 C2-C1-C11=102.9685
C3-C1-C11=122.2667 C3-C2-C11=126.3738 C4-C1-C11=103.4871
C4-C2-C11= 60.355 C3-C4-C11= 96.2015 C5-C1-C11=132.5938
C5-C2-C11= 96.2471 C5-C4-C11=130.1951 C1-C11-C6= 72.759
C6-C2-C11= 71.2015 C3-C6-C11=101.0324 C4-C11-C6= 73.0406
C1-C11-C7= 95.6326 C2-C11-C7= 72.1618 C4-C11-C7= 72.5841
C6-C7-C11=103.5166 C1-C11-C8= 72.9061 C2-C11-C8= 72.4687
C3-C8-C11= 85.2323 C8-C4-C11= 70.8318 C5-C8-C11= 92.8374
C8-C6-C11= 60.6429 C8-C7-C11=104.4211 C9-C4-C11= 93.9583
C9-C6-C11= 97.2633 C9-C7-C11=134.1879 C9-C8-C11=133.7749
C10-C2-C11=100.7374 C10-C4-C11= 84.269 C10-C6-C11=126.2477
C10-C7-C11=122.9895 C10-C8-C11= 96.2586 C1-C5-C12=120.2841
C2-C5-C12=111.8751 C3-C5-C12= 90.176 C4-C5-C12= 91.8095
C1-C8-C12=119.2447 C2-C8-C12= 99.9122 C3-C8-C12= 68.0201
C4-C8-C12= 92.341 C5-C8-C12= 63.4865 C6-C8-C12=100.5988
C7-C8-C12=136.1373 C3-C9-C12= 93.5194 C4-C9-C12= 94.1739
C5-C9-C12= 75.655 C6-C9-C12=146.6588 C7-C9-C12=151.7565
C8-C9-C12=114.5746 C2-C10-C12=121.3316 C3-C10-C12= 91.4815
C4-C10-C12= 68.8575 C5-C10-C12= 63.5419 C6-C10-C12=134.5809
C7-C10-C12= 98.5824 C8-C10-C12= 62.7454 C10-C9-C12=114.114

C11-C8-C12=153.2044 C3-C9-N13= 84.0652 C4-C9-N13=112.0006
C5-C9-N13= 82.7881 C6-C9-N13=128.2127 C7-C9-N13=162.94
C8-C9-N13=141.9351 C2-C10-N13=135.0095 C3-C10-N13= 92.2149
C4-C10-N13= 91.8435 C5-C10-N13= 75.9838 C6-C10-N13=161.8104
C7-C10-N13=125.4085 C8-C10-N13= 90.1372 C10-C9-N13= 90.3855
C5-C12-N13=106.6821 C8-C12-N13=142.2544 C9-C12-N13=112.9748
C10-C12-N13= 87.4183 C1-C6-O14=111.3473 C2-C6-O14=130.9101
C3-C6-O14= 91.77 C4-C6-O14= 80.4375 C1-C7-O14=125.7829
C2-C7-O14=106.5524 C4-C7-O14= 92.6486 C6-C7-O14= 82.0819
C1-C8-O14=138.4123 C2-C8-O14=106.2831 C3-C8-O14= 92.8007
C4-C8-O14=146.2529 C5-C8-O14=111.9495 C6-C8-O14= 78.304
C7-C8-O14= 88.6928 C3-C9-O14=143.7277 C4-C9-O14=141.8
C5-C9-O14=173.0335 C6-C9-O14= 97.9849 C7-C9-O14= 89.3314
C8-C9-O14=106.1244 C2-C10-O14=131.2527 C3-C10-O14=144.7554
C4-C10-O14= 92.0729 C5-C10-O14=110.8609 C6-C10-O14= 96.6751
C7-C10-O14= 69.7382 C10-C8-O14= 60.8538 C10-C9-O14=107.9771
C11-C6-O14=103.6901 C11-C7-O14=162.28 C11-C8-O14=126.3014
C5-C12-O14=103.6552 C6-O14-C12= 88.0436 C7-O14-C12= 93.4126
C8-O14-C12= 64.2467 C12-C9-O14=111.1973 C10-O14-C12= 63.6308
N13-C9-O14=103.7549 N13-C10-O14= 71.0564 N13-C12-O14=104.2985
C1-C5-O15=119.3621 C2-C5-O15=129.5266 C3-C5-O15=115.9535
C4-C5-O15= 80.8652 C1-C8-O15=120.3656 C2-C8-O15=115.8417
C3-C8-O15= 84.7458 C4-C8-O15= 83.8062 C5-C8-O15= 67.0001
C6-C8-O15=126.354 C7-C8-O15=163.3418 C3-C9-O15=100.704
C4-C9-O15= 75.8674 C5-C9-O15= 71.5147 C6-C9-O15=145.2427
C7-C9-O15=125.711 C8-C9-O15= 87.3883 C10-C5-O15= 82.9738
C10-C8-O15= 88.4089 C10-C9-O15=132.4919 C11-C8-O15=154.1148
C5-C12-O15= 88.1176 C8-C12-O15= 85.275 C9-C12-O15=116.2845
C10-C12-O15=136.4123 C5-O15-N13= 76.4079 C8-O15-N13= 91.8065
C9-N13-O15= 61.0396 C10-N13-O15= 87.8102 N13-C12-O15=130.7018
O14-C8-O15= 78.0187 O14-C9-O15=113.7782 O14-C12-O15=117.6946
C1-C3-O16= 85.2616 C2-C3-O16=118.7816 C1-C4-O16=114.9049
C2-C4-O16= 93.4227 C3-C4-O16= 61.6141 C1-C5-O16=136.549
C2-C5-O16=148.1548 C3-C5-O16=127.2928 C4-C5-O16=122.9236
C6-C3-O16=135.9245 C6-C4-O16=110.148 C7-C4-O16=140.0643
C8-C3-O16= 83.1723 C8-C4-O16=122.4594 C8-C5-O16=138.2732
C9-C3-O16= 90.0506 C9-C4-O16= 90.5101 C9-C5-O16=129.3955
C10-C3-O16=123.0151 C10-C4-O16= 84.8374 C10-C5-O16=141.5857
C11-C4-O16=151.4628 C12-C5-O16= 95.5003 O15-C5-O16= 81.939
C2-C1-H17=115.2687 C3-C1-H17=117.8837 C3-C2-H17=111.4106
C4-C1-H17=114.425 C2-H17-C4= 65.2028 C3-C4-H17= 86.7541
C5-C1-H17=106.495 C5-C2-H17= 76.1399 C3-C5-H17= 89.286
C5-C4-H17= 98.0319 C6-C1-H17=150.2624 C6-C2-H17=127.6157
C6-C4-H17= 83.045 C7-C1-H17=159.5861 C7-C2-H17= 89.678
C7-C4-H17= 89.4312 C8-C1-H17=150.6566 C8-C2-H17= 83.7676
C8-C4-H17=127.0278 C8-C5-H17= 80.1881 C9-C4-H17=135.579
C9-C5-H17=109.7523 C10-C2-H17=133.7992 C10-C4-H17=106.1704
C10-C5-H17=100.2438 C11-C1-H17=117.4083 C2-H17-C11= 65.2837
C4-H17-C11= 65.7208 C5-H17-C11= 88.1084 C6-C11-H17= 94.5961
C7-C11-H17=120.8915 C8-C11-H17= 94.836 C12-C5-H17=139.9701
O15-C5-H17=131.5033 O16-C4-H17=101.0669 O16-C5-H17=116.1349
C1-C2-H18=115.8928 C1-H18-C3= 68.0373 C3-C2-H18=116.8362
C4-C1-H18=123.5313 C4-C2-H18=147.9437 C4-C3-H18= 92.1026
C5-C1-H18= 88.26 C5-C2-H18=133.1441 C5-C3-H18=115.0427

C1-H18-C6= 65.3309 C6-C2-H18=119.509 C6-C3-H18= 61.0115
C4-C6-H18= 80.3631 C7-C1-H18= 94.2372 C7-C2-H18=137.7774
C7-C6-H18=117.6527 C8-C1-H18=112.9255 C8-C2-H18=169.4748
C8-C3-H18= 99.0807 C8-C6-H18=113.93 C9-C3-H18=120.6019
C9-C6-H18=124.298 C10-C2-H18=132.1166 C10-C3-H18=102.2893
C10-C6-H18=102.6392 C11-C1-H18=105.9348 C11-C2-H18=116.0362
C11-C6-H18= 80.5417 O14-C6-H18=152.1403 O16-C3-H18=123.6931
H17-C1-H18= 92.6341 H17-C2-H18= 92.995 C3-H18-H17= 82.5316
C4-H17-H18= 89.6981 C5-H17-H18= 72.662 C6-H18-H17= 90.3069
C11-H17-H18= 78.9821 C1-C2-H19=122.8582 C1-C3-H19=140.5099
C2-C3-H19=120.7485 C4-C2-H19= 90.6417 C4-C3-H19=149.477
C1-C5-H19= 98.9585 C2-H19-C5= 63.3284 C5-C3-H19=116.1197
C4-C5-H19=134.3496 C6-C2-H19=102.0068 C6-C3-H19=132.2403
C7-C2-H19=122.4543 C8-C2-H19= 96.9197 C8-C3-H19=164.4732
C8-C5-H19=113.6934 C9-C3-H19=133.8397 C9-C5-H19= 89.818
C2-C10-H19= 62.3391 C10-C3-H19=116.8585 C4-C10-H19= 80.8459
C5-H19-C10= 68.0606 C6-C10-H19=104.2415 C7-C10-H19=121.7247
C8-C10-H19=114.4029 C9-C10-H19=124.0599 C11-C2-H19=149.4563
C12-C5-H19= 95.9316 C12-C10-H19= 96.0807 N13-C10-H19= 85.3296
O14-C10-H19=155.1732 O15-C5-H19=120.1856 C2-H19-O16= 87.9807
O16-C3-H19= 91.8349 C4-O16-H19= 81.5506 O16-C5-H19=101.0355
C10-H19-O16= 91.1364 H17-C2-H19=116.7577 H17-C5-H19=100.9561
C1-H18-H19= 89.3074 H18-C2-H19= 93.4821 H18-C3-H19= 95.9236
C5-H19-H18= 83.1339 C6-H18-H19= 76.7315 C10-H19-H18= 76.3867
O16-H19-H18=103.2443 H17-H18-H19= 97.91 C2-C1-H20=124.823
C3-C1-H20= 88.7875 C1-C4-H20=117.3969 C2-C4-H20=153.4596
C3-C4-H20=148.7496 C1-H20-C5= 64.1184 C2-C5-H20= 98.0369
C3-C5-H20=136.153 C5-C4-H20=113.7548 C6-C1-H20=112.4581
C6-C4-H20=162.3186 C7-C1-H20= 91.5278 C7-C4-H20=130.0574
C1-H20-C8= 66.1474 C2-C8-H20= 82.5487 C3-C8-H20= 81.4641
C8-C4-H20=113.0399 C5-H20-C8= 68.9304 C6-C8-H20=115.3148
C7-C8-H20=116.7023 C9-C4-H20=127.3242 C9-C5-H20= 88.819
C9-C8-H20=122.7174 C10-C4-H20=157.3309 C10-C5-H20=113.606
C10-C8-H20=114.6586 C11-C1-H20=102.4198 C2-C11-H20= 77.1528
C11-C4-H20=111.5971 C5-H20-C11= 86.0965 C6-C11-H20= 92.1779
C7-C11-H20= 85.262 C11-C8-H20= 79.4962 C12-C5-H20= 94.3654
C12-C8-H20= 94.4004 O14-C8-H20=153.2432 O15-C5-H20= 73.8759
O15-C8-H20= 75.4477 C1-H20-O16= 87.9636 C3-O16-H20= 82.9851
O16-C4-H20= 87.3787 O16-C5-H20= 95.6705 C8-H20-O16= 93.6894
C11-H20-O16=114.053 H17-C1-H20= 94.3259 C2-H17-H20= 89.5468
H17-C4-H20= 96.2029 C5-H20-H17= 73.3334 C8-H20-H17= 90.701
C11-H17-H20= 76.4093 O16-H20-H17= 87.8529 H18-C1-H20=143.4884
H18-H17-H20=113.7319 H19-C5-H20=159.3985 H19-O16-H20=105.5748
C1-C2-H21=117.5814 C3-C2-H21=103.5167 C4-C2-H21=114.2856
C5-C2-H21=124.747 C1-C6-H21=135.489 C2-C6-H21=118.3106
C3-C6-H21=132.6669 C4-C6-H21=167.2265 C1-C7-H21= 94.2698
C2-H21-C7= 65.2143 C4-C7-H21=114.2105 C7-C6-H21=115.8324
C8-C2-H21= 80.5768 C8-C6-H21=148.603 C8-C7-H21=124.1013
C9-C6-H21=134.186 C9-C7-H21= 89.7368 C10-C2-H21= 60.9908
C3-C10-H21=103.575 C4-C10-H21= 99.1847 C5-C10-H21=119.0351
C10-C6-H21=118.8716 C7-H21-C10= 67.0914 C8-C10-H21= 92.5548
C9-C10-H21=118.3377 C11-C2-H21= 80.1115 C11-C6-H21=114.2597
C11-C7-H21=105.1805 C12-C10-H21=151.4344 N13-C10-H21=163.9464
O14-C6-H21=108.3479 O14-C7-H21= 87.197 O14-C10-H21= 96.7572

H17-C2-H21=135.5783 C1-H18-H21= 85.5446 H18-C2-H21= 94.9871
C3-H18-H21= 77.4241 H18-C6-H21= 94.2382 C7-H21-H18= 85.9286
C10-H21-H18= 76.7115 H17-H18-H21=109.056 H19-C2-H21=106.2741
H19-C10-H21=107.8248 H19-H18-H21= 89.7046 C1-C6-H22= 89.4944
C2-C6-H22=127.4233 C3-C6-H22=132.9914 C4-C6-H22= 82.8823
C1-C7-H22=159.6299 C2-C7-H22=150.7149 C4-C7-H22=149.2456
C6-C7-H22=114.9846 C1-C8-H22= 89.8087 C2-C8-H22= 83.5353
C3-C8-H22=107.2216 C4-C8-H22=127.5295 C5-C8-H22=135.095
C6-H22-C8= 65.3701 C8-C7-H22=113.3085 C3-C9-H22= 97.9577
C4-C9-H22= 77.6703 C5-C9-H22=104.8503 C9-C6-H22= 75.8333
C9-C7-H22=104.3898 C9-C8-H22= 99.5651 C10-C6-H22=110.6665
C10-C7-H22=117.1971 C10-C8-H22= 86.7273 C10-C9-H22= 85.1607
C1-C11-H22=120.8222 C2-C11-H22= 94.1079 C4-C11-H22= 94.1444
C6-H22-C11= 65.607 C11-C7-H22=117.4522 C8-H22-C11= 66.331
C9-H22-C11= 90.1808 C12-C8-H22=130.7632 C12-C9-H22=158.652
N13-C9-H22=169.0317 C6-H22-O14= 74.527 C7-H22-O14= 83.9865
O14-C8-H22= 72.279 C9-O14-H22= 81.8232 C10-O14-H22= 75.6847
C11-H22-O14=119.9745 C12-O14-H22=114.4706 O15-C8-H22=148.3008
O15-C9-H22=130.6118 H17-C11-H22=146.0796 H18-C6-H22=136.5015
H20-C8-H22=134.4055 H20-C11-H22=102.2549 C2-H21-H22= 90.2117
H21-C6-H22= 93.4406 H21-C7-H22= 92.8868 C8-H22-H21= 90.0642
C9-H22-H21= 74.5109 C10-H21-H22= 81.2104 C11-H22-H21= 78.4424
O14-H22-H21= 83.857 H18-H21-H22=109.7322 C1-C4-H23=116.6942
C2-C4-H23=114.584 C3-C4-H23=113.9358 C5-C4-H23=122.8856
C6-C4-H23= 82.0549 C1-C7-H23= 91.5604 C2-C7-H23=112.7699
C4-H23-C7= 66.8657 C6-C7-H23=125.6329 C1-C8-H23=127.6135
C2-C8-H23=160.3012 C3-C8-H23=157.1742 C4-C8-H23=110.2649
C5-C8-H23=127.8819 C6-C8-H23=153.2357 C7-C8-H23=116.4815
C3-C9-H23=110.2505 C4-H23-C9= 71.5871 C5-C9-H23= 85.9268
C6-C9-H23= 94.1808 C7-H23-C9= 66.4028 C9-C8-H23=112.4545
C10-C4-H23= 81.0703 C10-C7-H23= 89.5832 C10-C8-H23=150.7766
C10-C9-H23=129.0337 C1-C11-H23= 85.5358 C2-C11-H23= 92.0158
C11-C4-H23= 79.3013 C6-C11-H23= 77.1279 C11-C7-H23=102.1623
C11-C8-H23=109.5398 C9-H23-C11= 89.203 C4-H23-C12= 73.1595
C5-C12-H23= 71.8874 C7-H23-C12= 96.25 C12-C8-H23= 95.5933
C12-C9-H23=100.6544 C10-C12-H23= 75.5387 C11-H23-C12=112.5955
N13-C9-H23=130.9653 N13-C12-H23=160.5686 C4-H23-O14=103.0631
C6-O14-H23= 73.3553 C7-H23-O14= 69.5499 O14-C8-H23= 92.0191
O14-C9-H23= 91.4096 C10-O14-H23= 83.0046 C11-H23-O14= 99.5608
C12-O14-H23= 68.7075 C4-H23-O15= 76.1375 C5-O15-H23= 70.9391
C7-H23-O15=119.9418 C8-H23-O15= 82.9489 O15-C9-H23= 72.1951
C11-H23-O15=127.2668 C12-O15-H23= 85.157 N13-O15-H23=110.0399
O14-H23-O15= 75.2346 O16-C4-H23=124.7269 H17-C4-H23=134.1984
H17-C11-H23=102.8264 C1-H20-H23= 87.8499 H20-C4-H23= 85.9999
C5-H20-H23= 91.665 C7-H23-H20= 89.0589 H20-C8-H23= 84.2257
C9-H23-H20= 93.4885 C11-H23-H20= 66.9599 C12-H23-H20= 83.8799
O14-H23-H20=126.6212 O15-H23-H20= 74.8906 O16-H20-H23=110.5754
H17-H20-H23=110.9189 H21-C7-H23=145.0728 C4-H23-H22= 91.7726
C6-H22-H23= 90.2085 H22-C7-H23= 93.433 H22-C8-H23= 95.4974
C9-H23-H22= 74.8152 C11-H22-H23= 76.4365 C12-H23-H22=106.2643
O14-H23-H22= 62.8537 O15-H23-H22=132.4368 H20-H23-H22=112.5409
H21-H22-H23=114.7246 C1-C3-H24=121.1602 C2-C3-H24=103.0347
C4-C3-H24=114.7962 C5-C3-H24=125.8236 C1-C6-H24=122.4119
C2-C6-H24=101.3511 C6-C3-H24= 61.7861 C4-C6-H24= 97.2874

C7-C6-H24=123.4601 C8-C3-H24= 80.9516 C8-C6-H24= 90.8779
C3-H24-C9= 69.9684 C4-C9-H24=110.5089 C5-C9-H24= 87.8049
C6-H24-C9= 66.0376 C7-C9-H24= 95.3961 C8-C9-H24=127.7802
C2-C10-H24=130.6067 C3-C10-H24=113.8123 C4-C10-H24=163.464
C5-C10-H24=133.7467 C6-C10-H24=120.6163 C7-C10-H24=142.102
C8-C10-H24=151.069 C9-C10-H24=114.094 C11-C6-H24=149.7597
C3-H24-C12= 70.6045 C5-C12-H24= 72.6494 C6-H24-C12= 92.9442
C8-C12-H24= 74.4014 C12-C9-H24=102.8491 C12-C10-H24= 99.6159
C3-H24-N13= 82.1021 C6-H24-N13=118.5175 N13-C9-H24= 73.6255
C10-H24-N13= 83.5428 C12-N13-H24= 85.7816 C3-H24-O14=101.4904
C6-H24-O14= 74.3733 C7-O14-H24= 77.1941 C8-O14-H24= 83.0705
O14-C9-H24= 91.7361 O14-C10-H24= 91.8278 C12-O14-H24= 69.9245
N13-H24-O14= 68.9593 O15-C9-H24=129.6962 O15-C12-H24=157.4203
O15-N13-H24=109.3422 O16-C3-H24=128.7281 H18-C3-H24=106.8615
H18-C6-H24=104.6321 C2-H19-H24= 77.4673 H19-C3-H24= 90.9191
C5-H19-H24= 90.4446 C6-H24-H19= 79.1708 C9-H24-H19= 91.8011
H19-C10-H24= 88.9454 C12-H24-H19= 82.6257 N13-H24-H19= 83.2108
O14-H24-H19=124.6344 O16-H19-H24=108.7084 H18-H19-H24= 90.3324
C2-H21-H24= 75.7444 C3-H24-H21= 77.6971 H21-C6-H24= 95.2742
C7-H21-H24= 88.5871 C9-H24-H21= 85.6513 H21-C10-H24= 96.3023
C12-H24-H21=115.0054 N13-H24-H21=141.163 O14-H24-H21= 82.9711
H18-H21-H24= 88.0344 H19-H24-H21= 91.9251 H22-C6-H24=117.1692
H22-C9-H24= 98.4917 H22-O14-H24= 92.2154 H22-H21-H24= 97.014
H23-C9-H24=153.3174 H23-C12-H24= 93.5831 H23-O14-H24=106.3737
C2-C1-H25=129.511 C3-C1-H25=138.8647 C4-C1-H25= 91.3222
C2-C4-H25= 82.8781 C3-C4-H25=119.5584 C5-C1-H25=128.7052
C5-C4-H25=152.9884 C6-C1-H25= 94.1854 C6-C4-H25= 74.7454
C1-H25-C7= 62.321 C2-C7-H25= 94.5493 C4-C7-H25= 71.4069
C6-C7-H25=130.0293 C8-C1-H25= 71.5874 C2-C8-H25= 74.8781
C3-C8-H25=104.7574 C8-C4-H25= 73.3076 C5-C8-H25=103.06
C6-C8-H25= 83.0247 C8-C7-H25= 92.2008 C9-C4-H25=104.1191
C9-C7-H25=129.4168 C9-C8-H25=156.2865 C10-C4-H25=103.9521
C10-C7-H25=139.6581 C10-C8-H25=119.5038 C1-C11-H25=112.9395
C2-C11-H25=150.8992 C4-C11-H25= 93.6383 C6-C11-H25=150.825
C7-C11-H25=113.159 C8-C11-H25= 94.1982 C12-C8-H25=164.5829
O14-C7-H25=142.1242 O14-C8-H25=135.7105 O15-C8-H25=142.761
O16-C4-H25=163.8667 H17-C1-H25=102.7013 C2-H17-H25= 87.8491
C4-H17-H25= 67.131 C5-H17-H25= 96.1995 C7-H25-H17= 85.4445
C8-H25-H17= 79.5903 H17-C11-H25= 99.6153 H18-C1-H25=131.5482
H18-H17-H25=102.6984 H20-C1-H25= 81.4161 H20-C4-H25= 89.0297
C5-H20-H25=107.1038 C7-H25-H20= 77.7236 H20-C8-H25= 70.6918
C11-H25-H20= 84.0322 O16-H20-H25=134.9466 H20-H17-H25= 67.5687
H21-C7-H25=130.6026 C1-H25-H22= 85.4398 C4-H25-H22= 79.2103
C6-H22-H25= 88.2336 H22-C7-H25=102.5542 C8-H22-H25= 67.8838
C9-H22-H25= 97.9596 H22-C11-H25= 99.63 O14-H22-H25=124.3833
H17-H25-H22=108.223 H20-H25-H22= 95.1626 H21-H22-H25=102.1539
C1-H25-H23= 77.8055 H23-C4-H25= 70.6233 H23-C7-H25= 81.0791
H23-C8-H25= 87.0015 C9-H23-H25=110.4163 C11-H25-H23= 83.8207
C12-H23-H25=131.5064 O14-H23-H25=117.8408 O15-H23-H25=138.7003
H17-H25-H23= 95.5424 H20-H23-H25= 66.1603 H23-H22-H25= 67.4882
C2-C1-H26= 90.8219 C3-C1-H26=122.6507 C3-C2-H26=149.0869
C4-C1-H26=130.3941 C4-C2-H26= 83.3942 C5-C1-H26=150.2442
C5-C2-H26=119.238 C6-C1-H26= 71.2417 C6-C2-H26= 73.4306
C3-C6-H26=113.5771 C4-C6-H26= 74.9963 C1-H26-C7= 62.4595

C2-C7-H26= 71.1368 C4-C7-H26= 94.1192 C6-C7-H26= 90.8671
C8-C1-H26= 94.3197 C8-C2-H26= 75.5028 C8-C6-H26= 83.7043
C8-C7-H26=130.7913 C9-C6-H26=120.2546 C9-C7-H26=151.5121
C10-C2-H26=113.5567 C10-C6-H26=148.7593 C10-C7-H26=122.6101
C1-C11-H26=112.0616 C2-C11-H26= 92.9531 C4-C11-H26=149.8646
C6-C11-H26= 93.2763 C7-C11-H26=113.2229 C8-C11-H26=150.1074
O14-C6-H26=121.0493 O14-C7-H26=170.1646 H17-C1-H26=102.6288
C2-H17-H26= 66.6417 C4-H17-H26= 88.4036 C5-H17-H26=105.8266
C6-H26-H17= 79.822 C7-H26-H17= 85.673 H17-C11-H26= 98.9309
H18-C1-H26= 84.4165 H18-C2-H26= 94.0752 C3-H18-H26=103.121
H18-C6-H26= 72.5415 C7-H26-H18= 77.9826 C11-H26-H18= 83.4092
H18-H17-H26= 70.2162 H19-C2-H26=172.3949 H19-H18-H26=127.1527
H20-C1-H26=128.4563 H20-C11-H26=155.5825 H20-H17-H26=100.273
C1-H26-H21= 78.5237 H21-C2-H26= 72.2046 H21-C6-H26= 92.3668
H21-C7-H26= 83.5226 C10-H21-H26=103.064 C11-H26-H21= 83.3364
H17-H26-H21= 96.8298 H18-H21-H26= 64.4204 C1-H26-H22= 85.2303
C2-H26-H22= 79.0519 C6-H22-H26= 66.5522 H22-C7-H26=103.5726
C8-H22-H26= 88.5387 C9-H22-H26=107.5462 H22-C11-H26=100.6637
O14-H22-H26=136.3447 H17-H26-H22=108.0365 H18-H26-H22= 96.1248
H21-H22-H26= 69.2818 H23-C7-H26=127.8836 H23-C11-H26=156.7946
H23-H22-H26= 99.9365 H24-C6-H26=172.0501 H24-H21-H26=126.9218
C1-H26-H25= 66.5118 C2-H26-H25= 97.1464 C4-H25-H26= 96.5751
C6-H26-H25= 96.9453 C7-H25-H26= 66.343 C8-H25-H26= 96.3253
H25-C11-H26=109.3496 H17-H26-H25= 70.8093 H18-H26-H25=114.9035
H20-H25-H26=115.8331 H21-H26-H25=114.8782 H22-H25-H26= 71.0878
H23-H25-H26=115.9736 C5-C12-H27=114.1029 C8-C12-H27=168.5895
C9-C12-H27=141.8174 C10-C12-H27=115.2479 C9-N13-H27=148.8409
C10-N13-H27=165.2517 C12-N13-H27=112.436 O14-C12-H27=125.4948
C5-O15-H27= 90.58 C8-O15-H27=115.3575 C9-O15-H27= 83.5666
O15-C12-H27=101.8782 O15-N13-H27= 88.2218 H23-C12-H27=169.1746
H23-O15-H27=133.3242 H24-C12-H27= 96.8394 H24-N13-H27=160.4371
C3-C9-H28=137.8526 C4-C9-H28=165.6147 C5-C9-H28=159.2928
C6-C9-H28=113.7622 C7-C9-H28=115.2011 C8-C9-H28=131.0125
C2-C10-H28=150.2626 C3-C10-H28=146.253 C4-C10-H28=105.1616
C5-C10-H28=115.8627 C6-C10-H28=113.1454 C7-C10-H28= 88.7443
C8-C10-H28= 75.7323 C10-C9-H28=106.3859 C5-C12-H28=122.3067
C8-C12-H28= 78.7215 C12-C9-H28= 88.7085 C10-C12-H28= 68.1703
N13-C9-H28= 76.9546 C10-N13-H28= 61.3689 N13-C12-H28= 86.067
C6-O14-H28=132.7235 C7-O14-H28=163.2038 C8-O14-H28=145.0446
C9-O14-H28=110.5893 C10-O14-H28=106.836 C12-O14-H28= 80.8119
N13-H28-O14= 99.9523 O15-C9-H28=100.9914 O15-C12-H28=125.5075
O15-N13-H28= 83.7308 H19-C10-H28=142.4542 H21-C10-H28=107.6497
H22-C9-H28= 94.67 H22-O14-H28=162.9755 H23-C9-H28=110.6329
H23-C12-H28= 79.0368 H23-O14-H28=139.7493 C3-H24-H28=115.4905
C6-H24-H28= 94.5809 H24-C9-H28= 82.4604 C10-H24-H28= 82.6496
C12-H28-H24= 67.6729 H24-N13-H28= 60.7938 H24-O14-H28= 86.0107
H19-H24-H28=133.8327 H21-H24-H28=100.427 H27-C12-H28=103.6085
H27-N13-H28=132.1716 C1-C3-H29=105.6031 C2-C3-H29=136.301
C4-C3-H29= 80.5511 C1-C5-H29=151.405 C2-C5-H29=134.7338
C3-C5-H29=102.4442 C4-C5-H29=148.4093 C6-C3-H29=154.4848
C8-C3-H29=100.0709 C8-C5-H29=146.5035 C9-C3-H29= 97.5629
C9-C5-H29=119.3916 C10-C3-H29=124.5762 C10-C5-H29=117.724
C12-C5-H29= 88.304 O15-C5-H29= 85.7391 C3-O16-H29= 91.6115
C4-O16-H29=148.5026 C5-O16-H29=118.5082 H17-C5-H29=130.7351

H18-C3-H29=132.2783 C2-H19-H29=108.8081 C3-H19-H29= 84.2189
H19-C5-H29= 76.9191 C10-H19-H29=103.4596 O16-H29-H19= 88.8289
H18-H19-H29=122.2091 H20-C5-H29=121.244 H20-O16-H29=169.0374
H24-C3-H29=119.0802 H24-H19-H29=113.9302

Stoichiometry C12H13NO3
Framework group C1[X(C12H13NO3)]
Deg. of freedom 81
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.072457	0.945768	-0.359061
2	6	0	-1.734873	0.596529	1.127904
3	6	0	-0.195727	0.923218	1.354402
4	6	0	-0.648699	0.919396	-1.008612
5	6	0	0.160475	1.538005	0.060802
6	6	0	-1.411440	-0.936449	1.076090
7	6	0	-1.591317	-1.277288	-0.430123
8	6	0	-0.313975	-0.648790	-1.037751
9	6	0	0.777551	-0.980475	-0.025975
10	6	0	0.105354	-0.632819	1.295279
11	6	0	-2.726013	-0.344122	-0.876192
12	6	0	2.111124	-0.253192	-0.262692
13	7	0	2.854154	-0.193662	0.805093
14	8	0	0.949049	-2.419344	-0.075822
15	8	0	2.296164	0.222467	-1.434418
16	8	0	0.905488	2.568024	-0.133487
17	1	0	-2.612881	1.870106	-0.504512
18	1	0	-2.425188	0.968752	1.867176
19	1	0	0.131626	1.448894	2.235173
20	1	0	-0.533452	1.392245	-1.967573
21	1	0	-1.916868	-1.589119	1.768849
22	1	0	-1.695985	-2.326584	-0.649793
23	1	0	-0.056213	-0.956279	-2.035870
24	1	0	0.618749	-1.008216	2.160400
25	1	0	-2.877516	-0.340037	-1.949272
26	1	0	-3.668613	-0.550012	-0.381008
27	1	0	3.763967	0.212496	0.620951
28	1	0	1.809087	-2.672944	0.291572
29	1	0	1.518576	2.838467	0.573640

Rotational constants (GHZ): 0.9454103 0.6570686 0.5382905
Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,N-14,O-16,
O-16,O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1
Standard basis: 3-21+G* (6D, 7F)
There are 234 symmetry adapted basis functions of A symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be 262144 words long.
Raffenetti 1 integral format.

```
 Two-electron integral symmetry is turned on.
   234 basis functions      343 primitive gaussians
    58 alpha electrons       58 beta electrons
       nuclear repulsion energy      1230.5307570241 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   234 RedAO= T  NBF=   234
 NBsUse=   234 1.00D-04 NBFU=   234
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -736.887327244     A.U. after   17 cycles
             Convg  =    0.6272D-08             -V/T =  2.0022
             S**2   =   0.0000
 Range of M.O.s used for correlation:     1   234
 NBasis=   234 NAE=    58 NBE=    58 NFC=     0 NFV=     0
 NROrb=    234 NOA=    58 NOB=    58 NVA=   176 NVB=   176

 **** Warning!!: The largest alpha MO coefficient is  0.10566240D+03

          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   3 vectors were produced by pass 12.
   3 vectors were produced by pass 13.
 Inv2:  IOpt= 1 Iter= 1 AM= 7.19D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  42 with in-core refinement.
 G2DrvN: will do   29 atoms at a time, making    1 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  90 IRICut=      82 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
          There are  90 degrees of freedom in the 1st order CPHF.
  87 vectors were produced by pass  0.
```

```
 AX will form  87 AO Fock derivatives at one time.
  87 vectors were produced by pass  1.
  87 vectors were produced by pass  2.
  87 vectors were produced by pass  3.
  87 vectors were produced by pass  4.
  87 vectors were produced by pass  5.
  87 vectors were produced by pass  6.
  46 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   1 vectors were produced by pass  9.
 Inv2:  IOpt= 1 Iter= 1 AM= 4.31D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 659 with in-core refinement.

 ********************************************************************

            Population analysis using the SCF density.

 ********************************************************************

 Alpha  occ. eigenvalues --  -20.63376 -20.47526 -20.37554 -15.41271 -
11.40708
 Alpha  occ. eigenvalues --  -11.24220 -11.24088 -11.24029 -11.23564 -
11.23261
 Alpha  occ. eigenvalues --  -11.22923 -11.21110 -11.20520 -11.20310 -
11.19687
 Alpha  occ. eigenvalues --  -11.19440  -1.55532  -1.36927  -1.30631  -
1.27881
 Alpha  occ. eigenvalues --   -1.13779  -1.12411  -1.11289  -1.07945  -
0.96960
 Alpha  occ. eigenvalues --   -0.96014  -0.93208  -0.89612  -0.82862  -
0.81906
 Alpha  occ. eigenvalues --   -0.77126  -0.76849  -0.75108  -0.71799  -
0.70213
 Alpha  occ. eigenvalues --   -0.68867  -0.66906  -0.65695  -0.63831  -
0.61960
 Alpha  occ. eigenvalues --   -0.60476  -0.58185  -0.56367  -0.56197  -
0.53557
 Alpha  occ. eigenvalues --   -0.52738  -0.51527  -0.50826  -0.49990  -
0.49011
 Alpha  occ. eigenvalues --   -0.48467  -0.47466  -0.46627  -0.45738  -
0.43125
 Alpha  occ. eigenvalues --   -0.37861  -0.34916  -0.30795
 Alpha virt. eigenvalues --    0.02308   0.04122   0.05375   0.06394
0.06993
 Alpha virt. eigenvalues --    0.08169   0.08634   0.09373   0.10469
0.10569
 Alpha virt. eigenvalues --    0.11700   0.12391   0.13781   0.14052
0.14560
 Alpha virt. eigenvalues --    0.14697   0.15697   0.16774   0.17147
0.17629
 Alpha virt. eigenvalues --    0.17955   0.18706   0.19058   0.19306
0.19770
 Alpha virt. eigenvalues --    0.20125   0.20244   0.22773   0.23038
0.23417
```

```
 Alpha virt. eigenvalues --    0.23481   0.23831   0.24321   0.24666
0.25146
 Alpha virt. eigenvalues --    0.25609   0.26117   0.26289   0.26965
0.27266
 Alpha virt. eigenvalues --    0.27467   0.28016   0.28175   0.29484
0.29935
 Alpha virt. eigenvalues --    0.30470   0.31103   0.31384   0.32082
0.33085
 Alpha virt. eigenvalues --    0.33365   0.34345   0.34855   0.35126
0.36896
 Alpha virt. eigenvalues --    0.37188   0.37926   0.38902   0.39192
0.39787
 Alpha virt. eigenvalues --    0.41611   0.41971   0.42612   0.43472
0.44084
 Alpha virt. eigenvalues --    0.44346   0.45768   0.46168   0.47142
0.47431
 Alpha virt. eigenvalues --    0.47987   0.48840   0.49588   0.49874
0.51027
 Alpha virt. eigenvalues --    0.51157   0.51580   0.52635   0.53584
0.54713
 Alpha virt. eigenvalues --    0.54995   0.56380   0.56565   0.57177
0.58399
 Alpha virt. eigenvalues --    0.59159   0.60501   0.60769   0.61350
0.62957
 Alpha virt. eigenvalues --    0.63265   0.65174   0.65881   0.66598
0.67608
 Alpha virt. eigenvalues --    0.71160   0.73225   0.77303   0.86821
1.07367
 Alpha virt. eigenvalues --    1.08713   1.10315   1.11236   1.11715
1.12383
 Alpha virt. eigenvalues --    1.13782   1.15011   1.16257   1.16971
1.17523
 Alpha virt. eigenvalues --    1.17962   1.19201   1.19799   1.20567
1.21263
 Alpha virt. eigenvalues --    1.22192   1.22939   1.25209   1.25757
1.26611
 Alpha virt. eigenvalues --    1.28780   1.31413   1.33796   1.36191
1.38135
 Alpha virt. eigenvalues --    1.39490   1.43214   1.43459   1.44602
1.47668
 Alpha virt. eigenvalues --    1.48846   1.50704   1.52164   1.52469
1.53416
 Alpha virt. eigenvalues --    1.55939   1.57662   1.57826   1.58672
1.62420
 Alpha virt. eigenvalues --    1.65390   1.68902   1.69650   1.72394
1.76031
 Alpha virt. eigenvalues --    1.76825   1.83053   1.85965   1.91762
1.93338
 Alpha virt. eigenvalues --    2.00378   2.04451   2.10421   2.13465
2.21002
 Alpha virt. eigenvalues --    2.22122   2.22910   2.25306   2.29291
2.31002
 Alpha virt. eigenvalues --    2.34746   2.36860   2.40482   2.46032
2.50568
```

```
 Alpha virt. eigenvalues --    2.54797   2.69080   2.89903   3.01864
3.15602
 Alpha virt. eigenvalues --    3.19971   3.38995   3.74488   3.80141
3.89513
 Alpha virt. eigenvalues --    3.95523
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   15.178176  -9.190712   6.139408  -5.331201  -1.952980   5.670637
  2  C   -9.190712  24.330190 -16.585541   2.360124   7.645416 -13.771977
  3  C    6.139408 -16.585541  41.370394   8.407055 -29.940448  11.197497
  4  C   -5.331201   2.360124   8.407055  27.082732 -21.784927  -2.170592
  5  C   -1.952980   7.645416 -29.940448 -21.784927  50.403964  -3.951397
  6  C    5.670637 -13.771977  11.197497  -2.170592  -3.951397  23.113002
  7  C   -2.368471   4.520858  -1.876877   3.499425  -0.519522  -7.927859
  8  C    3.312506  -3.573939  -3.129539 -10.956415   8.748864   3.823116
  9  C    0.162440  -0.289734   5.592396   6.933658 -12.189897   4.409154
 10  C   -3.343507   9.960665 -15.707165  -3.660435  12.451503 -13.740099
 11  C   -2.137517   0.528257  -0.204965  -0.301258   0.765361  -0.131752
 12  C   -0.405715  -0.088009  -0.309789   0.916487  -2.680927  -0.868771
 13  N    0.102560  -0.259407   0.722094  -0.120927   0.077803   0.158109
 14  O    0.059166  -0.135099   0.096783  -0.132418   0.162170   0.102621
 15  O   -0.062646   0.023060   0.114759   0.278693  -0.241966   0.015377
 16  O   -0.058322  -0.138147   0.987325   0.818457  -1.358885   0.063592
 17  H    0.507792  -0.140038   0.016560  -0.128940   0.021152   0.028290
 18  H   -0.086476   0.540700  -0.110184   0.017724   0.007861  -0.103123
 19  H    0.033190  -0.073743   0.540474  -0.012907  -0.133808   0.044608
 20  H    0.005440  -0.034457   0.051009   0.529675  -0.154654   0.008024
 21  H   -0.019796  -0.079858   0.047782   0.005869   0.014100   0.559033
 22  H   -0.026874   0.029725  -0.002529   0.054222   0.003866  -0.095650
 23  H    0.031361  -0.002835   0.010596  -0.094278   0.010861  -0.029353
 24  H   -0.004180   0.020435  -0.005261   0.005078  -0.007318  -0.091995
 25  H   -0.074821   0.015453   0.015835   0.057639  -0.030539   0.025977
 26  H   -0.069114   0.000728  -0.006205   0.014565   0.005894   0.051406
 27  H   -0.001564   0.004557  -0.027500   0.020038  -0.038110  -0.003442
 28  H   -0.004498   0.010249  -0.007601   0.003430  -0.013119  -0.025282
 29  H    0.028547  -0.048527   0.107602   0.015907  -0.075091   0.021334
               7          8          9         10         11         12
  1  C   -2.368471   3.312506   0.162440  -3.343507  -2.137517  -0.405715
  2  C    4.520858  -3.573939  -0.289734   9.960665   0.528257  -0.088009
  3  C   -1.876877  -3.129539   5.592396 -15.707165  -0.204965  -0.309789
  4  C    3.499425 -10.956415   6.933658  -3.660435  -0.301258   0.916487
  5  C   -0.519522   8.748864 -12.189897  12.451503   0.765361  -2.680927
  6  C   -7.927859   3.823116   4.409154 -13.740099  -0.131752  -0.868771
  7  C   17.500685  -8.551454   1.265796   4.502297  -3.730558  -0.690816
  8  C   -8.551454  29.748894 -27.236756   9.417983   0.954368   2.378653
  9  C    1.265796 -27.236756  79.725307 -35.399882  -0.621876 -15.062111
 10  C    4.502297   9.417983 -35.399882  38.371769   0.358439   2.839927
 11  C   -3.730558   0.954368  -0.621876   0.358439  12.371299  -0.940789
 12  C   -0.690816   2.378653 -15.062111   2.839927  -0.940789  20.852610
 13  N   -0.046464   0.603980  -1.196460   0.308492   0.009181  -1.383289
 14  O   -0.039446   0.842385  -3.025935   1.195818  -0.044684   0.419054
 15  O   -0.042202   0.445273  -0.885956   0.176155   0.004052  -0.033122
 16  O   -0.009083  -0.072229  -0.164045  -0.148297  -0.013246   0.126133
 17  H    0.016358   0.050624  -0.001042  -0.000543  -0.027261   0.005124
```

18	H	-0.000752	0.009118	-0.003910	0.070773	0.020940	0.000857
19	H	-0.005244	0.012799	-0.011555	-0.043351	-0.004759	0.000533
20	H	0.031000	-0.081558	-0.012016	-0.004554	-0.008495	0.015565
21	H	-0.104445	0.042993	-0.038933	-0.104565	0.050284	-0.010728
22	H	0.549043	-0.166377	-0.000238	0.028004	-0.029543	0.003786
23	H	-0.039439	0.569915	-0.291802	0.136894	0.026698	0.006305
24	H	0.015725	0.081527	-0.361136	0.667113	0.002243	0.003994
25	H	-0.106836	0.035521	-0.024552	0.006249	0.392571	0.004922
26	H	-0.168190	0.066969	-0.013064	-0.013077	0.448177	-0.000636
27	H	0.002643	-0.031452	0.053845	0.014368	-0.000275	0.080624
28	H	0.022167	-0.021230	0.219221	-0.112455	0.001113	-0.037863
29	H	-0.002995	0.001030	0.034707	-0.042296	0.002504	-0.050132

		13	14	15	16	17	18
1	C	0.102560	0.059166	-0.062646	-0.058322	0.507792	-0.086476
2	C	-0.259407	-0.135099	0.023060	-0.138147	-0.140038	0.540700
3	C	0.722094	0.096783	0.114759	0.987325	0.016560	-0.110184
4	C	-0.120927	-0.132418	0.278693	0.818457	-0.128940	0.017724
5	C	0.077803	0.162170	-0.241966	-1.358885	0.021152	0.007861
6	C	0.158109	0.102621	0.015377	0.063592	0.028290	-0.103123
7	C	-0.046464	-0.039446	-0.042202	-0.009083	0.016358	-0.000752
8	C	0.603980	0.842385	0.445273	-0.072229	0.050624	0.009118
9	C	-1.196460	-3.025935	-0.885956	-0.164045	-0.001042	-0.003910
10	C	0.308492	1.195818	0.176155	-0.148297	-0.000543	0.070773
11	C	0.009181	-0.044684	0.004052	-0.013246	-0.027261	0.020940
12	C	-1.383289	0.419054	-0.033122	0.126133	0.005124	0.000857
13	N	8.941765	0.138145	-0.069879	0.024937	0.000027	0.000135
14	O	0.138145	8.915661	0.037702	0.002217	0.000062	0.000037
15	O	-0.069879	0.037702	9.099916	0.026633	0.000055	-0.000004
16	O	0.024937	0.002217	0.026633	8.335760	0.000066	0.000305
17	H	0.000027	0.000062	0.000055	0.000066	0.370865	-0.000401
18	H	0.000135	0.000037	-0.000004	0.000305	-0.000401	0.355782
19	H	0.004196	0.000320	0.000548	0.001123	-0.000028	0.000043
20	H	0.000030	0.000373	-0.001178	0.003670	-0.000030	-0.000012
21	H	0.000006	0.003528	0.000002	-0.000056	-0.000005	-0.000475
22	H	-0.000019	0.004389	0.000150	-0.000017	-0.000013	-0.000008
23	H	0.001452	0.014531	-0.000662	0.001013	-0.000003	0.000000
24	H	0.020312	0.007873	0.001628	0.001240	0.000000	-0.000031
25	H	0.000015	-0.000054	0.000022	0.000234	-0.000182	-0.000020
26	H	-0.000018	-0.000113	-0.000001	-0.000037	-0.000446	0.000190
27	H	0.203299	-0.004182	-0.022186	-0.000884	0.000000	0.000000
28	H	0.008535	0.178557	-0.000431	0.000127	0.000000	0.000000
29	H	0.005859	-0.000046	-0.002438	0.231624	-0.000003	0.000003

		19	20	21	22	23	24
1	C	0.033190	0.005440	-0.019796	-0.026874	0.031361	-0.004180
2	C	-0.073743	-0.034457	-0.079858	0.029725	-0.002835	0.020435
3	C	0.540474	0.051009	0.047782	-0.002529	0.010596	-0.005261
4	C	-0.012907	0.529675	0.005869	0.054222	-0.094278	0.005078
5	C	-0.133808	-0.154654	0.014100	0.003866	0.010861	-0.007318
6	C	0.044608	0.008024	0.559033	-0.095650	-0.029353	-0.091995
7	C	-0.005244	0.031000	-0.104445	0.549043	-0.039439	0.015725
8	C	0.012799	-0.081558	0.042993	-0.166377	0.569915	0.081527
9	C	-0.011555	-0.012016	-0.038933	-0.000238	-0.291802	-0.361136
10	C	-0.043351	-0.004554	-0.104565	0.028004	0.136894	0.667113
11	C	-0.004759	-0.008495	0.050284	-0.029543	0.026698	0.002243

12	C	0.000533	0.015565	-0.010728	0.003786	0.006305	0.003994
13	N	0.004196	0.000030	0.000006	-0.000019	0.001452	0.020312
14	O	0.000320	0.000373	0.003528	0.004389	0.014531	0.007873
15	O	0.000548	-0.001178	0.000002	0.000150	-0.000662	0.001628
16	O	0.001123	0.003670	-0.000056	-0.000017	0.001013	0.001240
17	H	-0.000028	-0.000030	-0.000005	-0.000013	-0.000003	0.000000
18	H	0.000043	-0.000012	-0.000475	-0.000008	0.000000	-0.000031
19	H	0.345854	-0.000011	-0.000068	0.000000	-0.000001	-0.000526
20	H	-0.000011	0.326287	0.000000	-0.000007	0.000359	-0.000001
21	H	-0.000068	0.000000	0.360779	-0.000379	-0.000005	-0.000242
22	H	0.000000	-0.000007	-0.000379	0.346433	0.000256	0.000013
23	H	-0.000001	0.000359	-0.000005	0.000256	0.329625	-0.000006
24	H	-0.000526	-0.000001	-0.000242	0.000013	-0.000006	0.332086
25	H	0.000000	0.000097	-0.000029	-0.000345	0.000143	0.000000
26	H	0.000000	-0.000019	0.000023	-0.000364	-0.000058	0.000000
27	H	0.000015	0.000000	0.000000	0.000000	-0.000001	-0.000122
28	H	0.000000	0.000000	0.000010	-0.000055	-0.000028	0.000549
29	H	-0.000490	0.000026	0.000000	0.000000	-0.000001	0.000003

		25	26	27	28	29
1	C	-0.074821	-0.069114	-0.001564	-0.004498	0.028547
2	C	0.015453	0.000728	0.004557	0.010249	-0.048527
3	C	0.015835	-0.006205	-0.027500	-0.007601	0.107602
4	C	0.057639	0.014565	0.020038	0.003430	0.015907
5	C	-0.030539	0.005894	-0.038110	-0.013119	-0.075091
6	C	0.025977	0.051406	-0.003442	-0.025282	0.021334
7	C	-0.106836	-0.168190	0.002643	0.022167	-0.002995
8	C	0.035521	0.066969	-0.031452	-0.021230	0.001030
9	C	-0.024552	-0.013064	0.053845	0.219221	0.034707
10	C	0.006249	-0.013077	0.014368	-0.112455	-0.042296
11	C	0.392571	0.448177	-0.000275	0.001113	0.002504
12	C	0.004922	-0.000636	0.080624	-0.037863	-0.050132
13	N	0.000015	-0.000018	0.203299	0.008535	0.005859
14	O	-0.000054	-0.000113	-0.004182	0.178557	-0.000046
15	O	0.000022	-0.000001	-0.022186	-0.000431	-0.002438
16	O	0.000234	-0.000037	-0.000884	0.000127	0.231624
17	H	-0.000182	-0.000446	0.000000	0.000000	-0.000003
18	H	-0.000020	0.000190	0.000000	0.000000	0.000003
19	H	0.000000	0.000000	0.000015	0.000000	-0.000490
20	H	0.000097	-0.000019	0.000000	0.000000	0.000026
21	H	-0.000029	0.000023	0.000000	0.000010	0.000000
22	H	-0.000345	-0.000364	0.000000	-0.000055	0.000000
23	H	0.000143	-0.000058	-0.000001	-0.000028	-0.000001
24	H	0.000000	0.000000	-0.000122	0.000549	0.000003
25	H	0.420728	-0.015385	0.000000	0.000000	0.000000
26	H	-0.015385	0.425681	0.000000	0.000000	0.000000
27	H	0.000000	0.000000	0.398341	-0.000065	0.000088
28	H	0.000000	0.000000	-0.000065	0.308010	0.000000
29	H	0.000000	0.000000	0.000088	0.000000	0.237148

Total atomic charges:

		1
1	C	-0.092830
2	C	0.421605
3	C	-1.503965
4	C	-0.326481

```
 5  C    0.754774
 6  C   -0.380486
 7  C    0.304653
 8  C   -1.325570
 9  C    4.434375
10  C   -2.186222
11  C   -1.738508
12  C    0.908120
13  N   -1.254469
14  O   -0.799416
15  O   -0.861355
16  O   -0.661208
17  H    0.281958
18  H    0.280930
19  H    0.302787
20  H    0.325434
21  H    0.275175
22  H    0.302532
23  H    0.318462
24  H    0.310997
25  H    0.277358
26  H    0.273091
27  H    0.351964
28  H    0.470659
29  H    0.535636
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
                1
 1  C    0.189128
 2  C    0.702535
 3  C   -1.201178
 4  C   -0.001047
 5  C    0.754774
 6  C   -0.105311
 7  C    0.607185
 8  C   -1.007109
 9  C    4.434375
10  C   -1.875225
11  C   -1.188059
12  C    0.908120
13  N   -0.902505
14  O   -0.328757
15  O   -0.861355
16  O   -0.125571
17  H    0.000000
18  H    0.000000
19  H    0.000000
20  H    0.000000
21  H    0.000000
22  H    0.000000
23  H    0.000000
24  H    0.000000
25  H    0.000000
26  H    0.000000
```

```
 27  H    0.000000
 28  H    0.000000
 29  H    0.000000
 Sum of Mulliken charges=   0.00000
 Electronic spatial extent (au):  <R**2>=  2442.9915
 Charge=     0.0000 electrons
 Dipole moment (Debye):
    X=    -7.9227    Y=     4.5715    Z=     4.0043  Tot=     9.9851
 Quadrupole moment (Debye-Ang):
   XX=  -105.0876   YY=   -89.2325   ZZ=   -99.5697
   XY=     2.3331   XZ=     7.3982   YZ=     5.5563
 Octapole moment (Debye-Ang**2):
  XXX=   -29.6555  YYY=    33.9761  ZZZ=     4.4064  XYY=    20.3897
  XXY=     4.9731  XXZ=    12.2087  XZZ=   -30.4397  YZZ=     3.6747
  YYZ=    19.7979  XYZ=    11.4726
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -1701.8455 YYYY=  -917.5012 ZZZZ=  -600.9671 XXXY=    21.7487
 XXXZ=    12.5392 YYYX=    28.2536 YYYZ=    26.5790 ZZZX=    11.8347
 ZZZY=     5.8941 XXYY=  -376.4048 XXZZ=  -453.7360 YYZZ=  -246.8080
 XXYZ=    26.3886 YYXZ=    29.7331 ZZXY=     3.3020
 N-N= 1.230530757024D+03 E-N=-4.184483225196D+03  KE= 7.353024291196D+02
  Exact polarizability: 134.230   5.473 119.055   7.720  -0.852 116.572
 Approx polarizability: 113.412   5.740 114.081   5.621  -2.378 118.245
 Full mass-weighted force constant matrix:
 Low frequencies ---  -93.7040   -0.8408   -0.1394    0.0001    0.0004
0.0007
 Low frequencies ---    0.5655  128.1886  146.1503
 ******    1 imaginary frequencies (negative Signs) ******
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                      1                      2                      3
                     ?A                     ?A                     ?A
 Frequencies --   -93.7040               128.1886               146.1503
 Red. masses --     8.7073                 5.2364                 6.2084
 Frc consts  --     0.0450                 0.0507                 0.0781
 IR Inten    --     2.4717                 6.2856                 2.5549
 Raman Activ --     1.7431                 0.1967                 0.2722
 Depolar     --     0.7479                 0.6936                 0.7433
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.02   0.01   0.05     0.15   0.06  -0.04     0.03   0.00  -
0.08
   2   6    -0.03  -0.04   0.04     0.10   0.06  -0.02    -0.09  -0.01  -
0.05
   3   6    -0.05  -0.02   0.06     0.14  -0.10  -0.01    -0.12   0.03
0.08
   4   6    -0.02   0.05   0.06     0.15  -0.11  -0.03     0.08   0.00
0.04
   5   6     0.00  -0.02   0.08     0.13  -0.08  -0.02     0.00   0.01
0.11
   6   6    -0.01  -0.04  -0.02    -0.04   0.02   0.01    -0.05   0.00  -
0.03
```

7	6	0.00	0.01	-0.03	-0.07	0.01	0.02	0.03	-0.01	-0.04
8	6	-0.01	0.04	-0.01	-0.01	-0.12	0.01	0.05	-0.02	0.04
9	6	0.00	0.03	-0.01	-0.02	-0.13	0.01	0.01	0.02	0.08
10	6	-0.01	-0.02	0.00	-0.01	-0.11	0.01	-0.05	0.04	0.06
11	6	-0.01	0.02	0.00	0.03	0.11	-0.01	0.07	0.00	-0.13
12	6	-0.01	0.05	-0.05	-0.11	0.03	0.01	-0.02	0.00	-0.11
13	7	-0.19	0.48	0.06	-0.12	0.20	0.01	0.17	0.00	-0.25
14	8	-0.01	0.03	-0.06	0.07	-0.11	-0.01	0.03	0.02	0.23
15	8	0.16	-0.37	-0.18	-0.19	0.07	0.01	-0.22	-0.03	-0.16
16	8	0.15	-0.14	0.07	-0.10	0.10	0.04	0.08	-0.04	0.20
17	1	-0.03	0.00	0.07	0.24	0.11	-0.07	0.04	0.00	-0.12
18	1	-0.05	-0.08	0.04	0.13	0.14	-0.04	-0.16	-0.03	-0.11
19	1	-0.05	-0.06	0.07	0.18	-0.12	-0.02	-0.21	0.03	0.11
20	1	-0.02	0.08	0.07	0.20	-0.13	-0.04	0.18	0.00	0.05
21	1	0.00	-0.07	-0.04	-0.11	0.09	0.02	-0.06	-0.01	-0.05
22	1	0.01	0.02	-0.07	-0.17	0.01	0.04	0.04	-0.01	-0.04
23	1	0.01	0.08	-0.01	-0.03	-0.17	0.02	0.10	0.00	0.05
24	1	-0.01	-0.04	-0.01	-0.05	-0.16	0.01	-0.10	0.04	0.08
25	1	0.00	0.05	0.00	0.04	0.10	-0.02	0.17	-0.01	-0.15
26	1	-0.01	-0.01	-0.01	0.00	0.21	-0.02	0.02	0.01	-0.22
27	1	-0.18	0.46	0.04	-0.19	0.35	0.00	0.14	-0.01	-0.42
28	1	0.01	-0.02	-0.14	0.06	-0.09	0.01	0.08	0.09	0.18
29	1	0.21	-0.26	0.07	-0.20	0.21	0.08	0.00	-0.07	0.29

	4	5	6
	?A	?A	?A
Frequencies --	166.7187	268.0693	305.3670
Red. masses --	6.3063	5.2632	4.7247
Frc consts --	0.1033	0.2228	0.2596
IR Inten --	17.9955	24.0529	1.1365
Raman Activ --	0.5748	1.3923	0.8008
Depolar --	0.4821	0.6879	0.6033

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.03	-0.01	0.00	-0.01	0.06	0.00	0.02	0.01	0.07
2	6	-0.02	0.00	-0.01	-0.04	0.05	0.01	0.04	-0.07	0.03
3	6	-0.03	-0.01	-0.03	-0.03	-0.02	0.02	0.02	-0.02	0.00
4	6	-0.05	0.00	-0.01	-0.01	-0.04	0.00	0.00	-0.01	0.01
5	6	0.05	-0.08	-0.05	-0.02	-0.04	0.02	0.01	-0.01	0.01
6	6	-0.03	0.00	0.01	-0.10	0.04	0.00	0.07	-0.06	-0.08
7	6	-0.04	-0.01	0.01	-0.13	0.03	0.02	-0.04	0.00	-0.09
8	6	-0.04	-0.02	0.00	-0.08	-0.06	0.00	-0.03	-0.04	-0.12
9	6	-0.02	0.00	0.01	-0.01	0.02	-0.02	-0.01	-0.01	-0.12
10	6	-0.03	-0.02	0.01	-0.07	-0.02	-0.01	0.05	0.02	-0.13
11	6	-0.04	-0.01	0.02	-0.09	0.10	0.02	-0.05	0.07	0.05
12	6	-0.07	0.11	0.04	-0.01	0.03	-0.03	0.00	0.01	-0.11
13	7	-0.04	0.07	0.03	-0.02	-0.13	0.00	-0.14	-0.01	0.00
14	8	0.10	0.03	-0.03	0.42	0.08	0.00	-0.04	-0.04	0.33
15	8	-0.15	0.27	0.10	0.12	-0.09	-0.04	0.13	0.13	-0.04
16	8	0.33	-0.29	-0.09	-0.05	-0.03	0.01	0.00	-0.01	0.02
17	1	-0.04	-0.01	0.00	0.05	0.10	-0.01	0.06	0.04	0.13
18	1	-0.01	0.01	0.00	-0.04	0.08	0.00	0.04	-0.13	0.07
19	1	-0.01	0.01	-0.04	-0.01	-0.03	0.02	0.06	-0.07	0.01
20	1	-0.05	-0.03	-0.02	0.02	-0.04	0.01	-0.04	0.04	0.03
21	1	-0.04	0.01	0.02	-0.11	0.06	0.02	0.14	-0.11	-0.08
22	1	-0.04	-0.02	0.02	-0.21	0.03	0.03	-0.12	0.01	-0.12
23	1	-0.04	-0.02	0.00	-0.12	-0.08	-0.01	-0.08	0.02	-0.15
24	1	-0.03	-0.01	0.01	-0.09	-0.05	-0.01	0.10	-0.01	-0.18
25	1	-0.05	-0.02	0.02	-0.11	0.11	0.02	-0.16	0.13	0.06
26	1	-0.03	-0.01	0.03	-0.09	0.16	0.04	-0.01	0.06	0.13

```
  27   1    -0.07   0.13   0.04     0.05  -0.28   0.04    -0.13   0.03
0.15
  28   1     0.09   0.09   0.03     0.49   0.42   0.08    -0.13   0.09
0.62
  29   1     0.52  -0.53  -0.16    -0.09   0.03   0.02    -0.01   0.00
0.03
                     7                      8                      9
                    ?A                     ?A                     ?A
 Frequencies --   329.3095               372.7468               385.8272
 Red. masses --     4.1254                 6.2958                 3.2833
 Frc consts  --     0.2636                 0.5154                 0.2880
 IR Inten    --     9.8276                16.8683                28.6117
 Raman Activ --     0.6120                 2.8397                 1.1760
 Depolar     --     0.4726                 0.2858                 0.6605
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.02   0.05   0.12     0.01   0.04  -0.05     0.06  -0.02
0.02
   2   6     0.00  -0.08   0.08    -0.05   0.05  -0.02    -0.04   0.00
0.05
   3   6     0.02  -0.06   0.05    -0.05  -0.06   0.03    -0.04   0.05
0.13
   4   6    -0.05   0.05   0.08     0.02  -0.12  -0.03     0.08  -0.07
0.11
   5   6    -0.02  -0.01   0.01    -0.03  -0.14   0.01     0.01  -0.03
0.11
   6   6    -0.03  -0.07  -0.08    -0.11   0.03   0.02    -0.01   0.01
0.07
   7   6     0.00   0.06  -0.13    -0.13   0.01   0.04     0.00  -0.03
0.07
   8   6     0.05   0.06   0.01    -0.05  -0.08   0.03    -0.01  -0.05
0.05
   9   6     0.02  -0.02   0.07     0.04  -0.01   0.02    -0.02   0.03  -
0.03
  10   6    -0.03  -0.08   0.03    -0.06  -0.04   0.03     0.01   0.03
0.03
  11   6     0.02   0.14  -0.09    -0.10   0.08   0.03     0.12   0.01  -
0.12
  12   6     0.02  -0.01   0.07     0.20   0.07  -0.01    -0.03   0.03  -
0.09
  13   7     0.13   0.05   0.00     0.29   0.15  -0.09    -0.12  -0.05  -
0.03
  14   8     0.03  -0.02   0.09    -0.14  -0.04  -0.02    -0.04   0.04  -
0.09
  15   8    -0.08  -0.05   0.04     0.26   0.15   0.01     0.07   0.07  -
0.06
  16   8    -0.08  -0.02  -0.25    -0.09  -0.12   0.02    -0.03  -0.04  -
0.13
  17   1     0.01   0.08   0.21     0.11   0.09  -0.10     0.10   0.00  -
0.02
  18   1     0.02  -0.15   0.14    -0.07   0.10  -0.06    -0.10  -0.01
0.00
  19   1     0.05  -0.08   0.05    -0.04  -0.03   0.01    -0.08   0.02
0.16
```

20	1	-0.11	0.09	0.09	0.10	-0.12	-0.01	0.15	-0.05
0.13									
21	1	-0.05	-0.14	-0.16	-0.14	0.08	0.04	0.03	0.01
0.10									
22	1	-0.04	0.08	-0.22	-0.22	0.01	0.07	-0.02	-0.03
0.10									
23	1	0.13	0.15	0.00	-0.08	-0.16	0.04	-0.06	-0.06
0.04									
24	1	-0.10	-0.12	0.05	-0.12	-0.08	0.05	0.04	0.02
0.00									
25	1	0.14	0.31	-0.10	-0.17	0.04	0.04	0.44	0.05
-0.17									
26	1	-0.03	0.04	-0.22	-0.08	0.17	0.11	-0.04	0.04
-0.41									
27	1	0.09	0.08	-0.12	0.23	0.23	-0.25	-0.07	-0.09
0.09									
28	1	0.11	0.00	-0.08	-0.11	-0.22	-0.21	-0.25	-0.02
0.35									
29	1	0.11	0.08	-0.45	-0.15	-0.05	0.04	-0.04	0.20
-0.22									

	10			11			12		
	?A			?A			?A		
Frequencies --	414.2597			451.0823			478.4809		
Red. masses --	1.2029			2.4030			5.8478		
Frc consts --	0.1216			0.2881			0.7888		
IR Inten --	120.2800			11.7845			14.2323		
Raman Activ --	1.2555			1.1791			5.9818		
Depolar --	0.7450			0.0885			0.1886		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.00	0.00	0.09	0.00	-0.05	0.03	-0.01	0.00
2 6	-0.01	0.00	0.01	-0.02	-0.02	-0.05	0.12	-0.02	0.00
3 6	-0.01	0.02	0.01	-0.06	0.02	0.09	0.17	-0.17	-0.05
4 6	0.01	0.00	0.02	0.12	-0.06	0.01	-0.03	-0.03	-0.11
5 6	0.00	0.01	0.02	0.03	-0.04	0.08	0.06	-0.20	-0.11
6 6	0.01	0.01	0.01	0.02	-0.03	-0.07	0.00	-0.05	0.03
7 6	0.00	0.00	0.02	0.04	-0.01	-0.07	0.01	-0.02	0.02
8 6	-0.01	-0.01	0.00	0.05	0.02	-0.04	-0.04	0.06	0.01
9 6	-0.01	-0.01	-0.02	-0.02	0.06	0.01	-0.09	0.22	0.06
10 6	0.01	0.01	-0.01	-0.02	0.02	0.02	0.00	-0.05	0.07
11 6	0.02	0.00	-0.03	-0.04	0.00	0.15	0.06	0.00	-0.06
12 6	-0.01	0.00	-0.02	-0.03	0.03	0.01	-0.06	0.13	0.03

13	7	-0.05	-0.02	0.00	-0.03	-0.03	0.01	-0.02	-0.05	0.00
14	8	-0.02	-0.03	0.07	-0.04	0.08	-0.02	-0.12	0.30	0.08
15	8	0.03	0.03	-0.01	-0.04	-0.02	-0.01	0.00	-0.04	-0.03
16	8	0.01	0.00	-0.01	-0.02	-0.04	-0.08	-0.09	-0.09	0.07
17	1	0.00	-0.01	-0.01	0.15	0.03	-0.08	0.02	-0.01	0.05
18	1	-0.02	0.00	0.00	-0.11	-0.07	-0.11	0.21	0.06	0.04
19	1	-0.02	0.01	0.02	-0.13	0.02	0.12	0.24	-0.05	-0.16
20	1	0.02	0.00	0.02	0.21	0.00	0.05	-0.07	0.00	-0.10
21	1	0.02	0.01	0.02	0.00	-0.05	-0.10	-0.07	0.00	0.03
22	1	0.00	-0.01	0.03	0.03	0.00	-0.11	0.04	-0.01	-0.02
23	1	-0.04	0.00	-0.01	0.13	0.01	-0.01	0.07	-0.07	0.08
24	1	0.04	0.00	-0.03	-0.02	-0.03	0.00	0.07	-0.16	-0.02
25	1	0.08	0.00	-0.04	-0.47	-0.08	0.21	0.25	0.03	-0.09
26	1	-0.01	0.00	-0.08	0.15	0.05	0.54	-0.03	0.00	-0.24
27	1	-0.05	0.01	0.04	0.00	-0.08	0.03	0.09	-0.29	0.01
28	1	0.40	0.04	-0.89	0.02	0.06	-0.18	-0.01	0.29	-0.17
29	1	-0.01	0.04	-0.01	-0.10	0.20	-0.10	-0.09	-0.20	0.11

		13			14			15		
		?A			?A			?A		
Frequencies --		523.6577			543.6393			597.9060		
Red. masses --		3.2159			6.3984			5.0693		
Frc consts --		0.5196			1.1142			1.0677		
IR Inten --		8.1324			1.9604			5.4347		
Raman Activ --		2.9809			5.6346			1.7300		
Depolar --		0.3491			0.2464			0.6823		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.06	0.01	0.09	-0.07	0.08	-0.03	0.05	0.07	-0.02
2	6	-0.01	-0.08	0.06	0.00	0.21	0.04	-0.01	-0.10	-0.05
3	6	-0.12	0.12	-0.06	0.05	-0.01	0.06	-0.13	-0.06	-0.11
4	6	0.02	-0.11	-0.06	-0.06	0.01	0.00	0.01	0.10	-0.11
5	6	-0.08	-0.02	-0.08	-0.17	-0.19	0.05	-0.09	0.02	-0.14

```
   6   6     0.11  -0.04   0.02     0.07   0.22  -0.04    -0.02  -0.12
0.07
   7   6    -0.03   0.00  -0.01     0.18   0.14  -0.03     0.07   0.08
0.03
   8   6     0.01  -0.09  -0.04     0.11   0.07  -0.07     0.09   0.08
0.18
   9   6     0.03   0.02  -0.02     0.08  -0.05  -0.04     0.05  -0.04
0.16
  10   6     0.08   0.13  -0.05     0.06   0.06  -0.01     0.03  -0.06
0.21
  11   6     0.02   0.16  -0.01     0.09  -0.02   0.02     0.06   0.13
0.07
  12   6     0.02  -0.01   0.05     0.03  -0.08  -0.04    -0.01   0.00  -
0.12
  13   7     0.03   0.00   0.05    -0.07  -0.02   0.03    -0.15  -0.05  -
0.04
  14   8    -0.01   0.03  -0.05     0.04  -0.09   0.01     0.02  -0.09  -
0.01
  15   8    -0.09  -0.04   0.04    -0.07   0.01  -0.02     0.08   0.08  -
0.11
  16   8     0.00  -0.08   0.05    -0.21  -0.26   0.05    -0.03  -0.01
0.00
  17   1     0.17   0.09   0.16    -0.09   0.04  -0.19     0.05   0.09
0.10
  18   1    -0.07  -0.15   0.04     0.02   0.19   0.07    -0.04  -0.07  -
0.09
  19   1    -0.11   0.19  -0.11     0.19   0.07  -0.04    -0.25   0.12  -
0.17
  20   1    -0.08  -0.13  -0.08     0.04   0.14   0.08    -0.01  -0.03  -
0.17
  21   1     0.26  -0.12   0.05     0.01   0.18  -0.12    -0.13  -0.14  -
0.02
  22   1    -0.19   0.03  -0.04     0.24   0.11   0.12     0.07   0.12  -
0.16
  23   1     0.01  -0.15  -0.02     0.09   0.12  -0.09     0.20   0.02
0.23
  24   1     0.16   0.25  -0.04    -0.01  -0.02  -0.01    -0.03   0.08
0.30
  25   1     0.14   0.25  -0.03     0.03  -0.02   0.03    -0.07   0.05
0.09
  26   1    -0.05   0.18  -0.14     0.15  -0.19   0.07     0.12   0.17
0.20
  27   1     0.02   0.03   0.05    -0.09   0.08   0.18    -0.11  -0.04
0.17
  28   1    -0.01  -0.03  -0.10     0.03  -0.08   0.02    -0.01  -0.14
0.01
  29   1    -0.38   0.06   0.31    -0.16  -0.30   0.01     0.03  -0.21
0.02
                      16                    17                    18
                      ?A                    ?A                    ?A
 Frequencies --    633.0410              674.5839              692.6373
 Red. masses --      3.3845                2.8854                2.0437
 Frc consts  --      0.7991                0.7736                0.5777
 IR Inten    --     11.3665               83.0578               86.0918
```

Raman Activ --		1.2205			3.4208			7.1407		
Depolar --		0.6621			0.2888			0.1257		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.04	-0.05	0.19	0.05	0.02	0.03	0.08	-0.01	0.03
2	6	-0.03	0.08	0.12	-0.06	0.01	0.06	-0.01	0.01	0.03
3	6	0.02	0.06	-0.04	-0.11	-0.08	-0.05	-0.02	0.02	0.00
4	6	-0.02	-0.13	0.02	0.06	0.09	-0.06	0.01	-0.01	-0.02
5	6	0.08	-0.01	-0.09	0.02	-0.01	-0.04	-0.06	0.02	-0.01
6	6	-0.11	0.07	-0.07	-0.08	-0.04	0.09	0.00	0.00	0.01
7	6	0.08	-0.01	-0.13	0.07	0.05	0.11	0.04	-0.02	-0.01
8	6	0.10	-0.07	-0.02	-0.02	0.09	-0.07	0.02	-0.05	-0.05
9	6	-0.01	-0.01	0.07	-0.05	-0.01	-0.09	-0.06	-0.01	-0.02
10	6	-0.15	0.02	0.04	-0.09	-0.06	-0.09	-0.04	0.04	-0.02
11	6	0.04	-0.05	0.02	0.14	-0.03	0.08	0.09	0.02	0.04
12	6	-0.02	0.03	-0.03	-0.03	-0.02	0.03	-0.13	-0.03	0.03
13	7	-0.04	-0.02	-0.04	0.04	0.02	-0.03	0.00	0.02	-0.09
14	8	-0.01	0.00	-0.03	0.01	-0.01	0.03	0.00	0.01	-0.01
15	8	0.06	0.03	-0.04	0.01	-0.01	0.05	0.06	-0.01	0.09
16	8	0.07	0.04	0.02	0.04	-0.04	-0.05	-0.06	0.03	0.03
17	1	-0.01	-0.05	0.07	-0.03	-0.03	0.03	0.09	-0.01	0.00
18	1	0.05	0.08	0.21	-0.06	0.11	0.00	-0.04	0.03	-0.02
19	1	0.15	0.07	-0.09	-0.05	-0.19	-0.01	0.02	0.03	-0.03
20	1	-0.27	-0.16	-0.03	0.02	0.17	-0.03	-0.03	0.00	-0.01
21	1	-0.18	0.00	-0.19	-0.06	-0.10	0.04	0.03	-0.04	-0.01
22	1	0.06	-0.03	-0.03	0.16	0.05	0.08	-0.02	-0.01	0.00
23	1	0.30	-0.05	0.03	-0.21	0.03	-0.10	0.04	-0.05	-0.04
24	1	-0.30	0.01	0.13	0.02	-0.03	-0.15	-0.01	0.04	-0.04
25	1	-0.03	0.19	0.04	0.19	-0.11	0.07	0.06	0.05	0.05

26	1	0.09	-0.27	0.04	0.13	-0.01	0.05	0.10	0.04	0.07
27	1	-0.03	-0.03	-0.01	-0.04	0.12	-0.16	-0.04	-0.02	-0.41
28	1	-0.01	-0.05	-0.06	0.03	0.12	0.09	0.02	0.06	-0.01
29	1	-0.28	0.20	0.25	-0.50	0.42	0.23	0.57	-0.53	-0.28

	19	20	21
	?A	?A	?A
Frequencies --	712.3710	794.5435	816.8337
Red. masses --	2.8570	4.9363	3.5728
Frc consts --	0.8542	1.8361	1.4045
IR Inten --	125.0144	19.6893	4.2089
Raman Activ --	0.5172	2.6385	7.5836
Depolar --	0.1353	0.7471	0.1383

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.06	-0.01	0.03	0.08	0.01	-0.01	-0.07	-0.01	-0.07
2	6	-0.06	0.03	0.05	0.19	0.01	-0.09	-0.13	0.00	0.16
3	6	-0.04	-0.06	-0.03	0.02	0.08	0.04	0.04	-0.04	-0.04
4	6	0.02	-0.01	-0.01	-0.10	0.08	0.00	0.13	-0.05	-0.02
5	6	-0.04	0.04	-0.01	-0.19	0.14	0.06	0.00	0.00	-0.01
6	6	-0.08	-0.01	0.02	0.01	0.05	-0.08	0.05	-0.04	0.09
7	6	0.01	-0.02	0.06	-0.01	-0.09	0.00	0.01	0.13	-0.01
8	6	0.04	-0.06	-0.03	-0.02	-0.10	-0.01	0.06	0.05	0.03
9	6	0.06	0.02	-0.05	-0.03	0.00	0.01	0.00	-0.01	0.01
10	6	-0.08	-0.03	-0.11	-0.01	-0.11	-0.01	0.03	0.03	-0.07
11	6	0.08	0.02	0.05	0.11	0.01	0.05	-0.12	-0.02	-0.08
12	6	0.16	0.08	-0.02	-0.12	0.33	0.08	-0.12	0.23	0.07
13	7	0.02	-0.02	0.13	0.03	-0.03	0.01	0.01	-0.02	-0.01
14	8	-0.03	0.02	0.01	-0.02	-0.13	0.00	-0.01	-0.10	0.00
15	8	-0.10	-0.01	-0.12	0.03	-0.04	-0.04	0.02	-0.04	-0.01
16	8	-0.02	0.06	0.01	0.02	-0.08	-0.02	0.01	0.01	0.00
17	1	0.07	-0.01	-0.03	-0.04	-0.05	0.06	0.05	0.05	-0.14
18	1	-0.07	0.12	0.00	0.14	-0.07	-0.11	-0.07	0.09	0.17

19	1	0.04	-0.16	0.00	-0.04	0.06	0.07	0.28	-0.17	-0.05
20	1	-0.05	-0.02	-0.02	-0.09	0.08	0.00	0.23	-0.10	-0.03
21	1	-0.04	-0.04	0.02	-0.14	0.24	-0.02	0.26	-0.28	0.02
22	1	-0.05	-0.02	0.09	-0.12	-0.08	0.03	0.13	0.12	-0.02
23	1	-0.05	-0.08	-0.05	0.02	-0.03	-0.02	0.08	0.00	0.05
24	1	-0.10	-0.04	-0.10	-0.05	-0.16	0.00	0.11	0.13	-0.07
25	1	0.07	0.02	0.06	0.12	0.04	0.05	-0.19	-0.11	-0.07
26	1	0.08	0.04	0.06	0.08	0.08	0.03	-0.07	-0.06	0.01
27	1	0.17	-0.18	0.51	0.21	-0.45	-0.07	0.16	-0.43	-0.14
28	1	-0.02	-0.07	-0.07	-0.04	-0.13	0.06	-0.02	-0.11	0.03
29	1	0.46	-0.36	-0.23	-0.32	0.15	0.19	0.06	-0.05	-0.02

	22			23			24		
	?A			?A			?A		
Frequencies --	824.4228			829.0544			849.9853		
Red. masses --	3.8979			4.9244			4.5263		
Frc consts --	1.5609			1.9942			1.9267		
IR Inten --	21.2986			1.8852			5.5829		
Raman Activ --	9.0217			7.3110			5.2583		
Depolar --	0.0657			0.0497			0.0311		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.10	0.07	0.06	0.16	-0.19	0.01	-0.08	0.04	-0.08
2 6	-0.06	-0.03	-0.05	0.13	-0.02	0.13	-0.01	0.04	0.15
3 6	-0.09	0.01	0.10	0.04	0.17	0.07	-0.02	-0.09	0.20
4 6	-0.01	0.05	-0.10	0.09	0.09	-0.13	-0.02	0.00	-0.22
5 6	0.22	-0.16	-0.04	-0.06	0.00	0.00	-0.13	0.14	0.00
6 6	0.08	0.03	-0.01	-0.12	-0.02	0.18	0.03	0.04	0.03
7 6	0.05	0.03	0.02	-0.08	-0.02	-0.10	0.01	0.06	0.01
8 6	-0.09	-0.05	-0.18	0.00	0.12	-0.18	0.11	-0.18	-0.12
9 6	-0.04	0.00	-0.02	-0.06	0.00	-0.02	0.04	0.02	0.01
10 6	0.03	0.03	0.17	-0.05	0.00	0.13	0.09	-0.17	0.08
11 6	0.03	-0.01	0.04	-0.12	-0.07	-0.09	-0.04	0.02	-0.02

12	6	-0.01	0.11	0.03	0.07	-0.03	-0.02	-0.01	-0.07	-0.01
13	7	0.03	0.01	0.04	0.02	0.01	0.04	-0.02	-0.01	-0.03
14	8	0.01	-0.11	-0.01	0.02	-0.07	0.00	-0.02	0.10	0.01
15	8	0.00	-0.01	-0.03	-0.02	0.02	-0.04	0.00	0.00	0.03
16	8	-0.02	0.08	0.01	-0.04	-0.04	0.01	0.09	0.05	-0.03
17	1	-0.17	0.04	0.10	0.18	-0.15	0.19	-0.09	0.03	-0.13
18	1	-0.12	-0.22	0.00	0.08	0.23	-0.04	-0.08	-0.02	0.13
19	1	-0.37	0.28	0.04	0.09	0.34	-0.05	0.00	-0.11	0.22
20	1	-0.04	0.21	-0.03	0.05	0.34	-0.02	-0.02	0.02	-0.22
21	1	-0.02	0.03	-0.09	-0.19	-0.02	0.15	-0.05	-0.03	-0.09
22	1	-0.01	0.03	0.08	0.12	-0.03	-0.12	-0.16	0.04	0.18
23	1	-0.16	-0.17	-0.17	0.05	0.08	-0.16	0.23	-0.38	-0.03
24	1	0.06	-0.08	0.10	0.05	0.06	0.10	0.13	-0.39	-0.03
25	1	0.17	-0.01	0.01	-0.15	0.05	-0.08	-0.02	-0.03	-0.03
26	1	-0.02	-0.12	-0.11	-0.13	0.06	-0.05	-0.04	-0.05	-0.04
27	1	0.17	-0.30	0.04	0.04	0.03	0.16	-0.13	0.23	-0.04
28	1	0.02	-0.05	0.01	0.05	0.08	0.04	-0.06	-0.01	-0.01
29	1	0.22	-0.01	-0.16	0.04	-0.13	-0.02	-0.04	0.07	0.07

	25	26	27
	?A	?A	?A
Frequencies --	872.7682	884.4599	906.5579
Red. masses --	3.0760	2.4070	2.7712
Frc consts --	1.3805	1.1094	1.3419
IR Inten --	3.7605	20.1781	6.4014
Raman Activ --	9.6915	2.1676	1.8875
Depolar --	0.0126	0.5177	0.5837

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.07	-0.09	0.00	-0.03	0.03	-0.11	0.05	0.07
2	6	-0.12	0.07	0.05	0.02	0.14	-0.06	0.12	0.00	0.02
3	6	0.12	0.00	0.04	-0.10	-0.11	-0.05	-0.07	-0.03	-0.10
4	6	-0.06	0.16	-0.01	-0.07	-0.03	0.08	0.18	0.16	-0.02

```
    5   6     0.02  -0.03   0.01     0.04   0.00   0.03     0.00  -0.02
0.05
    6   6     0.03  -0.14   0.05    -0.04  -0.02   0.14    -0.03   0.01  -
0.03
    7   6    -0.06  -0.16  -0.07     0.01  -0.06  -0.09    -0.06  -0.05
0.01
    8   6    -0.01  -0.09  -0.03     0.07  -0.01  -0.05     0.08  -0.11
0.00
    9   6    -0.01   0.00   0.06     0.01   0.00  -0.03     0.04  -0.01
0.05
   10   6    -0.04   0.12   0.04     0.13   0.00   0.03    -0.02   0.05  -
0.05
   11   6     0.11   0.03   0.03    -0.02   0.04  -0.02    -0.04  -0.06
0.01
   12   6     0.01  -0.01  -0.01    -0.02   0.03   0.01    -0.02   0.00
0.00
   13   7     0.00   0.00   0.00     0.00   0.00   0.00    -0.01  -0.01  -
0.02
   14   8     0.01  -0.02  -0.02    -0.01   0.00   0.00    -0.01   0.04  -
0.01
   15   8     0.00   0.01  -0.01     0.00  -0.01   0.01     0.00   0.00
0.00
   16   8     0.00  -0.02  -0.01     0.01   0.01  -0.01    -0.04  -0.04  -
0.01
   17   1    -0.21  -0.06  -0.22     0.02  -0.03  -0.07    -0.26  -0.01
0.20
   18   1    -0.15   0.15  -0.01     0.15   0.46  -0.09     0.34  -0.02
0.23
   19   1     0.41  -0.07  -0.03    -0.37  -0.14   0.06    -0.21  -0.05  -
0.04
   20   1     0.00   0.23   0.03    -0.20   0.01   0.08     0.50   0.23
0.06
   21   1     0.26  -0.22   0.14    -0.13   0.07   0.16    -0.03   0.08
0.03
   22   1    -0.28  -0.11  -0.23    -0.05  -0.05  -0.13    -0.16  -0.06
0.09
   23   1     0.14   0.00  -0.02     0.20   0.12  -0.06     0.18  -0.11
0.03
   24   1    -0.08   0.16   0.08     0.45   0.14  -0.10    -0.06   0.18
0.03
   25   1    -0.02  -0.02   0.04    -0.10   0.19  -0.01     0.05   0.00
0.00
   26   1     0.12   0.15   0.12     0.01   0.00   0.02    -0.08  -0.16  -
0.09
   27   1    -0.01   0.04   0.04     0.02  -0.07  -0.05    -0.04   0.06  -
0.01
   28   1     0.01  -0.05  -0.03    -0.01  -0.02   0.01    -0.03  -0.09  -
0.05
   29   1    -0.15   0.13   0.06     0.01   0.09  -0.04     0.06   0.03  -
0.13
                     28                    29                    30
                     ?A                    ?A                    ?A
 Frequencies --    912.7355              939.0494              969.6632
 Red. masses --      2.5180                1.4242                2.9782
```

Frc consts	--	1.2359			0.7399			1.6498		
IR Inten	--	7.3086			66.0449			17.5208		
Raman Activ	--	2.8515			0.3991			3.4562		
Depolar	--	0.3538			0.5128			0.5379		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.08	-0.11	0.05	-0.01	0.01	-0.01	0.08	-0.01	0.04
2	6	-0.08	-0.07	-0.08	-0.01	-0.01	-0.01	0.06	0.18	0.06
3	6	0.02	-0.09	0.01	0.01	0.03	-0.01	-0.13	-0.09	0.08
4	6	-0.04	0.09	-0.01	0.00	-0.02	0.02	0.01	-0.01	-0.09
5	6	0.03	-0.02	0.00	0.01	-0.02	0.00	0.00	0.00	-0.05
6	6	0.05	0.13	0.02	0.00	-0.01	0.02	0.14	-0.02	-0.12
7	6	-0.02	-0.01	0.08	0.01	0.01	0.00	-0.07	-0.08	-0.02
8	6	0.13	0.00	-0.06	-0.01	0.00	-0.01	-0.07	0.12	0.07
9	6	0.05	0.01	0.05	0.00	-0.01	-0.02	0.01	0.03	0.05
10	6	-0.04	0.06	-0.04	0.00	-0.01	0.01	-0.02	0.02	-0.03
11	6	-0.10	0.04	-0.01	0.01	0.01	0.00	-0.05	-0.07	0.04
12	6	-0.03	0.02	0.01	-0.04	0.11	0.04	-0.01	0.01	0.01
13	7	-0.02	-0.02	-0.03	0.04	-0.11	-0.01	0.00	-0.02	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	0.01	-0.05	0.00
15	8	0.01	0.00	0.00	0.01	-0.04	-0.03	0.01	0.00	-0.01
16	8	0.00	-0.01	-0.01	0.00	0.01	0.01	0.00	0.02	0.00
17	1	0.14	-0.05	0.22	0.00	0.01	-0.01	0.10	-0.01	-0.10
18	1	-0.28	-0.12	-0.25	0.01	0.00	0.00	0.03	0.27	-0.01
19	1	0.13	-0.22	0.04	-0.01	0.07	-0.03	-0.20	-0.11	0.12
20	1	-0.28	0.26	0.05	0.01	-0.01	0.02	-0.04	-0.09	-0.13
21	1	0.17	0.20	0.16	-0.03	-0.02	0.01	0.46	-0.13	0.01
22	1	0.00	-0.06	0.30	0.00	0.02	-0.03	0.09	-0.08	-0.09
23	1	0.28	0.01	-0.02	-0.03	0.01	-0.02	0.04	0.12	0.10
24	1	-0.21	-0.01	0.03	0.03	0.02	0.00	-0.32	-0.19	0.05

```
  25   1    -0.02   0.08  -0.02    -0.01   0.00   0.00     0.24   0.04  -
0.01
  26   1    -0.16   0.20  -0.07     0.02  -0.01   0.01    -0.21   0.02  -
0.24
  27   1    -0.07   0.08  -0.03    -0.36   0.88   0.19    -0.08   0.18
0.04
  28   1    -0.02  -0.10  -0.02    -0.02  -0.01   0.03     0.02  -0.02
0.02
  29   1    -0.06   0.09   0.00     0.08  -0.05  -0.05     0.05  -0.06  -
0.01
                      31                      32                      33
                      ?A                      ?A                      ?A
 Frequencies --    986.1105                999.1749                1012.1796
 Red. masses --      3.0328                  2.7821                   2.5328
 Frc consts  --      1.7376                  1.6365                   1.5289
 IR Inten    --     11.1453                 24.0880                  10.3551
 Raman Activ --      4.9210                  3.9242                   8.7158
 Depolar     --      0.4233                  0.1271                   0.3627
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.12  -0.03   0.03     0.04   0.07   0.06     0.08   0.19  -
0.03
   2   6     0.03  -0.03   0.06    -0.12   0.01   0.08     0.04   0.01
0.04
   3   6    -0.02  -0.16   0.03    -0.03   0.03   0.02    -0.03   0.04  -
0.02
   4   6    -0.03   0.07  -0.01     0.08   0.09   0.02    -0.08   0.02
0.06
   5   6    -0.02   0.03  -0.01     0.01  -0.04  -0.12     0.02  -0.01
0.00
   6   6    -0.05   0.07  -0.07    -0.04   0.11  -0.02    -0.01  -0.08
0.00
   7   6     0.02   0.09  -0.06    -0.05  -0.17  -0.05     0.12  -0.09
0.09
   8   6    -0.15  -0.11   0.07    -0.02   0.03   0.09     0.03  -0.05  -
0.05
   9   6    -0.03  -0.01   0.04     0.04   0.00  -0.05     0.04   0.00  -
0.02
  10   6     0.08   0.18   0.04     0.14  -0.10  -0.01    -0.06  -0.02
0.00
  11   6     0.03  -0.07  -0.10     0.02  -0.04  -0.06    -0.12  -0.03  -
0.11
  12   6     0.00   0.01   0.00    -0.02   0.02   0.01    -0.01   0.00
0.00
  13   7     0.02  -0.01   0.02     0.00   0.00   0.00    -0.01   0.00  -
0.01
  14   8     0.01  -0.01  -0.02    -0.01   0.02   0.02     0.00   0.01
0.00
  15   8     0.00   0.00  -0.01     0.00  -0.01   0.02     0.00   0.00
0.01
  16   8     0.01   0.00  -0.01    -0.02   0.01  -0.01    -0.01   0.00
0.00
  17   1     0.14   0.00   0.15     0.04   0.05  -0.01     0.40   0.41
0.08
```

18	1	-0.03	0.00	-0.01	-0.31	-0.30	0.06	0.17	0.06
0.14									
19	1	0.04	-0.30	0.09	0.09	0.24	-0.14	-0.07	0.10
-0.04									
20	1	-0.12	0.06	-0.03	0.08	-0.03	-0.03	-0.20	0.09
0.08									
21	1	-0.17	-0.03	-0.25	-0.12	0.33	0.13	0.03	-0.18
-0.06									
22	1	0.11	0.06	0.07	0.05	-0.20	0.03	0.35	-0.16
0.24									
23	1	-0.33	-0.22	0.05	0.02	0.24	0.03	-0.05	-0.02
-0.08									
24	1	0.16	0.30	0.04	0.22	-0.27	-0.13	-0.11	0.01
0.04									
25	1	-0.32	-0.09	-0.05	-0.25	0.03	-0.01	-0.21	-0.25
-0.10									
26	1	0.22	-0.14	0.24	0.10	0.06	0.15	-0.08	0.08
0.02									
27	1	-0.03	0.13	0.06	-0.01	0.00	-0.04	0.00	-0.04
-0.04									
28	1	0.00	-0.03	-0.02	-0.02	-0.02	0.02	-0.02	-0.07
-0.02									
29	1	-0.02	0.03	0.01	-0.06	-0.22	0.12	-0.02	0.01
0.00									

	34			35			36		
	?A			?A			?A		
Frequencies --	1013.1272			1031.9619			1041.1135		
Red. masses --	2.3960			2.0299			2.1522		
Frc consts --	1.4490			1.2737			1.3744		
IR Inten --	28.6823			1.4858			45.1807		
Raman Activ --	6.1926			4.6614			5.2802		
Depolar --	0.4262			0.6047			0.6018		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.05	-0.12	-0.08	-0.04	0.00	0.01	0.02	-0.06	0.09
2 6	0.01	0.02	0.09	0.04	-0.02	-0.02	-0.07	0.10	-0.09
3 6	-0.07	0.04	-0.08	-0.03	0.00	0.01	0.04	0.09	0.02
4 6	-0.04	0.07	0.12	-0.01	0.01	-0.02	0.02	0.07	-0.03
5 6	0.05	-0.05	-0.03	0.01	-0.01	0.00	0.00	-0.02	0.01
6 6	0.07	0.03	-0.04	0.11	0.07	0.14	-0.01	-0.09	-0.02
7 6	-0.10	0.12	0.01	0.07	0.00	-0.08	0.05	0.06	0.00
8 6	0.00	-0.05	-0.02	-0.04	-0.05	0.06	-0.03	-0.08	0.07
9 6	0.05	-0.04	0.01	-0.06	-0.01	0.00	0.10	-0.03	-0.02
10 6	0.01	-0.10	0.02	-0.11	-0.05	-0.05	0.03	-0.07	-0.02

```
  11   6     0.06  -0.01  -0.04     0.03   0.04  -0.10    -0.06  -0.01
0.00
  12   6    -0.01   0.01   0.00     0.02  -0.01  -0.01    -0.02   0.02
0.00
  13   7    -0.01   0.00  -0.01     0.02   0.01   0.01    -0.02   0.00  -
0.02
  14   8    -0.01   0.06   0.01     0.00   0.01   0.00    -0.01   0.06
0.01
  15   8     0.00   0.00   0.00     0.00   0.01  -0.02     0.00  -0.01
0.02
  16   8    -0.01   0.01   0.00     0.00   0.00   0.00    -0.02  -0.01
0.00
  17   1    -0.03  -0.19  -0.26    -0.11  -0.01   0.20    -0.03  -0.06
0.26
  18   1     0.14   0.12   0.16     0.05   0.05  -0.04    -0.23   0.40  -
0.39
  19   1    -0.22   0.24  -0.14    -0.14  -0.01   0.05     0.10   0.16  -
0.04
  20   1    -0.21   0.17   0.16     0.10  -0.08  -0.05     0.06   0.12
0.00
  21   1     0.21  -0.20  -0.15     0.41   0.12   0.40     0.04  -0.24  -
0.11
  22   1    -0.32   0.12   0.12     0.13   0.00  -0.12     0.15   0.06  -
0.09
  23   1    -0.02   0.07  -0.06    -0.07  -0.10   0.07    -0.30  -0.24
0.05
  24   1    -0.19  -0.15   0.11    -0.25  -0.21  -0.04     0.01  -0.11  -
0.03
  25   1    -0.11  -0.24  -0.01    -0.37   0.16  -0.04     0.01   0.20  -
0.01
  26   1     0.13   0.17   0.18     0.23  -0.12   0.23    -0.06  -0.18  -
0.08
  27   1     0.01  -0.05  -0.02     0.02   0.01   0.04     0.00  -0.07  -
0.07
  28   1    -0.04  -0.09  -0.02     0.02   0.12   0.01    -0.07  -0.20  -
0.04
  29   1    -0.03   0.01   0.01     0.01   0.02  -0.02    -0.02   0.00
0.00
                     37                    38                    39
                     ?A                    ?A                    ?A
 Frequencies --  1050.8313             1068.4450             1102.6062
 Red. masses --     4.3405                1.6967                1.9885
 Frc consts  --     2.8239                1.1412                1.4243
 IR Inten    --    13.3804                1.3449               60.1678
 Raman Activ --     1.5503                4.9732                8.2212
 Depolar     --     0.6946                0.7489                0.6892
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.03  -0.02  -0.06    -0.04  -0.11  -0.04    -0.01   0.03  -
0.01
   2   6     0.12  -0.06   0.05     0.01   0.01   0.05     0.02  -0.03
0.00
   3   6    -0.03   0.09   0.18    -0.01  -0.02  -0.01     0.00  -0.05
0.01
```

4	6	-0.15	0.00	-0.14	0.01	0.01	-0.02	0.01	-0.06	-0.01
5	6	0.14	-0.11	0.00	0.01	-0.01	0.01	-0.03	0.02	0.00
6	6	-0.18	-0.05	0.00	-0.01	0.01	-0.05	-0.01	0.02	0.06
7	6	-0.06	0.02	0.04	0.09	-0.09	0.04	-0.02	-0.02	-0.04
8	6	0.11	0.05	0.14	-0.04	0.01	0.01	-0.05	0.06	-0.08
9	6	0.15	0.08	-0.03	0.03	0.01	-0.02	0.19	-0.08	-0.01
10	6	0.00	0.09	-0.18	0.00	0.02	0.02	-0.03	0.04	0.05
11	6	0.06	0.02	-0.04	-0.02	0.13	-0.01	0.03	-0.02	0.01
12	6	-0.03	0.01	0.01	-0.01	0.01	0.00	-0.03	0.03	0.01
13	7	-0.04	-0.01	-0.04	0.00	0.00	0.00	-0.04	-0.01	-0.03
14	8	0.01	-0.05	0.00	0.00	0.00	0.00	0.01	0.07	0.02
15	8	-0.01	-0.02	0.04	0.00	-0.01	0.01	0.00	-0.01	0.02
16	8	-0.02	0.01	0.02	0.01	0.00	0.00	0.02	0.01	-0.01
17	1	-0.18	-0.09	0.06	-0.28	-0.28	-0.23	0.04	0.06	-0.01
18	1	0.13	-0.03	0.04	0.12	-0.01	0.17	0.03	-0.09	0.04
19	1	-0.15	0.12	0.21	-0.03	-0.01	-0.01	0.01	-0.09	0.03
20	1	-0.23	-0.05	-0.17	0.11	0.00	-0.01	0.03	-0.06	-0.01
21	1	-0.09	0.03	0.15	-0.09	-0.04	-0.15	0.00	0.20	0.25
22	1	-0.14	0.07	-0.13	0.41	-0.16	0.20	-0.06	0.02	-0.23
23	1	0.09	-0.16	0.20	-0.22	-0.04	-0.02	-0.42	0.16	-0.21
24	1	0.06	-0.08	-0.30	-0.05	0.04	0.06	-0.33	0.10	0.27
25	1	-0.18	-0.09	-0.01	-0.13	0.39	0.01	0.01	-0.02	0.01
26	1	0.18	0.02	0.18	-0.06	0.41	0.03	0.04	-0.08	0.01
27	1	-0.05	-0.03	-0.11	-0.01	-0.01	-0.02	-0.01	-0.10	-0.09
28	1	-0.03	-0.25	-0.03	-0.01	-0.05	-0.01	-0.12	-0.48	-0.09
29	1	0.09	0.13	-0.12	0.02	0.05	-0.03	-0.01	-0.04	0.04

	40	41	42
	?A	?A	?A

Frequencies --	1128.9317			1163.9017			1193.4705		
Red. masses --	2.0167			1.8916			2.0676		
Frc consts --	1.5144			1.5097			1.7351		
IR Inten --	48.6786			49.1745			50.9431		
Raman Activ --	2.6487			2.3217			3.2532		
Depolar --	0.6457			0.6199			0.6530		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.04	-0.02	0.01	0.03	-0.01	-0.07	0.01	-0.02	0.02
2 6	0.03	0.00	-0.05	0.05	-0.01	0.02	-0.06	0.01	-0.02
3 6	0.06	-0.07	0.10	-0.04	0.01	0.04	0.06	-0.05	-0.05
4 6	0.05	0.02	0.10	-0.02	0.07	0.06	0.06	-0.01	0.02
5 6	-0.04	0.01	-0.12	0.03	-0.03	-0.06	-0.03	0.04	0.02
6 6	-0.02	-0.05	0.00	0.00	0.00	0.05	-0.01	-0.01	0.00
7 6	0.00	0.02	0.05	0.05	0.05	-0.06	0.00	0.01	0.00
8 6	0.06	-0.03	-0.01	0.01	-0.08	0.05	-0.01	-0.02	0.00
9 6	0.00	0.02	-0.07	-0.03	-0.08	0.01	0.04	0.21	0.01
10 6	-0.04	0.11	0.03	-0.04	0.02	-0.05	-0.01	0.01	0.02
11 6	-0.01	0.02	-0.03	-0.08	-0.01	0.10	-0.01	0.00	0.01
12 6	0.00	0.00	0.00	0.00	0.00	0.00	0.04	-0.01	-0.02
13 7	0.00	0.00	0.00	0.01	0.00	0.01	-0.04	0.00	-0.06
14 8	0.00	-0.02	-0.01	0.00	0.04	0.00	0.01	-0.09	0.00
15 8	0.00	-0.01	0.00	0.01	0.01	-0.02	-0.02	-0.02	0.07
16 8	0.01	0.03	-0.05	0.00	0.02	-0.02	0.01	-0.01	0.00
17 1	-0.11	-0.05	0.10	0.09	-0.03	-0.38	0.20	0.04	-0.30
18 1	0.05	0.14	-0.11	-0.06	-0.31	0.08	0.15	-0.12	0.25
19 1	-0.29	0.20	0.08	0.01	-0.02	0.05	-0.25	0.24	-0.11
20 1	0.20	-0.18	0.02	-0.07	0.11	0.07	-0.21	0.30	0.14
21 1	0.03	-0.14	-0.06	-0.11	0.20	0.15	0.05	0.16	0.20
22 1	-0.11	0.02	0.11	0.25	0.10	-0.39	0.03	0.06	-0.25
23 1	-0.04	0.26	-0.13	-0.05	-0.08	0.03	-0.19	-0.36	0.06

24	1	-0.09	-0.23	-0.08	0.12	0.00	-0.16	-0.06	-0.23	-0.06
25	1	-0.08	-0.04	-0.02	0.28	0.09	0.04	0.00	0.07	0.01
26	1	0.03	0.04	0.05	-0.25	-0.01	-0.24	0.01	-0.13	-0.01
27	1	-0.01	0.01	-0.03	0.02	-0.01	0.01	-0.03	0.04	0.11
28	1	0.03	0.08	0.01	-0.02	-0.03	-0.02	0.02	-0.04	0.01
29	1	-0.25	-0.47	0.38	-0.11	-0.21	0.17	0.00	0.01	0.00

	43			44			45		
	?A			?A			?A		
Frequencies --	1210.6883			1223.8748			1234.6298		
Red. masses --	1.9724			2.0036			2.0489		
Frc consts --	1.7034			1.7682			1.8401		
IR Inten --	50.6338			6.9933			95.5091		
Raman Activ --	7.4589			3.3713			4.7458		
Depolar --	0.6649			0.4962			0.3864		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.03	-0.01	0.00	-0.04	-0.02	0.08	-0.01	0.03	0.02
2	6	0.07	0.03	-0.02	0.02	0.11	-0.06	-0.05	-0.03	-0.02
3	6	-0.09	0.06	0.01	-0.02	0.02	0.03	0.07	0.01	0.01
4	6	0.01	-0.03	0.06	0.07	-0.02	-0.02	0.02	-0.04	-0.01
5	6	0.01	-0.03	-0.04	-0.01	0.01	-0.01	-0.01	0.02	0.01
6	6	0.04	-0.02	0.01	0.04	-0.10	-0.05	-0.04	0.01	0.00
7	6	0.00	0.01	0.01	-0.03	0.00	0.09	-0.02	0.00	0.00
8	6	-0.05	0.00	-0.06	0.07	0.05	0.01	-0.06	0.04	-0.06
9	6	0.01	0.14	0.11	-0.02	-0.09	-0.03	-0.03	-0.02	0.16
10	6	-0.03	-0.07	-0.02	0.00	0.00	0.02	0.02	-0.01	-0.08
11	6	0.01	0.01	-0.03	0.02	0.01	-0.09	0.03	-0.01	0.00
12	6	0.03	-0.01	-0.02	-0.03	0.00	0.01	-0.04	-0.05	0.03
13	7	-0.03	0.00	-0.06	0.02	0.00	0.05	0.02	-0.01	0.09
14	8	0.02	-0.04	0.00	-0.02	0.02	0.00	0.04	0.03	0.00
15	8	0.00	-0.01	0.04	0.01	0.02	-0.05	0.02	0.05	-0.10
16	8	0.00	0.04	-0.03	-0.01	-0.01	-0.01	0.00	0.00	-0.02

17	1	-0.13	-0.05	0.08	-0.01	-0.05	-0.20	-0.04	0.00	-0.02
18	1	-0.11	-0.06	-0.14	0.00	-0.32	0.14	0.13	0.11	0.08
19	1	0.45	-0.45	0.11	0.17	-0.16	0.07	-0.37	0.13	0.10
20	1	0.13	0.07	0.12	-0.41	0.31	0.09	-0.08	0.19	0.09
21	1	-0.08	0.04	-0.02	-0.09	0.21	0.16	0.13	-0.08	0.03
22	1	-0.01	0.00	0.08	-0.05	0.05	-0.12	0.25	-0.04	0.09
23	1	0.00	-0.01	-0.05	-0.16	-0.26	0.04	0.09	-0.13	0.03
24	1	0.22	0.16	-0.07	0.00	0.14	0.08	0.21	-0.10	-0.23
25	1	-0.07	-0.04	-0.02	-0.25	-0.03	-0.05	0.00	-0.03	0.01
26	1	0.04	0.06	0.05	0.13	0.01	0.15	0.02	0.15	0.05
27	1	-0.01	0.03	0.16	-0.01	0.00	-0.15	-0.06	0.03	-0.32
28	1	-0.04	-0.29	-0.03	0.04	0.23	0.02	-0.10	-0.49	-0.05
29	1	-0.10	-0.34	0.22	-0.02	-0.10	0.04	-0.07	-0.17	0.12

		46			47			48		
		?A			?A			?A		
Frequencies --		1247.2491			1266.9687			1272.5277		
Red. masses --		2.0974			1.0686			1.4051		
Frc consts --		1.9223			1.0107			1.3406		
IR Inten --		35.3946			8.9856			35.2196		
Raman Activ --		4.9034			12.9816			1.4383		
Depolar --		0.3794			0.7455			0.5272		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	-0.03	-0.02	0.00	0.01	-0.02	-0.03	0.00	-0.04
2	6	0.03	0.01	0.02	0.02	-0.03	-0.01	-0.02	-0.06	0.02
3	6	-0.05	-0.01	-0.03	0.00	0.01	0.01	-0.02	0.03	-0.01
4	6	-0.01	0.03	0.03	-0.01	0.01	-0.02	-0.01	-0.02	0.00
5	6	0.00	0.00	-0.01	0.01	-0.01	0.00	0.01	-0.03	0.02
6	6	0.02	0.00	0.01	-0.02	-0.01	0.02	-0.05	0.05	-0.02
7	6	0.02	0.00	0.00	-0.01	-0.01	0.01	0.01	-0.03	-0.02
8	6	0.01	-0.04	0.02	-0.02	0.03	0.01	-0.01	0.01	0.01
9	6	0.04	0.15	-0.07	0.00	-0.01	0.01	0.02	0.02	-0.04

```
  10   6    -0.03  -0.01   0.05     0.00  -0.01  -0.01     0.09  -0.02
0.00
  11   6    -0.03   0.01   0.00     0.00   0.00   0.01     0.01   0.02
0.03
  12   6    -0.05  -0.07   0.04     0.00   0.00   0.00    -0.01   0.00
0.00
  13   7     0.02  -0.03   0.15     0.00   0.00   0.00     0.00  -0.01
0.04
  14   8     0.01  -0.04   0.01     0.00   0.00   0.00    -0.02  -0.02
0.00
  15   8     0.00   0.04  -0.10     0.00   0.00   0.00     0.00   0.00  -
0.01
  16   8     0.00  -0.01   0.02     0.00   0.01  -0.01     0.01   0.04  -
0.04
  17   1     0.08   0.02  -0.01     0.19   0.07  -0.34     0.08   0.09
0.15
  18   1    -0.09  -0.08  -0.05     0.00  -0.05  -0.02     0.14   0.32  -
0.03
  19   1     0.26  -0.03  -0.14    -0.03  -0.04   0.05     0.05  -0.20
0.11
  20   1     0.14  -0.16  -0.04    -0.02   0.14   0.04     0.04   0.29
0.16
  21   1    -0.08   0.06   0.00     0.09  -0.16  -0.05     0.09  -0.01
0.03
  22   1    -0.21   0.04  -0.04    -0.17  -0.07   0.41     0.05  -0.01  -
0.15
  23   1    -0.07   0.09  -0.04     0.03   0.10   0.00     0.06  -0.26
0.11
  24   1    -0.03  -0.09   0.01    -0.01   0.09   0.04    -0.33   0.06
0.28
  25   1     0.01   0.06   0.00    -0.08   0.52   0.02     0.09  -0.08
0.02
  26   1    -0.01  -0.19  -0.04     0.10  -0.50  -0.03    -0.01   0.00  -
0.02
  27   1    -0.17   0.09  -0.72     0.01  -0.01   0.01    -0.04   0.02  -
0.19
  28   1    -0.01  -0.15  -0.01     0.00   0.01   0.00     0.07   0.33
0.04
  29   1     0.06   0.18  -0.12    -0.04  -0.09   0.07    -0.12  -0.31
0.22
                     49                    50                    51
                     ?A                    ?A                    ?A
 Frequencies --  1301.5624             1312.0261             1333.9489
 Red. masses --     1.6715                2.0446                1.5069
 Frc consts  --     1.6683                2.0736                1.5799
 IR Inten    --    28.6168                7.2493               10.1768
 Raman Activ --     1.1935                1.7804                0.8796
 Depolar     --     0.6871                0.6951                0.7044
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.02   0.07   0.01    -0.08  -0.09  -0.06     0.04  -0.01  -
0.01
   2   6     0.06  -0.01   0.00     0.03   0.02   0.05     0.00   0.04
0.05
```

3	6	-0.03	-0.02	-0.01	-0.04	-0.02	0.00	0.04	-0.03	-0.03
4	6	-0.01	-0.03	0.06	0.01	0.00	0.02	-0.10	0.00	0.00
5	6	-0.01	0.01	-0.02	-0.01	0.00	-0.03	0.00	-0.02	0.03
6	6	-0.09	-0.05	-0.01	-0.06	-0.01	-0.06	-0.02	0.02	-0.07
7	6	-0.05	0.07	0.02	0.10	-0.06	0.07	-0.02	-0.01	0.01
8	6	0.02	-0.03	-0.08	-0.01	0.02	-0.04	0.09	0.03	-0.02
9	6	-0.01	0.02	0.05	-0.06	-0.05	0.13	0.01	0.00	0.04
10	6	0.11	0.02	-0.02	0.07	0.04	-0.04	-0.04	-0.06	0.02
11	6	0.01	-0.05	0.00	-0.01	0.10	0.00	0.00	-0.02	0.00
12	6	0.00	0.00	0.00	-0.01	-0.01	0.00	-0.01	-0.01	0.01
13	7	0.00	0.00	0.00	0.01	0.01	-0.02	0.00	0.00	0.00
14	8	-0.01	-0.01	-0.01	0.00	0.01	-0.01	-0.01	-0.01	-0.01
15	8	0.00	0.00	0.00	0.01	0.01	-0.01	0.00	0.01	-0.01
16	8	0.00	-0.01	0.02	0.01	0.00	0.02	0.01	0.03	-0.02
17	1	-0.30	-0.14	-0.17	0.36	0.20	0.18	-0.01	-0.02	0.13
18	1	-0.26	-0.10	-0.25	-0.10	0.10	-0.11	-0.18	-0.15	-0.02
19	1	0.15	0.11	-0.16	0.12	0.14	-0.15	-0.24	0.13	-0.02
20	1	0.05	-0.09	0.04	0.10	0.12	0.09	0.42	-0.10	0.01
21	1	0.22	-0.01	0.27	0.05	0.13	0.14	0.28	0.02	0.15
22	1	0.42	0.01	0.06	-0.28	0.04	-0.20	-0.05	0.01	-0.07
23	1	0.05	-0.04	-0.07	-0.23	0.12	-0.13	-0.38	-0.24	-0.06
24	1	-0.31	-0.17	0.15	-0.04	-0.35	-0.15	0.31	0.39	0.01
25	1	-0.05	0.22	0.01	0.02	-0.13	0.00	-0.02	0.10	0.00
26	1	0.00	0.04	0.01	0.08	-0.31	0.01	0.00	-0.03	0.00
27	1	-0.01	0.01	0.00	0.05	-0.01	0.18	-0.01	0.00	-0.02
28	1	0.04	0.17	0.02	0.00	0.02	0.01	0.03	0.17	0.02
29	1	0.07	0.16	-0.11	0.06	0.17	-0.10	-0.06	-0.09	0.09

		52			53			54		
		?A			?A			?A		
Frequencies --		1346.4415			1354.1370			1370.7503		
Red. masses --		1.4729			1.5493			1.5748		
Frc consts --		1.5733			1.6739			1.7434		
IR Inten --		6.5439			7.8016			16.5015		
Raman Activ --		2.1818			1.6004			3.2319		
Depolar --		0.7383			0.2814			0.1559		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	-0.03	0.02	-0.08	0.01	-0.04	0.00	-0.02	0.01
2	6	0.00	0.08	0.04	0.10	0.02	0.04	0.01	0.05	-0.02
3	6	0.04	-0.02	-0.03	0.01	-0.06	0.00	0.06	0.05	-0.01
4	6	-0.06	-0.01	-0.02	0.06	-0.06	0.01	0.05	0.04	-0.01
5	6	0.00	-0.01	0.02	-0.02	0.00	-0.01	0.04	0.04	-0.03
6	6	0.04	-0.07	0.03	-0.03	0.06	0.02	-0.08	0.04	0.04
7	6	0.03	0.02	0.04	-0.01	-0.03	-0.03	0.07	-0.02	0.00
8	6	-0.09	0.00	-0.02	-0.02	0.01	0.05	-0.03	-0.04	-0.02
9	6	0.01	0.00	-0.01	0.02	0.00	-0.06	0.02	0.04	0.05
10	6	0.03	0.00	-0.07	-0.06	-0.01	0.02	0.05	-0.05	-0.03
11	6	0.00	0.02	-0.03	0.02	0.03	0.01	-0.03	0.02	0.00
12	6	0.00	0.00	0.00	0.01	0.01	-0.01	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00
14	8	0.00	0.00	0.01	0.01	0.00	0.01	-0.02	-0.01	-0.01
15	8	0.00	0.00	0.00	-0.01	-0.01	0.01	0.00	0.00	0.00
16	8	0.01	0.02	-0.01	0.01	0.01	0.00	-0.04	-0.05	0.01
17	1	0.07	-0.01	0.01	-0.03	0.07	0.12	-0.02	-0.04	-0.04
18	1	-0.28	-0.27	-0.04	-0.41	-0.17	-0.34	-0.13	-0.34	0.05
19	1	-0.29	0.12	0.01	-0.05	0.22	-0.15	-0.30	-0.28	0.31
20	1	0.36	0.07	0.07	-0.26	0.39	0.20	-0.24	-0.20	-0.16
21	1	-0.37	0.17	-0.04	0.19	-0.29	-0.15	0.23	-0.30	-0.05
22	1	-0.05	0.04	-0.04	0.07	-0.06	0.02	-0.17	0.03	-0.12

23	1	0.47	-0.01	0.13	0.12	-0.05	0.10	-0.10	0.25	-0.12
24	1	-0.31	0.12	0.17	0.14	0.19	-0.01	-0.12	0.15	0.16
25	1	-0.04	-0.04	-0.03	0.05	-0.15	0.01	0.03	-0.17	-0.01
26	1	0.05	-0.04	0.04	0.00	0.03	-0.01	-0.05	0.04	-0.03
27	1	0.00	0.00	-0.02	-0.01	0.00	-0.04	-0.02	0.01	-0.05
28	1	0.00	-0.04	-0.01	-0.02	-0.09	-0.01	0.04	0.19	0.02
29	1	-0.03	-0.05	0.05	0.04	0.06	-0.04	0.00	-0.03	-0.04

	55	56	57
	?A	?A	?A
Frequencies --	1381.9348	1392.1228	1405.0164
Red. masses --	1.4844	1.3429	1.6144
Frc consts --	1.6702	1.5334	1.8776
IR Inten --	44.8592	1.2677	11.3396
Raman Activ --	2.5783	1.5350	2.7209
Depolar --	0.6699	0.7461	0.6625

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.06	0.00	0.00	-0.01	0.00	0.08	0.03	-0.01
2	6	0.02	-0.06	0.07	-0.01	-0.04	0.04	-0.02	0.02	-0.05
3	6	0.03	0.00	0.00	0.02	-0.01	0.03	-0.03	-0.04	0.03
4	6	0.03	-0.02	0.01	0.05	0.02	-0.01	0.00	-0.06	-0.04
5	6	0.01	0.02	-0.03	0.00	-0.01	0.01	-0.04	-0.04	0.04
6	6	0.09	-0.01	0.04	0.00	-0.04	-0.09	-0.03	0.00	0.02
7	6	0.01	-0.03	-0.04	0.02	0.03	0.00	0.09	0.02	-0.02
8	6	0.03	0.02	0.00	-0.04	-0.04	0.00	-0.04	-0.02	0.03
9	6	0.03	0.01	0.09	0.00	0.02	-0.01	0.05	-0.01	0.05
10	6	-0.02	0.00	-0.06	-0.02	-0.05	0.00	0.00	0.00	-0.04
11	6	-0.01	-0.02	0.00	-0.02	0.07	0.00	-0.04	-0.03	0.00
12	6	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.00
13	7	-0.01	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.01
14	8	-0.02	-0.02	-0.02	0.00	0.00	0.00	-0.02	-0.01	-0.01
15	8	0.00	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00

```
  16   8    -0.01  -0.02   0.01     0.00   0.00   0.00     0.03   0.04  -
0.02
  17   1    -0.19  -0.07  -0.14    -0.08  -0.07  -0.11    -0.36  -0.20
0.18
  18   1    -0.21   0.28  -0.31     0.01   0.31  -0.11     0.20  -0.13
0.23
  19   1    -0.20   0.03   0.06    -0.06   0.13  -0.02     0.21   0.28  -
0.25
  20   1    -0.15   0.07   0.04    -0.23  -0.10  -0.10    -0.06   0.28
0.12
  21   1    -0.46   0.18  -0.19     0.09   0.39   0.38     0.07  -0.03
0.07
  22   1    -0.21  -0.04   0.11     0.14  -0.01   0.14    -0.35   0.05
0.08
  23   1    -0.38  -0.08  -0.07     0.16   0.25  -0.04    -0.01   0.32  -
0.07
  24   1    -0.08   0.01  -0.03     0.12   0.42   0.12     0.05   0.03  -
0.06
  25   1    -0.04   0.00   0.00     0.07  -0.22  -0.01     0.01   0.04  -
0.02
  26   1    -0.06   0.06  -0.06     0.05  -0.23   0.00    -0.09   0.08  -
0.04
  27   1    -0.02   0.00  -0.07    -0.01   0.00  -0.03    -0.03   0.00  -
0.10
  28   1     0.06   0.29   0.04     0.00   0.00  -0.01     0.05   0.25
0.03
  29   1     0.03   0.03  -0.05    -0.01  -0.01   0.00    -0.01  -0.03
0.06
                     58                    59                    60
                     ?A                    ?A                    ?A
 Frequencies --  1410.6105             1423.6679             1433.5309
 Red. masses --     1.6211                1.4586                1.4296
 Frc consts  --     1.9006                1.7418                1.7309
 IR Inten    --     7.8287                2.6597                2.0491
 Raman Activ --     6.9527                1.1073                1.2463
 Depolar     --     0.6296                0.7330                0.7473
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.08  -0.06   0.00    -0.05  -0.01   0.13     0.03   0.03
0.06
   2   6    -0.01   0.04  -0.04     0.03  -0.04  -0.04     0.00  -0.04
0.02
   3   6     0.00   0.00   0.04    -0.01  -0.01   0.02     0.02   0.04  -
0.05
   4   6    -0.01   0.00  -0.03    -0.03   0.02  -0.01    -0.05  -0.06  -
0.06
   5   6    -0.03  -0.03  -0.02    -0.03  -0.02  -0.01    -0.02  -0.02  -
0.02
   6   6     0.03  -0.03   0.03    -0.04   0.01   0.01     0.00   0.03  -
0.03
   7   6    -0.10   0.03  -0.05     0.08   0.01  -0.06    -0.02   0.00
0.06
   8   6     0.01  -0.06   0.01    -0.02   0.02   0.01     0.02  -0.06
0.04
```

```
    9   6     0.06   0.01   0.07     0.01  -0.01   0.00     0.01   0.00  -
0.01
   10   6    -0.01  -0.01  -0.04     0.00   0.00   0.00    -0.02   0.01
0.05
   11   6     0.06   0.00   0.02     0.00  -0.02  -0.02    -0.01   0.02  -
0.03
   12   6     0.02   0.01   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   13   7    -0.02  -0.01   0.01     0.00   0.00   0.00     0.00   0.00
0.00
   14   8    -0.03  -0.01  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
   15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   16   8     0.02   0.02   0.01     0.01   0.01   0.00     0.01   0.01
0.01
   17   1     0.43   0.26   0.12     0.26   0.05  -0.57    -0.10  -0.11  -
0.28
   18   1     0.09  -0.09   0.13     0.00   0.08  -0.13    -0.05   0.10  -
0.10
   19   1     0.03   0.06   0.00     0.12   0.05  -0.06    -0.12  -0.27
0.19
   20   1     0.11   0.09   0.03     0.28  -0.02   0.00     0.26   0.41
0.19
   21   1    -0.12   0.00  -0.04     0.17  -0.04   0.12     0.05  -0.02  -
0.04
   22   1     0.44  -0.07   0.20    -0.28   0.00   0.20     0.14   0.06  -
0.30
   23   1    -0.14   0.33  -0.15     0.01  -0.16   0.07     0.01   0.46  -
0.12
   24   1     0.02   0.10  -0.01     0.03   0.04   0.00     0.13  -0.17  -
0.11
   25   1     0.06  -0.04   0.03     0.02  -0.28  -0.02    -0.04  -0.08  -
0.02
   26   1     0.05   0.15   0.06    -0.07   0.40   0.04     0.04  -0.09
0.03
   27   1    -0.05   0.00  -0.16     0.00   0.00  -0.02     0.00   0.00  -
0.02
   28   1     0.06   0.34   0.04     0.00   0.02   0.00     0.00   0.02
0.01
   29   1     0.05   0.12  -0.06     0.03   0.06  -0.03     0.05   0.09  -
0.06
                      61                    62                    63
                      ?A                    ?A                    ?A
 Frequencies --   1436.5801             1455.8154             1477.8733
 Red. masses --      1.4989                1.4812                2.0402
 Frc consts  --      1.8226                1.8496                2.6254
 IR Inten    --      5.3706               13.7548              100.5505
 Raman Activ --      3.4663                1.3773                4.5740
 Depolar     --      0.7407                0.6764                0.1576
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.02  -0.01  -0.02     0.05   0.00   0.05     0.01  -0.01  -
0.03
```

2	6	0.00	0.04	0.03	0.00	0.00	-0.04	0.00	-0.01	0.00
3	6	0.01	0.03	-0.07	-0.02	-0.02	0.01	0.00	0.01	0.01
4	6	-0.02	-0.03	-0.01	-0.02	0.01	0.01	0.01	0.01	0.07
5	6	0.02	0.03	0.01	0.00	-0.01	0.03	0.00	0.04	-0.09
6	6	-0.02	-0.08	-0.01	0.01	0.04	0.05	-0.01	0.01	-0.03
7	6	0.01	0.03	-0.12	-0.06	-0.05	-0.02	0.01	0.00	0.04
8	6	0.01	0.01	0.03	0.02	0.03	-0.02	-0.12	0.04	-0.07
9	6	0.01	-0.01	-0.03	0.02	-0.01	0.03	0.16	-0.07	0.04
10	6	0.00	0.05	0.06	0.00	0.01	-0.02	-0.08	0.02	0.04
11	6	-0.01	0.04	0.03	-0.03	0.13	-0.01	0.00	0.00	-0.01
12	6	0.00	0.01	0.00	0.00	0.00	0.00	0.05	0.04	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	-0.04	-0.01	0.00
14	8	0.00	0.00	0.00	-0.01	0.00	0.00	-0.04	0.00	-0.01
15	8	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	-0.01	0.01
16	8	-0.01	-0.02	0.00	0.01	0.01	-0.01	-0.01	-0.03	0.03
17	1	-0.10	-0.05	0.18	-0.16	-0.18	-0.21	-0.02	-0.01	0.06
18	1	-0.11	-0.17	0.04	0.08	-0.09	0.06	0.06	0.05	0.03
19	1	-0.11	-0.25	0.14	0.14	0.12	-0.13	-0.02	-0.12	0.10
20	1	0.05	0.15	0.08	0.08	-0.14	-0.06	0.08	-0.09	0.03
21	1	0.05	0.16	0.28	-0.06	-0.21	-0.22	0.09	0.02	0.05
22	1	-0.01	-0.12	0.59	0.24	-0.09	0.01	-0.01	0.03	-0.09
23	1	-0.11	-0.06	0.03	-0.07	-0.18	0.01	0.43	-0.31	0.16
24	1	0.01	-0.37	-0.12	-0.03	-0.05	-0.03	0.35	-0.14	-0.27
25	1	0.14	-0.27	0.00	0.09	-0.51	-0.03	0.00	0.12	0.00
26	1	-0.01	-0.05	-0.03	0.12	-0.51	0.01	0.04	-0.10	0.03
27	1	0.00	0.00	0.00	-0.01	0.00	-0.02	-0.07	-0.02	-0.23
28	1	0.00	0.00	0.01	0.02	0.09	0.01	0.08	0.44	0.06

```
  29   1    -0.01  -0.05   0.02    -0.03  -0.05   0.05     0.07   0.13  -
0.12
                     64                     65                     66
                     ?A                     ?A                     ?A
 Frequencies --  1497.4389              1514.0925              1632.1621
 Red. masses --     2.2398                 2.7300                 8.2537
 Frc consts  --     2.9590                 3.6874                12.9547
 IR Inten    --    43.7791               113.5473               490.2095
 Raman Activ --     3.6082                13.2536                13.3067
 Depolar     --     0.6105                 0.4528                 0.2145
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.03   0.00   0.02     0.03   0.00  -0.01     0.00   0.00
0.00
   2   6     0.04   0.00   0.04    -0.02   0.00  -0.02     0.01   0.01
0.00
   3   6    -0.01   0.00  -0.10     0.01   0.00   0.06     0.01   0.02  -
0.03
   4   6     0.01   0.03  -0.06    -0.01  -0.02   0.04     0.03   0.03
0.01
   5   6     0.02  -0.04   0.20    -0.03   0.00  -0.13    -0.11  -0.12
0.04
   6   6     0.00   0.00  -0.01     0.00   0.00   0.00    -0.01  -0.01  -
0.01
   7   6     0.00   0.00   0.03     0.02  -0.01  -0.01     0.00   0.00  -
0.01
   8   6     0.00  -0.01  -0.01     0.05   0.03   0.01    -0.01   0.00
0.01
   9   6    -0.01  -0.04   0.05    -0.16  -0.03   0.01    -0.07  -0.02  -
0.06
  10   6    -0.01   0.05   0.03     0.04  -0.03  -0.03     0.03   0.03
0.01
  11   6     0.02  -0.02  -0.01    -0.02   0.02   0.00     0.03   0.01
0.02
  12   6     0.12   0.08  -0.08     0.22   0.12  -0.10     0.28  -0.05
0.59
  13   7    -0.04  -0.03   0.03    -0.08  -0.04   0.02    -0.20  -0.01  -
0.26
  14   8     0.00   0.00  -0.01     0.03   0.02   0.01     0.01   0.01
0.00
  15   8    -0.02  -0.03   0.06    -0.04  -0.04   0.08     0.01   0.06  -
0.18
  16   8     0.00   0.03  -0.06     0.00  -0.01   0.04     0.05   0.06  -
0.01
  17   1     0.11   0.07  -0.11    -0.09  -0.06   0.07     0.00   0.00
0.01
  18   1    -0.21  -0.02  -0.18     0.12   0.01   0.11    -0.03  -0.02  -
0.02
  19   1     0.02   0.02  -0.13    -0.04  -0.03   0.11    -0.05  -0.12
0.07
  20   1    -0.26  -0.28  -0.25     0.16   0.14   0.14    -0.17  -0.09  -
0.06
  21   1     0.00   0.00  -0.01     0.01   0.00   0.00     0.03   0.00
0.02
```

22	1	0.03	0.03	-0.10	-0.08	-0.02	0.06	-0.01	0.00	0.02
23	1	0.02	0.14	-0.06	-0.13	-0.11	0.01	-0.01	-0.06	0.04
24	1	0.08	-0.31	-0.18	-0.12	0.19	0.15	-0.01	-0.06	0.01
25	1	-0.07	0.05	0.00	0.03	-0.04	0.00	-0.32	-0.08	0.06
26	1	0.00	0.08	0.00	0.00	-0.09	-0.01	-0.14	-0.02	-0.30
27	1	-0.13	0.04	-0.43	-0.20	0.06	-0.62	-0.19	-0.12	-0.15
28	1	0.00	0.05	0.01	-0.06	-0.30	-0.04	-0.01	0.01	0.02
29	1	-0.14	-0.31	0.22	0.11	0.22	-0.16	0.03	0.05	0.00

	67	68	69
	?A	?A	?A
Frequencies --	1636.6211	1646.9335	3215.8697
Red. masses --	1.1563	3.9698	1.0588
Frc consts --	1.8248	6.3441	6.4518
IR Inten --	60.5660	283.8509	31.4962
Raman Activ --	14.9698	7.2266	139.2982
Depolar --	0.4759	0.0579	0.1920

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.01	0.00	-0.02	-0.01	0.02	0.01	-0.01	0.00
2	6	0.00	0.00	0.00	-0.01	-0.02	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	-0.06	-0.06	0.04	0.00	0.00	0.00
4	6	0.00	0.00	-0.01	-0.07	-0.06	-0.06	0.00	0.00	0.00
5	6	0.02	0.02	0.01	0.27	0.32	0.02	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
7	6	0.00	-0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00
8	6	0.01	0.00	0.00	0.00	-0.03	0.02	0.00	0.00	0.00
9	6	-0.01	0.00	0.00	-0.01	-0.01	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	-0.02	-0.01	0.00	0.00	0.00
11	6	-0.08	-0.02	-0.04	0.04	0.00	0.01	-0.06	-0.01	-0.02
12	6	0.03	0.00	0.05	0.07	0.01	0.08	0.00	0.00	0.00
13	7	-0.02	0.00	-0.02	-0.04	-0.01	-0.04	0.00	0.00	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

15	8	0.00	0.00	-0.01	0.00	0.00	-0.02	0.00	0.00	0.00
16	8	-0.01	-0.01	0.00	-0.12	-0.14	0.00	0.00	0.00	0.00
17	1	-0.01	0.01	-0.01	0.08	0.03	-0.05	-0.06	0.10	-0.02
18	1	-0.02	0.00	-0.02	0.04	0.04	0.02	0.00	0.00	0.00
19	1	0.02	0.02	-0.03	0.26	0.31	-0.27	0.00	0.00	0.00
20	1	-0.01	0.01	0.00	0.28	0.26	0.11	0.00	0.00	0.00
21	1	-0.01	0.00	-0.02	0.01	0.01	0.00	-0.01	-0.01	0.01
22	1	-0.01	-0.01	-0.01	0.05	0.02	-0.03	-0.01	-0.05	-0.01
23	1	-0.03	0.01	-0.01	0.01	0.17	-0.04	0.00	0.00	-0.01
24	1	0.00	0.00	0.00	0.02	0.10	0.03	0.00	0.00	0.00
25	1	0.67	0.16	-0.13	-0.23	-0.07	0.04	0.07	-0.01	0.62
26	1	0.28	0.07	0.64	-0.09	0.04	-0.19	0.66	0.15	-0.36
27	1	-0.02	-0.01	-0.02	-0.05	0.00	-0.07	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00	0.00
29	1	-0.02	-0.04	0.02	-0.16	-0.37	0.12	0.00	0.00	0.00

	70			71			72		
	?A			?A			?A		
Frequencies --	3263.0854			3275.4379			3299.1228		
Red. masses --	1.1063			1.0881			1.0892		
Frc consts --	6.9404			6.8777			6.9846		
IR Inten --	18.0302			23.7479			12.1473		
Raman Activ --	89.7692			107.4875			67.3977		
Depolar --	0.7494			0.3497			0.7307		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.00	0.00	0.04	-0.07	0.01	0.01	-0.01	0.00
2 6	0.00	0.00	0.00	-0.01	0.01	0.01	0.03	-0.02	-0.04
3 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01
4 6	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00
5 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6 6	0.00	0.00	0.00	0.00	0.00	0.00	-0.03	-0.04	0.04
7 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00

8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01
11	6	-0.04	-0.01	0.09	0.01	0.00	0.01	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	1	0.03	-0.04	0.01	-0.48	0.82	-0.13	-0.09	0.15	-0.03
18	1	-0.01	0.00	0.01	0.15	-0.08	-0.15	-0.39	0.21	0.42
19	1	0.00	0.00	0.00	0.00	0.01	0.01	-0.04	-0.07	-0.12
20	1	0.00	0.00	0.00	0.00	-0.03	0.06	0.00	-0.01	0.02
21	1	0.00	0.00	0.00	-0.01	-0.02	0.02	0.35	0.45	-0.47
22	1	0.00	0.01	0.00	0.01	0.05	0.01	-0.01	-0.14	-0.03
23	1	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.01
24	1	0.00	0.00	0.00	0.00	0.00	0.00	0.03	-0.03	0.06
25	1	-0.11	0.00	-0.76	-0.01	0.00	-0.10	0.00	0.00	-0.02
26	1	0.55	0.12	-0.28	-0.05	-0.01	0.03	-0.01	0.00	0.01
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	73			74			75		
	?A			?A			?A		
Frequencies --	3310.3021			3323.5952			3327.1815		
Red. masses --	1.0892			1.0892			1.0899		
Frc consts --	7.0324			7.0885			7.1090		
IR Inten --	25.9334			12.8581			10.4254		
Raman Activ --	121.1200			73.6988			178.2479		
Depolar --	0.4320			0.3176			0.1282		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z

1	6	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.00
2	6	0.04	-0.02	-0.04	0.02	-0.01	-0.02	-0.01	0.01	0.01
3	6	0.01	0.01	0.03	-0.02	-0.04	-0.06	0.01	0.01	0.02
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.02	0.03	-0.03	0.00	0.00	0.00	-0.01	-0.02	0.02
7	6	0.00	-0.02	0.00	0.00	-0.03	-0.01	-0.01	-0.07	-0.02
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	-0.01
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	1	-0.06	0.11	-0.02	-0.02	0.03	-0.01	0.04	-0.06	0.01
18	1	-0.42	0.23	0.45	-0.19	0.10	0.20	0.14	-0.08	-0.15
19	1	-0.10	-0.17	-0.29	0.27	0.42	0.73	-0.07	-0.11	-0.19
20	1	0.00	-0.01	0.02	-0.01	-0.02	0.04	0.00	0.00	0.00
21	1	-0.27	-0.35	0.37	0.00	-0.01	0.00	0.15	0.19	-0.21
22	1	0.03	0.29	0.06	0.03	0.31	0.06	0.09	0.83	0.17
23	1	0.01	-0.01	-0.03	0.01	-0.02	-0.06	0.05	-0.06	-0.21
24	1	-0.02	0.02	-0.03	-0.06	0.04	-0.09	0.04	-0.03	0.07
25	1	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.04
26	1	-0.01	0.00	0.01	0.01	0.00	0.00	0.04	0.01	-0.02
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  29   1     0.00   0.00   0.00     0.01   0.00   0.00     0.00   0.00
0.00
                     76                     77                     78
                     ?A                     ?A                     ?A
 Frequencies --  3343.8970              3355.5207              3367.5041
 Red. masses --     1.0887                 1.0890                 1.0903
 Frc consts  --     7.1727                 7.2241                 7.2845
 IR Inten    --     2.6135                 0.6552                 1.4187
 Raman Activ --    36.6619               134.0409               127.4244
 Depolar     --     0.7256                 0.1145                 0.1229
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   2   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   3   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.01  -
0.01
   4   6     0.01   0.02  -0.05     0.01   0.03  -0.05     0.00   0.00
0.01
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.01  -
0.01
   7   6     0.00   0.01   0.00     0.00  -0.01   0.00     0.00   0.00
0.00
   8   6    -0.01   0.02   0.06     0.01  -0.02  -0.05     0.00   0.00
0.01
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00    -0.01   0.00  -0.01    -0.04   0.03  -
0.07
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  17   1     0.02  -0.04   0.00     0.03  -0.05   0.01    -0.01   0.01
0.00
  18   1     0.00   0.00   0.00     0.02  -0.01  -0.02    -0.03   0.01
0.03
  19   1    -0.01  -0.01  -0.02     0.00   0.00  -0.01     0.04   0.06
0.10
  20   1    -0.07  -0.30   0.63    -0.07  -0.30   0.63     0.01   0.03  -
0.06
```

21	1	-0.01	-0.02	0.02	0.01	0.01	-0.01	-0.06	-0.07	0.07
22	1	-0.02	-0.17	-0.03	0.02	0.13	0.03	0.00	-0.04	-0.01
23	1	0.16	-0.19	-0.64	-0.16	0.19	0.63	0.02	-0.03	-0.09
24	1	-0.01	0.01	-0.02	0.06	-0.05	0.11	0.46	-0.34	0.79
25	1	0.00	0.00	-0.01	0.00	0.00	0.02	0.00	0.00	0.00
26	1	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	79			80			81		
	?A			?A			?A		
Frequencies --	3609.1278			3775.7350			3847.5500		
Red. masses --	1.0729			1.0670			1.0669		
Frc consts --	8.2340			8.9620			9.3054		
IR Inten --	6.3295			281.9474			91.5689		
Raman Activ --	211.7814			92.2988			87.1604		
Depolar --	0.3376			0.2711			0.2337		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12 6	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
13 7	-0.06	-0.03	0.01	0.00	0.00	0.00	0.00	0.00	0.00

```
  14   8     0.00   0.00   0.00     0.00   0.00   0.00    -0.06   0.02  -
0.02
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   8     0.00   0.00   0.00     0.04   0.02   0.04     0.00   0.00
0.00
  17   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  18   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  19   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  20   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  21   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  22   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  23   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  24   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  25   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  27   1     0.91   0.39  -0.14     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.01   0.00   0.00     0.88  -0.28
0.37
  29   1     0.00   0.00   0.00    -0.63  -0.30  -0.71     0.01   0.00
0.01

 --------------------
 - Thermochemistry -
 --------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Atom  1 has atomic number  6 and mass  12.00000
 Atom  2 has atomic number  6 and mass  12.00000
 Atom  3 has atomic number  6 and mass  12.00000
 Atom  4 has atomic number  6 and mass  12.00000
 Atom  5 has atomic number  6 and mass  12.00000
 Atom  6 has atomic number  6 and mass  12.00000
 Atom  7 has atomic number  6 and mass  12.00000
 Atom  8 has atomic number  6 and mass  12.00000
 Atom  9 has atomic number  6 and mass  12.00000
 Atom 10 has atomic number  6 and mass  12.00000
 Atom 11 has atomic number  6 and mass  12.00000
 Atom 12 has atomic number  6 and mass  12.00000
 Atom 13 has atomic number  7 and mass  14.00307
 Atom 14 has atomic number  8 and mass  15.99491
 Atom 15 has atomic number  8 and mass  15.99491
 Atom 16 has atomic number  8 and mass  15.99491
 Atom 17 has atomic number  1 and mass   1.00783
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 Atom 18 has atomic number  1 and mass   1.00783
 Atom 19 has atomic number  1 and mass   1.00783
 Atom 20 has atomic number  1 and mass   1.00783
 Atom 21 has atomic number  1 and mass   1.00783
 Atom 22 has atomic number  1 and mass   1.00783
 Atom 23 has atomic number  1 and mass   1.00783
 Atom 24 has atomic number  1 and mass   1.00783
 Atom 25 has atomic number  1 and mass   1.00783
 Atom 26 has atomic number  1 and mass   1.00783
 Atom 27 has atomic number  1 and mass   1.00783
 Atom 28 has atomic number  1 and mass   1.00783
 Atom 29 has atomic number  1 and mass   1.00783
 Molecular mass:   219.08954 amu.
 Principal axes and moments of inertia in atomic units:
                           1         2         3
     EIGENVALUES --  1908.95014 2746.65572 3352.72724
           X            0.99978   0.00785   0.01954
           Y           -0.00804   0.99992   0.01003
           Z           -0.01946  -0.01019   0.99976
 THIS MOLECULE IS AN ASYMMETRIC TOP.
 ROTATIONAL SYMMETRY NUMBER  1.
 WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
           MAY CAUSE SIGNIFICANT ERROR
 ROTATIONAL TEMPERATURES (KELVIN)      0.04537     0.03153     0.02583
 ROTATIONAL CONSTANTS (GHZ)            0.94541     0.65707     0.53829
    1 IMAGINARY FREQUENCIES IGNORED.
 Zero-point vibrational energy     662426.8 (Joules/Mol)
                                  158.32381 (Kcal/Mol)
 WARNING-- EXPLICIT CONSIDERATION OF  14 DEGREES OF FREEDOM AS
           VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
 VIBRATIONAL TEMPERATURES:    184.43   210.28   239.87   385.69   439.35
          (KELVIN)            473.80   536.30   555.12   596.02   649.00
                              688.42   753.42   782.17   860.25   910.80
                              970.57   996.54  1024.94  1143.16  1175.23
                             1186.15  1192.82  1222.93  1255.71  1272.53
                             1304.33  1313.22  1351.07  1395.12  1418.78
                             1437.58  1456.29  1457.66  1484.75  1497.92
                             1511.90  1537.25  1586.40  1624.27  1674.59
                             1717.13  1741.90  1760.87  1776.35  1794.50
                             1822.87  1830.87  1872.65  1887.70  1919.24
                             1937.22  1948.29  1972.19  1988.28  2002.94
                             2021.49  2029.54  2048.33  2062.52  2066.91
                             2094.58  2126.32  2154.47  2178.43  2348.30
                             2354.72  2369.56  4626.89  4694.82  4712.60
                             4746.67  4762.76  4781.88  4787.04  4811.09
                             4827.82  4845.06  5192.70  5432.41  5535.73

 Zero-point correction=                           0.252305
(Hartree/Particle)
 Thermal correction to Energy=                    0.262099
 Thermal correction to Enthalpy=                  0.263043
 Thermal correction to Gibbs Free Energy=         0.217262
 Sum of electronic and zero-point Energies=           -736.635022
 Sum of electronic and thermal Energies=              -736.625228
```

Sum of electronic and thermal Enthalpies= -736.624284
Sum of electronic and thermal Free Energies= -736.670065

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	164.470	43.467	96.355
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	42.056
ROTATIONAL	0.889	2.981	31.242
VIBRATIONAL	162.692	37.505	23.056
VIBRATION 1	0.611	1.925	2.973
VIBRATION 2	0.617	1.907	2.722
VIBRATION 3	0.624	1.883	2.472
VIBRATION 4	0.673	1.732	1.609
VIBRATION 5	0.696	1.664	1.387
VIBRATION 6	0.712	1.617	1.263
VIBRATION 7	0.744	1.528	1.068
VIBRATION 8	0.755	1.500	1.016
VIBRATION 9	0.778	1.439	0.912
VIBRATION 10	0.810	1.359	0.793
VIBRATION 11	0.835	1.298	0.714
VIBRATION 12	0.879	1.198	0.602
VIBRATION 13	0.899	1.154	0.558
VIBRATION 14	0.956	1.036	0.453

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.116678D-99	-99.933012	-230.104264
TOTAL V=0	0.131361D+17	16.118465	37.114137
VIB (BOT)	0.609884-114	-114.214753	-262.989187
VIB (BOT) 1	0.159108D+01	0.201692	0.464413
VIB (BOT) 2	0.138893D+01	0.142680	0.328533
VIB (BOT) 3	0.121007D+01	0.082809	0.190676
VIB (BOT) 4	0.721650D+00	-0.141673	-0.326215
VIB (BOT) 5	0.620890D+00	-0.206985	-0.476601
VIB (BOT) 6	0.567632D+00	-0.245933	-0.566282
VIB (BOT) 7	0.487510D+00	-0.312016	-0.718444
VIB (BOT) 8	0.466702D+00	-0.330960	-0.762063
VIB (BOT) 9	0.425718D+00	-0.370878	-0.853978
VIB (BOT) 10	0.379837D+00	-0.420403	-0.968014
VIB (BOT) 11	0.349994D+00	-0.455939	-1.049839
VIB (BOT) 12	0.307210D+00	-0.512565	-1.180224
VIB (BOT) 13	0.290432D+00	-0.536956	-1.236386
VIB (BOT) 14	0.250277D+00	-0.601578	-1.385185
VIB (V=0)	0.686632D+02	1.836724	4.229214
VIB (V=0) 1	0.216779D+01	0.336018	0.773710
VIB (V=0) 2	0.197619D+01	0.295828	0.681169
VIB (V=0) 3	0.180930D+01	0.257510	0.592939
VIB (V=0) 4	0.137794D+01	0.139230	0.320590
VIB (V=0) 5	0.129719D+01	0.113002	0.260197
VIB (V=0) 6	0.125644D+01	0.099143	0.228285
VIB (V=0) 7	0.119833D+01	0.078577	0.180930
VIB (V=0) 8	0.118397D+01	0.073340	0.168871
VIB (V=0) 9	0.115669D+01	0.063215	0.145559
VIB (V=0) 10	0.112791D+01	0.052276	0.120370
VIB (V=0) 11	0.111032D+01	0.045450	0.104652

```
VIB (V=0) 12    0.108684D+01          0.036165          0.083272
VIB (V=0) 13    0.107823D+01          0.032712          0.075321
VIB (V=0) 14    0.105914D+01          0.024954          0.057458
ELECTRONIC      0.100000D+01          0.000000          0.000000
TRANSLATIONAL   0.127466D+09          8.105393         18.663357
ROTATIONAL      0.150089D+07          6.176348         14.221567
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6           0.000000079   -0.000001530    0.000004694
   2          6           0.000003368    0.000002794   -0.000000209
   3          6          -0.000004786   -0.000006110    0.000007005
   4          6           0.000003481    0.000005804    0.000003623
   5          6          -0.000001148   -0.000001242   -0.000009296
   6          6           0.000000251   -0.000001492   -0.000000397
   7          6           0.000002514   -0.000001655    0.000000199
   8          6          -0.000004011   -0.000003945   -0.000002070
   9          6          -0.000002260    0.000001782   -0.000003536
  10          6          -0.000002415    0.000003856    0.000005195
  11          6           0.000000365    0.000001672   -0.000003339
  12          6          -0.000004768   -0.000003450    0.000010401
  13          7          -0.000003239    0.000006939   -0.000006529
  14          8           0.000003231    0.000001402    0.000001045
  15          8           0.000003055    0.000001922   -0.000009173
  16          8           0.000007393   -0.000005547    0.000003924
  17          1          -0.000000161    0.000000330   -0.000000804
  18          1          -0.000000407   -0.000000452    0.000000190
  19          1           0.000000426    0.000001227   -0.000000026
  20          1          -0.000001046   -0.000001544   -0.000002306
  21          1           0.000000355    0.000000246   -0.000000326
  22          1          -0.000000678    0.000000298   -0.000000545
  23          1           0.000000068    0.000000007    0.000000189
  24          1           0.000000576   -0.000000890   -0.000000667
  25          1           0.000000187   -0.000000155    0.000000135
  26          1           0.000000705   -0.000000163    0.000000249
  27          1           0.000001346   -0.000000009    0.000001692
  28          1          -0.000000883   -0.000002862    0.000000335
  29          1          -0.000001596    0.000002770    0.000000349
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000010401 RMS     0.000003262
-------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------
  1  C         0.000000(   1)     -0.000002(  30)      0.000005(  59)
  2  C         0.000003(   2)      0.000003(  31)      0.000000(  60)
  3  C        -0.000005(   3)     -0.000006(  32)      0.000007(  61)
  4  C         0.000003(   4)      0.000006(  33)      0.000004(  62)
  5  C        -0.000001(   5)     -0.000001(  34)     -0.000009(  63)
  6  C         0.000000(   6)     -0.000001(  35)      0.000000(  64)
  7  C         0.000003(   7)     -0.000002(  36)      0.000000(  65)
  8  C        -0.000004(   8)     -0.000004(  37)     -0.000002(  66)
```

```
  9  C        -0.000002(   9)      0.000002(  38)     -0.000004(  67)
 10  C        -0.000002(  10)      0.000004(  39)      0.000005(  68)
 11  C         0.000000(  11)      0.000002(  40)     -0.000003(  69)
 12  C        -0.000005(  12)     -0.000003(  41)      0.000010(  70)
 13  N        -0.000003(  13)      0.000007(  42)     -0.000007(  71)
 14  O         0.000003(  14)      0.000001(  43)      0.000001(  72)
 15  O         0.000003(  15)      0.000002(  44)     -0.000009(  73)
 16  O         0.000007(  16)     -0.000006(  45)      0.000004(  74)
 17  H         0.000000(  17)      0.000000(  46)     -0.000001(  75)
 18  H         0.000000(  18)      0.000000(  47)      0.000000(  76)
 19  H         0.000000(  19)      0.000001(  48)      0.000000(  77)
 20  H        -0.000001(  20)     -0.000002(  49)     -0.000002(  78)
 21  H         0.000000(  21)      0.000000(  50)      0.000000(  79)
 22  H        -0.000001(  22)      0.000000(  51)     -0.000001(  80)
 23  H         0.000000(  23)      0.000000(  52)      0.000000(  81)
 24  H         0.000001(  24)     -0.000001(  53)     -0.000001(  82)
 25  H         0.000000(  25)      0.000000(  54)      0.000000(  83)
 26  H         0.000001(  26)      0.000000(  55)      0.000000(  84)
 27  H         0.000001(  27)      0.000000(  56)      0.000002(  85)
 28  H        -0.000001(  28)     -0.000003(  57)      0.000000(  86)
 29  H        -0.000002(  29)      0.000003(  58)      0.000000(  87)
--------------------------------------------------------------------------
Internal  Forces:  Max     0.000010401 RMS     0.000003262

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   1 out of a maximum of  97
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
    Eigenvalues ---   -0.00326   0.00306   0.00491   0.00658   0.00684
    Eigenvalues ---    0.01155   0.01357   0.01769   0.02460   0.02598
    Eigenvalues ---    0.03373   0.04117   0.04273   0.04564   0.04642
    Eigenvalues ---    0.04704   0.04905   0.04983   0.05018   0.05132
    Eigenvalues ---    0.05186   0.05358   0.05501   0.05778   0.05865
    Eigenvalues ---    0.05942   0.06079   0.06903   0.06947   0.07847
    Eigenvalues ---    0.08364   0.10079   0.10609   0.11123   0.13711
    Eigenvalues ---    0.14865   0.15957   0.16997   0.18758   0.19107
    Eigenvalues ---    0.20107   0.21133   0.25015   0.26483   0.28549
    Eigenvalues ---    0.31665   0.33418   0.34519   0.37634   0.39098
    Eigenvalues ---    0.40274   0.43301   0.43565   0.48921   0.50579
    Eigenvalues ---    0.50628   0.53156   0.55879   0.57501   0.58161
    Eigenvalues ---    0.63427   0.66386   0.69040   0.71826   0.73684
    Eigenvalues ---    0.84202   0.88047   0.90147   0.95163   0.96469
    Eigenvalues ---    0.97580   0.99810   1.02883   1.03393   1.06092
    Eigenvalues ---    1.07118   1.09076   1.12358   1.13659   1.36800
    Eigenvalues ---    1.39961
Eigenvalue   1 out of range, new value =    0.003256 Eigenvector:
                          1
          X1         -0.01779
          Y1          0.00619
          Z1          0.03611
          X2         -0.02819
          Y2         -0.02794
```

Z2	0.02997
X3	-0.04920
Y3	-0.01004
Z3	0.05053
X4	-0.01406
Y4	0.03752
Z4	0.04650
X5	-0.00056
Y5	-0.01842
Z5	0.07148
X6	-0.00647
Y6	-0.02322
Z6	-0.00914
X7	-0.00312
Y7	0.01114
Z7	-0.01739
X8	-0.00906
Y8	0.03160
Z8	-0.00174
X9	-0.00495
Y9	0.03286
Z9	-0.00916
X10	-0.00774
Y10	-0.00720
Z10	0.00189
X11	-0.00627
Y11	0.01449
Z11	-0.00072
X12	0.00083
Y12	0.01915
Z12	-0.06643
X13	-0.20057
Y13	0.49495
Z13	0.04928
X14	-0.01691
Y14	0.02604
Z14	-0.03868
X15	0.21155
Y15	-0.47781
Z15	-0.21509
X16	0.15870
Y16	-0.13668
Z16	0.05421
X17	-0.02382
Y17	0.00574
Z17	0.05344
X18	-0.04683
Y18	-0.05915
Z18	0.02783
X19	-0.04533
Y19	-0.03508
Z19	0.06313
X20	-0.00831
Y20	0.06468

Z20	0.05901
X21	0.00402
Y21	-0.04709
Z21	-0.02385
X22	0.00529
Y22	0.01556
Z22	-0.04327
X23	0.00460
Y23	0.05889
Z23	-0.00610
X24	-0.00684
Y24	-0.01446
Z24	-0.00255
X25	-0.00143
Y25	0.03674
Z25	-0.00156
X26	-0.00680
Y26	-0.00243
Z26	-0.00931
X27	-0.16186
Y27	0.40204
Z27	0.02207
X28	-0.00856
Y28	-0.01935
Z28	-0.09275
X29	0.18622
Y29	-0.21313
Z29	0.06486

Angle between quadratic step and forces= 74.80 degrees.
Linear search not attempted -- first point.
TrRot= 0.000008 -0.000015 -0.000011 -0.000002 0.000004 -0.000002

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
X1	-3.93366	0.00000	0.00000	0.00003	0.00005	-3.93362
Y1	1.72787	0.00000	0.00000	0.00003	0.00003	1.72790
Z1	-0.73034	0.00000	0.00000	0.00006	0.00006	-0.73028
X2	-3.30989	0.00000	0.00000	-0.00004	-0.00002	-3.30990
Y2	1.10889	0.00000	0.00000	-0.00004	-0.00004	1.10886
Z2	2.09210	0.00000	0.00000	0.00005	0.00005	2.09215
X3	-0.41313	0.00000	0.00000	-0.00010	-0.00007	-0.41320
Y3	1.76917	-0.00001	0.00000	-0.00006	-0.00007	1.76909
Z3	2.53588	0.00001	0.00000	0.00013	0.00012	2.53600
X4	-1.23292	0.00000	0.00000	0.00006	0.00007	-1.23285
Y4	1.69903	0.00001	0.00000	0.00003	0.00001	1.69904
Z4	-1.93581	0.00000	0.00000	0.00009	0.00008	-1.93573
X5	0.26454	0.00000	0.00000	0.00006	0.00008	0.26461
Y5	2.91126	0.00000	0.00000	-0.00008	-0.00010	2.91117
Z5	0.08333	-0.00001	0.00000	0.00015	0.00014	0.08346
X6	-2.66034	0.00000	0.00000	-0.00004	-0.00003	-2.66036
Y6	-1.78071	0.00000	0.00000	-0.00005	-0.00005	-1.78076
Z6	2.03288	0.00000	0.00000	-0.00001	-0.00002	2.03287
X7	-2.96889	0.00000	0.00000	-0.00003	-0.00003	-2.96892
Y7	-2.46211	0.00000	0.00000	0.00001	0.00000	-2.46211
Z7	-0.80833	0.00000	0.00000	-0.00003	-0.00003	-0.80835

X8	-0.56151	0.00000	0.00000	-0.00003	-0.00003	-0.56154
Y8	-1.25632	0.00000	0.00000	-0.00001	-0.00003	-1.25635
Z8	-1.95124	0.00000	0.00000	0.00001	0.00000	-1.95124
X9	1.49365	0.00000	0.00000	-0.00002	-0.00002	1.49363
Y9	-1.83389	0.00000	0.00000	0.00004	0.00001	-1.83388
Z9	-0.01580	0.00000	0.00000	-0.00001	-0.00002	-0.01583
X10	0.19486	0.00000	0.00000	-0.00003	-0.00002	0.19484
Y10	-1.16472	0.00000	0.00000	-0.00003	-0.00005	-1.16477
Z10	2.46303	0.00001	0.00000	0.00003	0.00002	2.46305
X11	-5.12901	0.00000	0.00000	0.00002	0.00002	-5.12900
Y11	-0.73677	0.00000	0.00000	0.00007	0.00008	-0.73670
Z11	-1.68877	0.00000	0.00000	-0.00004	-0.00003	-1.68879
X12	3.99920	0.00000	0.00000	-0.00006	-0.00006	3.99914
Y12	-0.43194	0.00000	0.00000	0.00007	0.00004	-0.43190
Z12	-0.45920	0.00001	0.00000	-0.00018	-0.00021	-0.45941
X13	5.38542	0.00000	0.00000	-0.00038	-0.00037	5.38505
Y13	-0.27772	0.00001	0.00000	0.00101	0.00097	-0.27675
Z13	1.56821	-0.00001	0.00000	-0.00002	-0.00005	1.56816
X14	1.85378	0.00000	0.00000	0.00003	0.00002	1.85380
Y14	-4.54939	0.00000	0.00000	0.00003	0.00001	-4.54938
Z14	-0.07565	0.00000	0.00000	-0.00002	-0.00004	-0.07569
X15	4.35502	0.00000	0.00000	0.00025	0.00025	4.35527
Y15	0.44572	0.00000	0.00000	-0.00085	-0.00088	0.44484
Z15	-2.68096	-0.00001	0.00000	-0.00049	-0.00052	-2.68148
X16	1.64992	0.00001	0.00000	0.00033	0.00036	1.65028
Y16	4.87159	-0.00001	0.00000	-0.00028	-0.00030	4.87129
Z16	-0.29539	0.00000	0.00000	0.00020	0.00018	-0.29522
X17	-4.97527	0.00000	0.00000	0.00006	0.00008	-4.97519
Y17	3.45780	0.00000	0.00000	0.00005	0.00005	3.45785
Z17	-1.03366	0.00000	0.00000	0.00005	0.00006	-1.03360
X18	-4.63465	0.00000	0.00000	-0.00009	-0.00007	-4.63471
Y18	1.81130	0.00000	0.00000	-0.00009	-0.00009	1.81121
Z18	3.47044	0.00000	0.00000	0.00002	0.00003	3.47047
X19	0.17907	0.00000	0.00000	-0.00009	-0.00005	0.17902
Y19	2.78977	0.00000	0.00000	-0.00008	-0.00009	2.78967
Z19	4.19342	0.00000	0.00000	0.00014	0.00013	4.19355
X20	-1.01215	0.00000	0.00000	0.00008	0.00008	-1.01207
Y20	2.57431	0.00000	0.00000	0.00003	0.00002	2.57433
Z20	-3.75652	0.00000	0.00000	0.00009	0.00008	-3.75644
X21	-3.60988	0.00000	0.00000	-0.00004	-0.00003	-3.60991
Y21	-3.01122	0.00000	0.00000	-0.00007	-0.00007	-3.01129
Z21	3.34873	0.00000	0.00000	-0.00004	-0.00003	3.34870
X22	-3.13755	0.00000	0.00000	-0.00007	-0.00009	-3.13764
Y22	-4.45209	0.00000	0.00000	0.00002	0.00002	-4.45207
Z22	-1.20180	0.00000	0.00000	-0.00008	-0.00008	-1.20187
X23	-0.05171	0.00000	0.00000	0.00000	-0.00001	-0.05172
Y23	-1.85277	0.00000	0.00000	0.00002	0.00000	-1.85277
Z23	-3.82658	0.00000	0.00000	0.00000	-0.00001	-3.82658
X24	1.16095	0.00000	0.00000	-0.00003	-0.00001	1.16094
Y24	-1.84238	0.00000	0.00000	-0.00009	-0.00011	-1.84249
Z24	4.11367	0.00000	0.00000	0.00000	-0.00001	4.11366
X25	-5.39902	0.00000	0.00000	0.00007	0.00006	-5.39897
Y25	-0.75628	0.00000	0.00000	0.00011	0.00012	-0.75616
Z25	-3.71875	0.00000	0.00000	-0.00004	-0.00003	-3.71878

X26	-6.91255	0.00000	0.00000	0.00000	0.00000	-6.91256
Y26	-1.13826	0.00000	0.00000	0.00008	0.00009	-1.13817
Z26	-0.76265	0.00000	0.00000	-0.00008	-0.00006	-0.76271
X27	7.09735	0.00000	0.00000	-0.00030	-0.00029	7.09707
Y27	0.50815	0.00000	0.00000	0.00080	0.00075	0.50891
Z27	1.22491	0.00000	0.00000	-0.00010	-0.00014	1.22477
X28	3.47945	0.00000	0.00000	-0.00002	-0.00003	3.47942
Y28	-4.99925	0.00000	0.00000	-0.00005	-0.00007	-4.99932
Z28	0.63702	0.00000	0.00000	0.00004	0.00002	0.63703
X29	2.79093	0.00000	0.00000	0.00015	0.00018	2.79111
Y29	5.41321	0.00000	0.00000	-0.00024	-0.00027	5.41294
Z29	1.04395	0.00000	0.00000	0.00034	0.00032	1.04426

Item		Value	Threshold	Converged?
Maximum	Force	0.000010	0.000450	YES
RMS	Force	0.000003	0.000300	YES
Maximum	Displacement	0.000973	0.001800	YES
RMS	Displacement	0.000204	0.001200	YES

Predicted change in Energy=-3.041485D-09
Optimization completed.
   -- Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1|1|UNPC-UNK|Freq|RHF|3-21+G*|C12H13N1O3|PCUSER|14-Mar-2002|0||#N RHF/
3-21+G* FREQ||Freq calc of output str of m1s13Nbotts2||0,1|C,-2.081605
0172,0.9143499569,-0.3864779569|C,-1.7515170172,0.5868019569,1.1070920
431|C,-0.2186210172,0.9362019569,1.3419300431|C,-0.6524320172,0.899086
9569,-1.0243889569|C,0.1399859828,1.5405739569,0.0440940431|C,-1.40778
90172,-0.9423110431,1.0757560431|C,-1.5710690172,-1.3028950431,-0.4277
479569|C,-0.2971400172,-0.6648170431,-1.0325509569|C,0.7904069828,-0.9
704530431,-0.0083619569|C,0.1031159828,-0.6163430431,1.3033780431|C,-2
.7141570172,-0.3898830431,-0.8936569569|C,2.1162849828,-0.2285740431,-
0.2429999569|N,2.8498429828,-0.1469650431,0.8298630431|O,0.9809789828,
-2.4074360431,-0.0400329569|O,2.3045749828,0.2358639569,-1.4187029569|
O,0.8730979828,2.5779329569,-0.1563159569|H,-2.6328010172,1.8297909569
,-0.5469919569|H,-2.4525490172,0.9584969569,1.8364780431|H,0.094760982
8,1.4762809569,2.2190610431|H,-0.5356070172,1.3622659569,-1.9878669569
|H,-1.9102660172,-1.5934710431,1.7720720431|H,-1.6603220172,-2.3559440
431,-0.6359629569|H,-0.0273630172,-0.9804460431,-2.0249379569|H,0.6143
499828,-0.9749470431,2.1768630431|H,-2.8570400172,-0.4002080431,-1.967
8769569|H,-3.6579660172,-0.6023400431,-0.4035759569|H,3.7557579828,0.2
689019569,0.6481930431|H,1.8412479828,-2.6454890431,0.3370940431|H,1.4
768979828,2.8645459569,0.5524320431||Version=x86-Win32-G98RevA.7|HF=-7
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,1.5295605|DipoleDeriv=0.1699591,-0.0593268,0.0242046,-0.0934835,0.119
681,-0.034376,-0.029934,-0.0472983,-0.007726,0.2165931,0.0146475,-0.07
59774,0.1010354,0.0429782,0.0073397,-0.0226292,0.0727319,0.0404759,-0.
2849532,-0.058044,0.0720418,-0.1072641,-0.4759233,0.1647103,0.0574906,
0.2382642,-0.0704648,-0.2355419,-0.0779094,-0.020845,-0.0749372,-0.336
8858,-0.1099952,-0.0080815,-0.1687852,-0.0145,1.0530229,0.6704053,-0.0
19672,0.5245211,1.4219121,-0.0618354,-0.1028186,-0.2058357,0.6132719,0
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,0.006375,0.3297102,0.0919618,-0.0713138,0.0566138,-0.0038729,0.351356

2,-0.3273718,0.005573,-0.3389393,0.5981143,0.1074612,-0.0100607,0.0575
509,0.2610689,0.0734107,0.0189895,0.0394123,-0.0138316,0.342902,-0.091
4891,0.0244658,-0.0547008,-0.0548039,0.0267548,0.0612748,-0.0522856,0.
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7,-0.0352878,-0.0135837,-0.0202993,0.0611469,0.0777782,0.0034707,0.012
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77,-0.00000035|||@

GARLIC THEN HAVE POWER TO SAVE FROM DEATH

```
 BEAR WITH IT THOUGH IT MAKETH UNSAVORY BREATH,
 AND SCORN NOT GARLIC LIKE SOME THAT THINK
 IT ONLY MAKETH MEN WINK AND DRINK AND STINK.
   --  SIR JOHN HARRINGTON,
       "THE ENGLISHMAN'S DOCTOR", 1609
 Job cpu time:  0 days 20 hours 31 minutes  5.0 seconds.
 File lengths (MBytes):  RWF=  320 Int=    0 D2E=    0 Chk=    6 Scr=
1
 Normal termination of Gaussian 98.
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Std input@99.9899degrees-optcyc=200-ts search

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 C                  2             B2    1             A1
 C                  1             B3    2             A2    3
D1
 C                  3             B4    2             A3    1
D2
 C                  2             B5    1             A4    4
D3
 C                  6             B6    2             A5    1
D4
 C                  7             B7    6             A6    2
D5
 C                  8             B8    7             A7    6
D6
 C                  9             B9    8             A8    7
D7
 C                  7            B10    6             A9    2
D8
 C                  9            B11    8            A10    7
D9
 N                 12            B12    9            A11    8
D10
 O                  9            B13    8            A12    7
D11
 O                 12            B14    9            A13    8
D12
 O                  5            B15    3            A14    2
D13
 H                  1            B16    2            A15    6
D14
 H                  2            B17    1            A16   11
D15
 H                  3            B18    2            A17    1
D16
 H                  4            B19    1            A18    2
D17
 H                  6            B20    2            A19    1
D18
 H                  7            B21    6            A20    2
D19
 H                  8            B22    7            A21    6
D20
 H                 10            B23    9            A22    8
D21
 H                 11            B24    7            A23    6
D22
```

H	11	B25	7	A24	6
D23					
H	13	B26	12	A25	9
D24					
H	14	B27	9	A26	8
D25					
H	16	B28	5	A27	3
D26					

B1	1.564717
B2	1.584904
B3	1.567442
B4	1.472080
B5	1.566723
B6	1.555423
B7	1.547340
B8	1.523357
B9	1.522423
B10	1.535171
B11	1.537291
B12	1.301977
B13	1.451222
B14	1.276758
B15	1.283882
B16	1.080815
B17	1.077828
B18	1.077060
B19	1.075598
B20	1.077613
B21	1.076997
B22	1.075642
B23	1.073687
B24	1.083715
B25	1.084466
B26	1.012944
B27	0.969015
B28	0.973026
A1	107.076565
A2	101.291452
A3	101.646458
A4	103.327009
A5	102.913394
A6	101.279232
A7	103.955821
A8	102.043884
A9	103.572297
A10	114.884077
A11	112.652973
A12	106.003607
A13	116.237986
A14	127.672529
A15	115.201558
A16	115.745611
A17	120.860092

```
  A18          117.387093
  A19          118.380035
  A20          114.998876
  A21          116.521654
  A22          114.038114
  A23          113.123246
  A24          113.261962
  A25          112.462642
  A26          110.476233
  A27          118.903974
  D1            21.110514
  D2             4.893245
  D3           -73.707757
  D4             0.018329
  D5            74.754961
  D6            40.399217
  D7           -46.072452
  D8           -33.285509
  D9          -171.113060
  D10          159.240351
  D11           66.201494
  D12          -20.759750
  D13          144.690939
  D14          162.190111
  D15          -99.391835
  D16          135.847431
  D17         -163.148066
  D18         -129.175491
  D19         -162.754796
  D20          164.822715
  D21          166.890891
  D22          170.783834
  D23          -64.057040
  D24          174.621947
  D25          158.925183
  D26            0.000630

1  2 1.0  4 1.0  11 1.0  17 1.0
2  3 1.0  6 1.0  18 1.0
3  5 1.0  10 1.0  19 1.0
4  5 1.0  8 1.0  20 1.0
5  16 2.0
6  7 1.0  10 1.0  21 1.0
7  8 1.0  11 1.0  22 1.0
8  9 1.0  23 1.0
9  10 1.0  12 1.0  14 1.0
10  24 1.0
11  25 1.0  26 1.0
12  13 2.0  15 2.0
13  27 1.0
14  28 1.0
15
16  29 1.0
17
```

```
%nproc=2
# opt=(gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity optcyc=100

TS2

0  1
 C                  0.000000    0.000000    0.000000
 C                  0.000000    0.000000    1.564280
 C                  1.519540    0.000000    2.043361
 C                  1.439481   -0.535188   -0.304057
 C                  2.218699    0.152757    0.748689
 C                 -0.119514   -1.520598    1.928085
 C                 -0.156355   -2.207383    0.534469
 C                  1.322804   -2.080856    0.094379
 C                  2.114804   -2.362319    1.367452
 C                  1.367980   -1.531545    2.401070
 C                 -0.903361   -1.193675   -0.344817
 C                  3.603436   -2.001426    1.311231
 N                  4.092390   -1.945395    0.116016
 O                  1.904308   -3.762839    1.679047
 O                  4.150649   -1.744422    2.452679
 O                  3.196895    0.958769    0.504736
 H                 -0.232135    0.948948   -0.461685
 H                 -0.656991    0.712151    2.036223
 H                  1.845559    0.655754    2.832839
 H                  1.821953   -0.382167   -1.297027
 H                 -0.888862   -1.820553    2.620567
 H                 -0.517216   -3.222469    0.537052
 H                  1.634526   -2.703189   -0.725168
 H                  1.614801   -1.768511    3.419205
 H                 -0.883181   -1.447187   -1.398331
 H                 -1.929697   -1.031813   -0.033913
 H                  5.083018   -1.732849    0.107776
 H                  2.611284   -4.113357    2.240223
 H                  3.723240    1.276557    1.261058

 1  2 1.0  4 1.0  11 1.0  17 1.0
 2  3 1.0  6 1.0  18 1.0
 3  5 1.0  10 1.0  19 1.0
 4  5 1.0  8 1.0  20 1.0
 5  16 1.5
 6  7 1.0  10 1.0  21 1.0
 7  8 1.0  11 1.0  22 1.0
 8  9 1.0  23 1.0
 9  10 1.0  12 1.0  14 1.0
 10  24 1.0
 11  25 1.0  26 1.0
 12  13 2.0  15 1.5
 13  27 1.0
 14  28 1.0
 15
 16  29 1.0
 17
 18
```

```
 Entering Gaussian System, Link 0=g98
 Input=mech1s13ts2F.gjf
 Output=mech1s13ts2F.out
 Initial command:
 /usr/g98/l1.exe /usr/scratch/Singh/Gau-3499.inp -
scrdir=/usr/scratch/Singh/
 Default is to use a total of   2 processors:
                                2 via shared-memory
                                1 via Linda
 Entering Link 1 = /usr/g98/l1.exe PID=      3517.
```

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

Cite this work as:
Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

```
**********************************************
Gaussian 98:  DEC-AXP-OSF/1-G98RevA.7 11-Apr-1999
                 15-Oct-2001
**********************************************
%nproc=2
Will use up to    2 processors via shared memory.
%chk=mech1s13ts2F
%nosave
-------------------
#N RHF/3-21+G* FREQ
-------------------
1/10=4,30=1,38=1/1,3;
2/17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
```

```
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;
------------------------------
Freq calc of output str of TS2
------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                    -1.63935   1.37132  -0.83138
C                    -1.51501   1.31307   0.72686
C                     0.03513   1.2096    1.08023
C                    -0.2628    0.76756  -1.26903
C                     0.63698   1.37081  -0.26145
C                    -1.695    -0.21087   1.04947
C                    -1.88307  -0.84211  -0.35814
C                    -0.43869  -0.78284  -0.91297
C                     0.43395  -1.1557    0.28146
C                    -0.17788  -0.32323   1.39903
C                    -2.63631   0.24412  -1.14012
C                     1.93214  -0.87743   0.11588
N                     2.327    -0.80458  -1.11275
O                     0.16639  -2.55277   0.56339
O                     2.5826   -0.69436   1.21669
O                     1.63866   2.12894  -0.55794
H                    -1.85089   2.34838  -1.24145
H                    -2.08912   2.04305   1.27373
H                     0.4611    1.81608   1.86145
H                     0.04792   0.93565  -2.28436
H                    -2.42327  -0.49257   1.79221
H                    -2.30202  -1.83464  -0.35922
H                    -0.23047  -1.3908   -1.77504
H                     0.13464  -0.61148   2.38539
H                    -2.71497   0.02928  -2.19947
H                    -3.6233    0.45188  -0.74149
H                     3.32467  -0.64804  -1.19478
H                     0.89375  -2.96322   1.05336
H                     2.24134   2.38818   0.16291

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  97 maximum allowed number of steps= 174.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

--------------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
--------------------------------------------------------------------------
  1   1  C     0  -1.639354          1.371321         -0.831383
  2   2  C     0  -1.515014          1.313071          0.726859
  3   3  C     0   0.035128          1.209597          1.080234
```

4	4	C	0	-0.262796	0.767556	-1.269031
5	5	C	0	0.636975	1.370814	-0.261452
6	6	C	0	-1.695000	-0.210866	1.049468
7	7	C	0	-1.883074	-0.842111	-0.358138
8	8	C	0	-0.438689	-0.782844	-0.912973
9	9	C	0	0.433951	-1.155704	0.281461
10	10	C	0	-0.177878	-0.323229	1.399025
11	11	C	0	-2.636311	0.244122	-1.140121
12	12	C	0	1.932142	-0.877433	0.115876
13	13	N	0	2.327000	-0.804578	-1.112755
14	14	O	0	0.166385	-2.552766	0.563389
15	15	O	0	2.582600	-0.694360	1.216687
16	16	O	0	1.638659	2.128944	-0.557940
17	17	H	0	-1.850893	2.348377	-1.241453
18	18	H	0	-2.089117	2.043046	1.273730
19	19	H	0	0.461099	1.816082	1.861453
20	20	H	0	0.047920	0.935649	-2.284359
21	21	H	0	-2.423267	-0.492566	1.792214
22	22	H	0	-2.302019	-1.834639	-0.359218
23	23	H	0	-0.230471	-1.390804	-1.775038
24	24	H	0	0.134635	-0.611477	2.385393
25	25	H	0	-2.714972	0.029281	-2.199471
26	26	H	0	-3.623305	0.451876	-0.741487
27	27	H	0	3.324675	-0.648038	-1.194785
28	28	H	0	0.893747	-2.963222	1.053356
29	29	H	0	2.241336	2.388180	0.162912

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.639354	1.371321	-0.831383
2	6	0	-1.515014	1.313071	0.726859
3	6	0	0.035128	1.209597	1.080234
4	6	0	-0.262796	0.767556	-1.269031
5	6	0	0.636975	1.370814	-0.261452
6	6	0	-1.695000	-0.210866	1.049468
7	6	0	-1.883074	-0.842111	-0.358138
8	6	0	-0.438689	-0.782844	-0.912973
9	6	0	0.433951	-1.155704	0.281461
10	6	0	-0.177878	-0.323229	1.399025
11	6	0	-2.636311	0.244122	-1.140121
12	6	0	1.932142	-0.877433	0.115876
13	7	0	2.327000	-0.804578	-1.112755
14	8	0	0.166385	-2.552766	0.563389
15	8	0	2.582600	-0.694360	1.216687
16	8	0	1.638659	2.128944	-0.557940
17	1	0	-1.850893	2.348377	-1.241453
18	1	0	-2.089117	2.043046	1.273730
19	1	0	0.461099	1.816082	1.861453
20	1	0	0.047920	0.935649	-2.284359
21	1	0	-2.423267	-0.492566	1.792214
22	1	0	-2.302019	-1.834639	-0.359218

23	1	0	-0.230471	-1.390804	-1.775038
24	1	0	0.134635	-0.611477	2.385393
25	1	0	-2.714972	0.029281	-2.199471
26	1	0	-3.623305	0.451876	-0.741487
27	1	0	3.324675	-0.648038	-1.194785
28	1	0	0.893747	-2.963222	1.053356
29	1	0	2.241336	2.388180	0.162912

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.564280	0.000000			
3	C	2.546434	1.593273	0.000000		
4	C	1.565561	2.418515	2.408985	0.000000	
5	C	2.346593	2.368787	1.479302	1.479434	0.000000
6	C	2.458458	1.568074	2.238751	2.895507	3.107786
7	C	2.276542	2.440798	3.155617	2.458873	3.355150
8	C	2.467526	2.870607	2.857831	1.600455	2.493948
9	C	3.452951	3.176742	2.528190	2.566790	2.592155
10	C	3.159452	2.217480	1.580049	2.883670	2.508178
11	C	1.536171	2.426020	3.605372	2.433963	3.571540
12	C	4.325481	4.129709	2.980662	3.072737	2.621918
13	N	4.532734	4.757068	3.757497	3.033657	2.883268
14	O	4.539223	4.218829	3.799965	3.816608	4.036868
15	O	5.127039	4.589134	3.183282	4.051207	3.199265
16	O	3.375520	3.501715	2.469843	2.444291	1.290750
17	H	1.080529	2.249206	3.200645	2.240939	2.847019
18	H	2.254995	1.077741	2.290086	3.380526	3.200040
19	H	3.443992	2.333526	1.076837	3.379846	2.176217
20	H	2.268886	3.413597	3.375751	1.075030	2.151396
21	H	3.312380	2.284782	3.073756	3.953070	4.129747
22	H	3.307604	3.421552	4.098982	3.428937	4.349963
23	H	3.241107	3.901344	3.871073	2.217117	3.266487
24	H	4.174467	3.029185	2.242689	3.926131	3.344789
25	H	2.197656	3.413418	4.439894	2.724690	4.097704
26	H	2.188497	2.709721	4.156554	3.416281	4.384617
27	H	5.371355	5.564283	4.409947	3.857378	3.488639
28	H	5.362566	4.918883	4.260325	4.544203	4.536356
29	H	4.133084	3.947665	2.664187	3.308710	1.946559

		6	7	8	9	10
6	C	0.000000				
7	C	1.554090	0.000000			
8	C	2.399303	1.548419	0.000000		
9	C	2.452547	2.424052	1.525516	0.000000	
10	C	1.560921	2.502909	2.371625	1.521939	0.000000
11	C	2.426393	1.535828	2.436349	3.661545	3.579531
12	C	3.804217	3.844712	2.586178	1.532785	2.530969
13	N	4.604801	4.277333	2.772981	2.377134	3.579826
14	O	3.030763	2.824152	2.382936	1.450123	2.405751
15	O	4.308085	4.737525	3.697495	2.388343	2.791277
16	O	4.378556	4.611907	3.594430	3.597892	3.625283
17	H	3.438365	3.310664	3.450618	4.451782	4.112005
18	H	2.299074	3.321081	3.935891	4.193145	3.044304
19	H	3.068649	4.181832	3.906593	3.365802	2.280084

20	H	3.932769	3.255687	2.251822	3.332598	3.899113
21	H	1.077682	2.244550	3.367618	3.299366	2.285835
22	H	2.233720	1.077324	2.210185	2.890839	3.144480
23	H	3.393367	2.244943	1.075233	2.173918	3.349203
24	H	2.300598	3.413400	3.352206	2.193695	1.074091
25	H	3.413740	2.200429	2.737899	4.180303	4.417045
26	H	2.713873	2.202218	3.419901	4.482417	4.129594
27	H	5.515879	5.278095	3.776307	3.285317	4.370495
28	H	3.778504	3.768575	3.224265	2.018504	2.870093
29	H	4.799559	5.264697	4.288992	3.979926	3.838270

		11	12	13	14	15
11	C	0.000000				
12	C	4.868899	0.000000			
13	N	5.072966	1.292577	0.000000		
14	O	4.310410	2.474854	3.245593	0.000000	
15	O	5.802786	1.291664	2.346013	3.117461	0.000000
16	O	4.708169	3.094910	3.063852	5.034220	3.465743
17	H	2.248342	5.153596	5.235694	5.598935	5.912408
18	H	3.059775	5.102975	5.771167	5.168497	5.414941
19	H	4.590692	3.530727	4.381251	4.567128	3.349449
20	H	2.998764	3.549463	3.097621	4.504746	4.619400
21	H	3.030955	4.682715	5.576848	3.529976	5.042882
22	H	2.245620	4.366930	4.801735	2.731287	5.257682
23	H	2.977276	2.918219	2.706093	2.641191	4.165192
24	H	4.565024	2.907313	4.132891	2.662575	2.713904
25	H	1.083774	5.270544	5.224726	4.754218	6.344924
26	H	1.084540	5.776256	6.092836	5.009224	6.607690
27	H	6.027627	1.926032	1.013207	4.085823	2.523493
28	H	5.249734	2.511503	3.377276	0.968296	2.833132
29	H	5.485100	3.280556	3.439240	5.373895	3.275508

		16	17	18	19	20
16	O	0.000000				
17	H	3.562627	0.000000			
18	H	4.154360	2.544823	0.000000		
19	H	2.708872	3.905979	2.626887	0.000000	
20	H	2.633424	2.586299	4.295725	4.258360	0.000000
21	H	5.375386	4.195439	2.609561	3.695161	4.976445
22	H	5.592711	4.298776	4.212872	5.088611	4.111311
23	H	4.166965	4.109983	4.953875	4.897597	2.397768
24	H	4.293624	5.084985	3.636944	2.504823	4.920132
25	H	5.104636	2.653797	4.063258	5.456298	2.909000
26	H	5.525804	2.643506	2.991096	5.031770	4.011531
27	H	3.310566	5.980567	6.530286	4.859273	3.798994
28	H	5.392710	6.404084	5.831703	4.866411	5.201630
29	H	0.974706	4.326681	4.483956	2.526178	3.593057

		21	22	23	24	25
21	H	0.000000				
22	H	2.538607	0.000000			
23	H	4.282578	2.548107	0.000000		
24	H	2.628471	3.868630	4.248510	0.000000	
25	H	4.036207	2.651652	2.893015	5.436158	0.000000
26	H	2.958328	2.668348	3.996877	5.003020	1.769003
27	H	6.479596	5.810841	3.677968	4.795347	6.159991
28	H	4.201504	3.671782	3.425810	2.807361	5.706033

29	H	5.719426	6.224701	4.913879	4.286672	5.975805
		26	27	28	29	
26	H	0.000000				
27	H	7.049093	0.000000			
28	H	5.940380	4.040250	0.000000		
29	H	6.241893	3.497940	5.589847	0.000000	

Interatomic angles:

C1-C2-C3=107.499	C2-C1-C4=101.1989	C1-C4-C3= 76.4295
C2-C3-C4= 71.0526	C2-C1-C5= 71.3943	C1-C5-C3= 79.9587
C2-C3-C5=100.8125	C1-C4-C5=100.7847	C2-C5-C4= 73.8406
C3-C5-C4=109.0155	C1-C2-C6=103.4153	C1-C6-C3= 65.4608
C3-C2-C6= 90.1678	C4-C1-C6= 89.1735	C4-C2-C6= 90.5733
C4-C3-C6= 76.9734	C5-C1-C6= 80.5611	C5-C2-C6=102.3454
C5-C3-C6=111.7834	C5-C4-C6= 83.8735	C2-C1-C7= 76.4218
C3-C1-C7= 81.5233	C3-C2-C7=100.8338	C4-C1-C7= 77.1312
C4-C2-C7= 60.7951	C3-C4-C7= 80.8134	C5-C1-C7= 93.0468
C5-C2-C7= 88.4558	C5-C4-C7=114.5447	C1-C7-C6= 77.3148
C2-C6-C7=102.844	C3-C6-C7=111.327	C4-C7-C6= 89.4205
C2-C1-C8= 87.808	C3-C1-C8= 69.4765	C2-C3-C8= 74.2929
C1-C4-C8=102.4019	C2-C4-C8= 88.7396	C3-C4-C8= 88.5326
C5-C1-C8= 62.3432	C2-C5-C8= 72.3086	C3-C5-C8= 88.129
C5-C4-C8=108.0793	C1-C6-C8= 61.0411	C2-C6-C8= 90.1894
C3-C6-C8= 75.9861	C4-C8-C6= 90.4913	C5-C8-C6= 78.8312
C1-C7-C8= 77.7858	C2-C7-C8= 89.1304	C3-C8-C7= 86.068
C4-C8-C7=102.6687	C5-C8-C7=109.9851	C6-C7-C8=101.3099
C1-C3-C9= 85.7545	C2-C3-C9= 98.289	C1-C4-C9=111.0252
C2-C4-C9= 79.1085	C4-C3-C9= 62.5949	C1-C5-C9= 88.5733
C2-C5-C9= 79.4963	C5-C3-C9= 75.595	C5-C4-C9= 74.2787
C1-C6-C9= 89.3532	C2-C6-C9=102.1423	C3-C6-C9= 65.0325
C4-C9-C6= 70.4194	C5-C9-C6= 76.0003	C1-C7-C9= 94.4909
C2-C7-C9= 81.5354	C3-C9-C7= 79.1375	C4-C7-C9= 63.4215
C5-C9-C7= 83.887	C6-C7-C9= 72.4154	C1-C8-C9=117.7639
C2-C8-C9= 86.8852	C3-C9-C8= 85.8982	C4-C8-C9=110.3708
C5-C8-C9= 76.1017	C6-C8-C9= 73.5834	C7-C8-C9=104.104
C1-C2-C10=112.1703	C1-C3-C10= 97.1476	C2-C3-C10= 88.6587
C1-C4-C10= 85.0162	C4-C2-C10= 76.7913	C4-C3-C10= 90.1188
C1-C5-C10= 81.1287	C5-C2-C10= 66.2121	C5-C3-C10=110.0941
C4-C5-C10= 88.7328	C1-C6-C10=101.2831	C2-C6-C10= 90.2562
C3-C10-C6= 90.9174	C4-C10-C6= 74.7489	C5-C10-C6= 96.8279
C1-C7-C10= 82.6136	C7-C2-C10= 64.7932	C3-C10-C7= 98.7031
C4-C7-C10= 71.0603	C5-C10-C7= 84.0639	C7-C6-C10=106.9309
C1-C8-C10= 81.4942	C2-C10-C8= 77.361	C3-C10-C8= 90.3519
C4-C8-C10= 90.9774	C5-C8-C10= 62.0008	C6-C10-C8= 71.8656
C7-C8-C10= 76.1539	C2-C10-C9=115.0526	C3-C10-C9=109.1649
C4-C9-C10= 85.6754	C5-C10-C9= 75.6826	C6-C10-C9=105.4061
C7-C9-C10= 74.8546	C8-C9-C10=102.1978	C2-C1-C11=102.9714
C3-C1-C11=122.0754	C3-C2-C11=126.2814	C4-C1-C11=103.3838
C4-C2-C11= 60.3194	C3-C4-C11= 96.2238	C5-C1-C11=132.7039
C5-C2-C11= 96.2897	C5-C4-C11=130.1433	C1-C11-C6= 72.8099
C6-C2-C11= 71.1591	C3-C6-C11=101.1415	C4-C11-C6= 73.1306
C1-C11-C7= 95.644	C2-C11-C7= 72.1286	C4-C11-C7= 72.5906
C6-C7-C11=103.4881	C1-C11-C8= 72.8523	C2-C11-C8= 72.3665
C3-C8-C11= 85.4516	C8-C4-C11= 70.896	C5-C8-C11= 92.8316
C8-C6-C11= 60.6424	C8-C7-C11=104.3578	C9-C4-C11= 94.1045

C9-C6-C11= 97.2625 C9-C7-C11=133.9978 C9-C8-C11=133.7889
C10-C2-C11=100.7683 C10-C4-C11= 84.1667 C10-C6-C11=126.345
C10-C7-C11=123.0222 C10-C8-C11= 96.2228 C1-C3-C12=102.7148
C2-C3-C12=126.365 C4-C3-C12= 68.5745 C1-C5-C12=120.9523
C2-C5-C12=111.5813 C3-C5-C12= 88.6819 C4-C5-C12= 92.7968
C6-C3-C12= 92.4724 C1-C8-C12=117.7002 C2-C8-C12= 98.2315
C3-C8-C12= 66.1743 C4-C8-C12= 91.3286 C5-C8-C12= 62.1124
C6-C8-C12= 99.401 C7-C8-C12=135.3317 C3-C9-C12= 91.0585
C4-C9-C12= 93.6714 C5-C9-C12= 73.9707 C6-C9-C12=144.3267
C7-C9-C12=151.9192 C8-C9-C12=115.4779 C2-C10-C12=120.7045
C3-C10-C12= 89.871 C4-C10-C12= 68.7957 C5-C10-C12= 62.7042
C6-C10-C12=135.44 C7-C10-C12= 99.5934 C8-C10-C12= 63.5774
C10-C9-C12=111.8981 C11-C8-C12=151.5716 C1-C5-N13=119.8051
C2-C5-N13=129.5907 C3-C5-N13=115.0896 C4-C5-N13= 81.2426
C1-C8-N13=119.6389 C2-C8-N13=114.8876 C3-C8-N13= 83.7051
C4-C8-N13= 83.2205 C5-C8-N13= 66.1348 C6-C8-N13=125.6643
C7-C8-N13=162.916 C3-C9-N13= 99.9471 C4-C9-N13= 75.5938
C5-C9-N13= 70.7807 C6-C9-N13=144.8895 C7-C9-N13=125.968
C8-C9-N13= 87.7199 C10-C5-N13= 82.8947 C10-C8-N13= 87.8263
C10-C9-N13=132.0689 C11-C8-N13=153.6668 C3-C12-N13=117.5477
C5-C12-N13= 88.0387 C8-C12-N13= 84.2515 C9-C12-N13=114.2994
C10-C12-N13=136.4049 C1-C7-O14=125.3854 C2-C7-O14=106.2819
C4-C7-O14= 92.2473 C6-C7-O14= 82.1064 C1-C8-O14=138.7198
C2-C8-O14=106.4745 C3-C8-O14= 92.5002 C4-C8-O14=146.042
C5-C8-O14=111.7176 C6-C8-O14= 78.6544 C7-C8-O14= 89.2224
C3-C9-O14=144.1747 C4-C9-O14=142.1129 C5-C9-O14=173.8183
C6-C9-O14= 98.6329 C7-C9-O14= 89.9751 C8-C9-O14=106.3885
C2-C10-O14=131.6716 C3-C10-O14=144.0649 C4-C10-O14= 91.9136
C5-C10-O14=110.4562 C6-C10-O14= 97.3547 C7-C10-O14= 70.2151
C10-C8-O14= 60.7934 C10-C9-O14=108.0612 C11-C7-O14=161.889
C11-C8-O14=126.8616 C3-C12-O14= 87.7877 C5-C12-O14=104.7171
C7-O14-C12= 92.7927 C8-O14-C12= 64.2998 C12-C9-O14=112.1018
C10-O14-C12= 62.4547 N13-C8-O14= 77.6175 N13-C9-O14=113.7828
N13-C12-O14=115.3399 C3-C9-O15= 80.6469 C4-C9-O15=109.6337
C5-C9-O15= 79.8211 C6-C9-O15=125.7254 C7-C9-O15=159.7598
C8-C9-O15=140.7148 C2-C10-O15=132.4275 C3-C10-O15= 88.9964
C4-C10-O15= 91.0874 C5-C10-O15= 74.0536 C6-C10-O15=162.9713
C7-C10-O15=126.8945 C8-C10-O15= 91.1064 C10-C9-O15= 88.1929
C3-C12-O15= 86.8773 C5-C12-O15=104.4699 C8-C12-O15=142.7034
C9-C12-O15=115.2064 C10-C12-O15= 87.5195 C5-N13-O15= 74.6476
C8-N13-O15= 92.1066 C9-N13-O15= 60.7471 C10-O15-N13= 87.9003
N13-C12-O15=130.4103 O14-C9-O15=106.0193 O14-C10-O15= 73.2956
O14-C12-O15=107.5258 C1-C3-O16= 84.5699 C2-C3-O16=117.412
C1-C4-O16=112.8227 C2-C4-O16= 92.1242 C3-C4-O16= 61.1763
C1-C5-O16=134.1784 C2-C5-O16=144.6048 C3-C5-O16=126.0206
C4-C5-O16=123.7137 C6-C3-O16=136.7861 C6-C4-O16=109.8793
C7-C4-O16=140.3044 C8-C3-O16= 84.523 C8-C4-O16=124.0779
C8-C5-O16=141.437 C9-C3-O16= 92.0786 C9-C4-O16= 91.7439
C9-C5-O16=132.9512 C10-C3-O16=125.6231 C10-C4-O16= 85.3312
C10-C5-O16=143.2156 C11-C4-O16=149.6514 C12-C3-O16= 68.459
C12-C5-O16= 98.8214 N13-C5-O16= 85.4374 C2-C1-H17=115.2949
C3-C1-H17=118.1033 C3-C2-H17=111.671 C4-C1-H17=114.5049
C2-H17-C4= 65.1802 C3-C4-H17= 86.9159 C5-C1-H17=106.3963
C5-C2-H17= 76.0737 C3-C5-H17= 89.6618 C5-C4-H17= 97.7573

C6-C1-H17=150.21 C6-C2-H17=127.6072 C6-C4-H17= 82.9916
C7-C1-H17=159.5708 C7-C2-H17= 89.7082 C7-C4-H17= 89.4418
C8-C1-H17=150.7056 C8-C2-H17= 83.8092 C8-C4-H17=127.0666
C8-C5-H17= 80.1941 C9-C4-H17=135.5205 C9-C5-H17=109.7747
C10-C2-H17=134.025 C10-C4-H17=106.0407 C10-C5-H17=100.1309
C11-C1-H17=117.3985 C2-H17-C11= 65.2869 C4-H17-C11= 65.663
C5-H17-C11= 88.1886 C6-C11-H17= 94.6258 C7-C11-H17=120.901
C8-C11-H17= 94.7958 C12-C5-H17=140.862 N13-C5-H17=132.0391
O16-C4-H17= 98.9058 O16-C5-H17=113.416 C1-C2-H18=115.97
C1-H18-C3= 68.1427 C3-C2-H18=116.7255 C4-C1-H18=123.4507
C4-C2-H18=147.9231 C4-C3-H18= 91.975 C5-C1-H18= 88.0981
C5-C2-H18=132.7761 C5-C3-H18=114.4786 C1-H18-C6= 65.3368
C6-C2-H18=119.5193 C6-C3-H18= 61.0026 C4-C6-H18= 80.3066
C7-C1-H18= 94.2559 C7-C2-H18=138.013 C7-C6-H18=117.7626
C8-C1-H18=112.8284 C8-C2-H18=169.7778 C8-C3-H18= 99.1415
C8-C6-H18=113.7818 C9-C3-H18=120.898 C9-C6-H18=123.8508
C10-C2-H18=131.8514 C10-C3-H18=102.179 C10-C6-H18=102.4355
C11-C1-H18=106.0667 C11-C2-H18=116.278 C11-C6-H18= 80.6589
C12-C3-H18=150.7521 O16-C3-H18=121.5203 H17-C1-H18= 92.6296
H17-C2-H18= 93.023 C3-H18-H17= 82.7225 C4-H17-H18= 89.6485
C5-H17-H18= 72.5661 C6-H18-H17= 90.2962 C11-H17-H18= 79.0741
C1-C2-H19=122.9306 C1-C3-H19=140.2615 C2-C3-H19=120.6102
C4-C2-H19= 90.6538 C4-C3-H19=149.2896 C1-C5-H19= 99.1189
C2-H19-C5= 63.2583 C5-C3-H19=115.8278 C4-C5-H19=134.3189
C6-C2-H19=101.9267 C6-C3-H19=132.301 C7-C2-H19=122.2875
C8-C2-H19= 96.7546 C8-C3-H19=164.6297 C8-C5-H19=113.3703
C9-C3-H19=133.9262 C9-C5-H19= 89.3572 C2-C10-H19= 62.491
C10-C3-H19=116.9577 C4-C10-H19= 80.8506 C5-H19-C10= 68.4589
C6-C10-H19=104.4927 C7-C10-H19=121.8584 C8-C10-H19=114.2277
C9-C10-H19=123.3312 C11-C2-H19=149.3791 C12-C3-H19=112.1673
C12-C5-H19= 94.3001 C12-C10-H19= 94.2804 N13-C5-H19=119.3253
O14-C10-H19=154.1421 O15-C10-H19= 82.0013 C2-H19-O16= 87.6367
O16-C3-H19= 90.8433 C4-O16-H19= 81.7982 O16-C5-H19= 99.5911
C10-H19-O16= 92.8114 H17-C2-H19=116.9191 H17-C5-H19=101.2395
C1-H18-H19= 89.3981 H18-C2-H19= 93.3471 H18-C3-H19= 95.7771
C5-H19-H18= 82.9857 C6-H18-H19= 76.7441 C10-H19-H18= 76.3274
O16-H19-H18=102.2521 H17-H18-H19= 98.0834 C2-C1-H20=124.8659
C3-C1-H20= 88.8274 C1-C4-H20=117.249 C2-C4-H20=153.3552
C3-C4-H20=148.9385 C1-H20-C5= 64.0638 C2-C5-H20= 97.9687
C3-C5-H20=136.0022 C5-C4-H20=113.8092 C6-C1-H20=112.5313
C6-C4-H20=162.1858 C7-C1-H20= 91.4922 C7-C4-H20=129.9931
C1-H20-C8= 66.1612 C2-C8-H20= 82.6297 C3-C8-H20= 81.7709
C8-C4-H20=113.1633 C5-H20-C8= 68.9546 C6-C8-H20=115.4259
C7-C8-H20=116.6802 C9-C4-H20=127.5328 C9-C5-H20= 88.759
C9-C8-H20=122.6668 C10-C4-H20=157.5902 C10-C5-H20=113.3857
C10-C8-H20=114.9633 C11-C1-H20=102.2994 C2-C11-H20= 77.1921
C11-C4-H20=111.4384 C5-H20-C11= 86.1552 C6-C11-H20= 92.3106
C7-C11-H20= 85.318 C11-C8-H20= 79.4238 C12-C5-H20= 95.5737
C12-C8-H20= 94.1341 N13-C5-H20= 74.3509 N13-C8-H20= 75.3199
O14-C8-H20=152.7828 C1-H20-O16= 86.6964 C3-O16-H20= 82.7601
O16-C4-H20= 87.87 O16-C5-H20= 96.6212 C8-H20-O16= 94.4214
C11-H20-O16=113.2687 H17-C1-H20= 94.3694 C2-H17-H20= 89.531
H17-C4-H20= 96.0934 C5-H20-H17= 73.2242 C8-H20-H17= 90.7237
C11-H17-H20= 76.3151 O16-H20-H17= 86.0786 H18-C1-H20=143.4513

H18-H17-H20=113.6867 H19-C5-H20=159.4718 H19-O16-H20=105.7
C1-C2-H21=117.5365 C3-C2-H21=103.416 C4-C2-H21=114.3538
C5-C2-H21=125.0961 C1-C6-H21=135.3001 C2-C6-H21=118.255
C3-C6-H21=132.7361 C4-C6-H21=167.02 C1-C7-H21= 94.2154
C2-H21-C7= 65.2087 C4-C7-H21=114.302 C7-C6-H21=115.8674
C8-C2-H21= 80.7003 C8-C6-H21=148.787 C8-C7-H21=124.182
C9-C6-H21=134.5659 C9-C7-H21= 89.8514 C10-C2-H21= 61.0008
C3-C10-H21=103.8273 C4-C10-H21= 99.105 C5-C10-H21=118.8842
C10-C6-H21=118.924 C7-H21-C10= 67.0663 C8-C10-H21= 92.5967
C9-C10-H21=118.7299 C11-C2-H21= 80.0311 C11-C6-H21=114.1293
C11-C7-H21=105.0473 C12-C10-H21=152.8625 O14-C7-H21= 87.4995
O14-C10-H21= 97.5656 O15-C10-H21=166.6192 H17-C2-H21=135.4351
C1-H18-H21= 85.5022 H18-C2-H21= 94.9863 C3-H18-H21= 77.4048
H18-C6-H21= 94.1971 C7-H21-H18= 85.9948 C10-H21-H18= 76.5887
H17-H18-H21=108.962 H19-C2-H21=106.2767 H19-C10-H21=108.0535
H19-H18-H21= 89.7654 C1-C6-H22= 89.5134 C2-C6-H22=127.4393
C3-C6-H22=132.8368 C4-C6-H22= 82.8241 C1-C7-H22=159.5821
C2-C7-H22=150.7586 C4-C7-H22=149.2032 C6-C7-H22=114.9724
C1-C8-H22= 89.8248 C2-C8-H22= 83.5826 C3-C8-H22=107.2663
C4-C8-H22=127.5459 C5-C8-H22=135.1635 C6-H22-C8= 65.3523
C8-C7-H22=113.4315 C3-C9-H22= 98.0738 C4-C9-H22= 77.596
C5-C9-H22=104.8696 C9-C6-H22= 76.0167 C9-C7-H22=104.6424
C9-C8-H22= 99.7746 C10-C6-H22=110.6726 C10-C7-H22=117.1701
C10-C8-H22= 86.5998 C10-C9-H22= 84.8785 C1-C11-H22=120.8472
C2-C11-H22= 94.098 C4-C11-H22= 94.1476 C6-H22-C11= 65.5962
C11-C7-H22=117.4104 C8-H22-C11= 66.2874 C9-H22-C11= 90.0316
C12-C8-H22=130.9792 C12-C9-H22=160.6934 N13-C8-H22=148.7784
N13-C9-H22=131.178 C6-H22-O14= 74.4849 C7-H22-O14= 83.7104
O14-C8-H22= 72.8652 C9-O14-H22= 81.2441 C10-O14-H22= 75.1871
C11-H22-O14=119.6956 C12-O14-H22=113.9376 O15-C9-H22=169.6071
H17-C11-H22=146.103 H18-C6-H22=136.6846 H20-C8-H22=134.2623
H20-C11-H22=102.2928 C2-H21-H22= 90.2088 H21-C6-H22= 93.4964
H21-C7-H22= 92.9144 C8-H22-H21= 90.0583 C9-H22-H21= 74.5272
C10-H21-H22= 81.1685 C11-H22-H21= 78.3587 O14-H22-H21= 84.0241
H18-H21-H22=109.8272 C1-C4-H23=116.8756 C2-C4-H23=114.5492
C3-C4-H23=113.5407 C5-C4-H23=122.9239 C6-C4-H23= 82.0102
C1-C7-H23= 91.583 C2-C7-H23=112.6666 C4-H23-C7= 66.8765
C6-C7-H23=125.5808 C1-C8-H23=127.905 C2-C8-H23=160.637
C3-C8-H23=157.114 C4-C8-H23=110.3704 C5-C8-H23=127.8937
C6-C8-H23=153.1201 C7-C8-H23=116.5053 C3-C9-H23=110.6003
C4-H23-C9= 71.5351 C5-C9-H23= 86.0557 C6-C9-H23= 94.1627
C7-H23-C9= 66.5153 C9-C8-H23=112.2577 C10-C4-H23= 80.9379
C10-C7-H23= 89.5556 C10-C8-H23=150.4437 C10-C9-H23=129.1187
C1-C11-H23= 85.4904 C2-C11-H23= 91.8674 C11-C4-H23= 79.4526
C6-C11-H23= 77.0549 C11-C7-H23=102.2715 C11-C8-H23=109.771
C9-H23-C11= 89.1892 C3-C12-H23= 82.0199 C4-H23-C12= 72.041
C5-C12-H23= 72.0325 C7-H23-C12= 95.3692 C12-C8-H23= 96.9354
C12-C9-H23=102.4844 C10-C12-H23= 75.4757 C11-H23-C12=111.3492
C4-H23-N13= 75.3468 C5-N13-H23= 71.4428 C7-H23-N13=119.2289
C8-H23-N13= 82.2013 N13-C9-H23= 72.8146 C11-H23-N13=126.3372
C12-N13-H23= 86.0846 C4-H23-O14=103.2032 C7-H23-O14= 70.0826
O14-C8-H23= 91.581 O14-C9-H23= 91.337 C10-O14-H23= 83.0107
C11-H23-O14=100.0318 C12-O14-H23= 69.4696 N13-H23-O14= 74.7291
O15-C9-H23=131.7805 O15-C12-H23=161.8696 O15-N13-H23=110.8642

O16-C4-H23=126.6739 H17-C4-H23=134.4169 H17-C11-H23=102.8293
C1-H20-H23= 87.9334 H20-C4-H23= 86.1268 C5-H20-H23= 91.6226
C7-H23-H20= 88.9911 H20-C8-H23= 84.3406 C9-H23-H20= 93.47
C11-H23-H20= 66.8161 C12-H23-H20= 83.1604 N13-H23-H20= 74.4589
O14-H23-H20=126.6891 O16-H20-H23=111.7487 H17-H20-H23=111.0445
H21-C7-H23=145.0742 C4-H23-H22= 91.7708 C6-H22-H23= 90.164
H22-C7-H23= 93.4663 H22-C8-H23= 95.4547 C9-H23-H22= 75.0299
C11-H22-H23= 76.5005 C12-H23-H22=105.8477 N13-H23-H22=132.0728
O14-H23-H22= 63.4859 H20-H23-H22=112.4215 H21-H22-H23=114.6856
C1-C3-H24=121.1733 C2-C3-H24=103.0016 C4-C3-H24=115.0888
C5-C3-H24=126.7458 C1-C6-H24=122.5695 C2-C6-H24=101.3859
C6-C3-H24= 61.7759 C4-C6-H24= 97.4949 C7-C6-H24=123.4677
C8-C3-H24= 81.2067 C8-C6-H24= 90.9752 C3-H24-C9= 69.4731
C4-C9-H24=110.8803 C5-C9-H24= 88.2669 C6-H24-C9= 66.0955
C7-C9-H24= 95.195 C8-C9-H24=127.7521 C2-C10-H24=130.6805
C3-C10-H24=113.979 C4-C10-H24=163.6875 C5-C10-H24=134.0022
C6-C10-H24=120.515 C7-C10-H24=141.9339 C8-C10-H24=151.0719
C9-C10-H24=114.2409 C11-C6-H24=149.9051 C3-H24-C12= 69.3548
C5-C12-H24= 74.2458 C6-H24-C12= 93.1147 C8-C12-H24= 74.9547
C12-C9-H24=101.0657 C12-C10-H24= 99.4534 N13-C9-H24=129.3848
N13-C12-H24=157.777 C3-H24-O14=101.2054 C6-H24-O14= 74.8754
C7-O14-H24= 76.8796 C8-O14-H24= 83.073 O14-C9-H24= 91.5685
O14-C10-H24= 91.641 C12-O14-H24= 68.8191 C3-H24-O15= 79.2926
C6-H24-O15=118.2038 O15-C9-H24= 72.4987 C10-H24-O15= 82.8294
C12-O15-H24= 85.2447 N13-O15-H24=109.3146 O14-H24-O15= 70.8703
O16-C3-H24=131.2574 H18-C3-H24=106.7086 H18-C6-H24=104.5013
C2-H19-H24= 77.4332 H19-C3-H24= 91.0072 C5-H19-H24= 90.9332
C6-H24-H19= 79.2472 C9-H24-H19= 91.2628 H19-C10-H24= 89.0838
C12-H24-H19= 81.071 O14-H24-H19=124.1887 O15-H24-H19= 79.7443
O16-H19-H24=110.8185 H18-H19-H24= 90.2294 C2-H21-H24= 75.7668
C3-H24-H21= 77.8046 H21-C6-H24= 95.2615 C7-H21-H24= 88.5646
C9-H24-H21= 85.8461 H21-C10-H24= 96.198 C12-H24-H21=115.4449
O14-H24-H21= 83.6939 O15-H24-H21=141.4431 H18-H21-H24= 87.9476
H19-H24-H21= 92.0508 H22-C6-H24=117.1128 H22-C9-H24= 98.1455
H22-O14-H24= 91.6432 H22-H21-H24= 96.9417 H23-C9-H24=153.1773
H23-C12-H24= 93.6538 H23-O14-H24=106.4577 C2-C1-H25=129.5152
C3-C1-H25=138.6242 C4-C1-H25= 91.193 C2-C4-H25= 82.9319
C3-C4-H25=119.6066 C5-C1-H25=128.7444 C5-C4-H25=152.9254
C6-C1-H25= 94.139 C6-C4-H25= 74.735 C1-H25-C7= 62.3456
C2-C7-H25= 94.5496 C4-C7-H25= 71.3301 C6-C7-H25=130.0033
C8-C1-H25= 71.6061 C2-C8-H25= 74.9369 C3-C8-H25=104.9967
C8-C4-H25= 73.416 C5-C8-H25=103.0142 C6-C8-H25= 83.0088
C8-C7-H25= 92.158 C9-C4-H25=104.3326 C9-C7-H25=129.3011
C9-C8-H25=156.3467 C10-C4-H25=103.8842 C10-C7-H25=139.7249
C10-C8-H25=119.4732 C1-C11-H25=112.893 C2-C11-H25=150.8225
C4-C11-H25= 93.5339 C6-C11-H25=150.8155 C7-C11-H25=113.1463
C8-C11-H25= 94.1887 C12-C8-H25=163.7296 N13-C8-H25=142.9095
O14-C7-H25=141.9321 O14-C8-H25=136.265 O16-C4-H25=161.8733
H17-C1-H25=102.716 C2-H17-H25= 87.839 C4-H17-H25= 67.0358
C5-H17-H25= 96.2422 C7-H25-H17= 85.4621 C8-H25-H17= 79.565
H17-C11-H25= 99.6036 H18-C1-H25=131.7156 H18-H17-H25=102.7951
H20-C1-H25= 81.2604 H20-C4-H25= 88.8523 C5-H20-H25=107.1955
C7-H25-H20= 77.8033 H20-C8-H25= 70.5567 C11-H25-H20= 84.1355
O16-H20-H25=134.0888 H20-H17-H25= 67.4268 H21-C7-H25=130.4685

C1-H25-H22= 85.4691 C4-H25-H22= 79.2406 C6-H22-H25= 88.2239
H22-C7-H25=102.5318 C8-H22-H25= 67.8459 C9-H22-H25= 97.8229
H22-C11-H25= 99.6256 O14-H22-H25=124.0552 H17-H25-H22=108.2421
H20-H25-H22= 95.2415 H21-H22-H25=102.0699 C1-H25-H23= 77.7663
H23-C4-H25= 70.8167 H23-C7-H25= 81.1961 H23-C8-H25= 87.2481
C9-H23-H25=110.3758 C11-H25-H23= 83.7753 C12-H23-H25=130.1761
N13-H23-H25=137.8333 O14-H23-H25=118.3517 H17-H25-H23= 95.5303
H20-H23-H25= 65.9382 H23-H22-H25= 67.577 C2-C1-H26= 90.8879
C3-C1-H26=122.5884 C3-C2-H26=148.9291 C4-C1-H26=130.2822
C4-C2-H26= 83.3369 C5-C1-H26=150.3802 C5-C2-H26=119.2421
C6-C1-H26= 71.1964 C6-C2-H26= 73.34 C3-C6-H26=113.7804
C4-C6-H26= 74.9605 C1-H26-C7= 62.4611 C2-C7-H26= 71.1988
C4-C7-H26= 94.1045 C6-C7-H26= 90.8383 C8-C1-H26= 94.3411
C8-C2-H26= 75.5302 C8-C6-H26= 83.7133 C8-C7-H26=130.7122
C9-C6-H26=120.279 C9-C7-H26=151.315 C10-C2-H26=113.5092
C10-C6-H26=148.8663 C10-C7-H26=122.5992 C1-C11-H26=112.0975
C2-C11-H26= 93.0587 C4-C11-H26=149.9659 C6-C11-H26= 93.2841
C7-C11-H26=113.2453 C8-C11-H26=150.1536 O14-C7-H26=170.4589
H17-C1-H26=102.592 C2-H17-H26= 66.6958 C4-H17-H26= 88.3606
C5-H17-H26=105.9298 C6-H26-H17= 79.8405 C7-H26-H17= 85.6783
H17-C11-H26= 98.9281 H18-C1-H26= 84.6058 H18-C2-H26= 94.3453
C3-H18-H26=103.0173 H18-C6-H26= 72.7321 C7-H26-H18= 77.8764
C11-H26-H18= 83.2671 H18-H17-H26= 70.3807 H19-C2-H26=172.2459
H19-H18-H26=127.0652 H20-C1-H26=128.3004 H20-C11-H26=155.5993
H20-H17-H26=100.174 C1-H26-H21= 78.5549 H21-C2-H26= 72.074
H21-C6-H26= 92.2064 H21-C7-H26= 83.4012 C10-H21-H26=103.1498
C11-H26-H21= 83.3666 H17-H26-H21= 96.8367 H18-H21-H26= 64.6322
C1-H26-H22= 85.2391 C2-H26-H22= 79.0147 C6-H22-H26= 66.5466
H22-C7-H26=103.5247 C8-H22-H26= 88.4975 C9-H22-H26=107.4061
H22-C11-H26=100.6602 O14-H22-H26=136.1541 H17-H26-H22=108.0504
H18-H26-H22= 96.047 H21-H22-H26= 69.191 H23-C7-H26=127.9854
H23-C11-H26=156.7751 H23-H22-H26=100.0032 H24-C6-H26=172.228
H24-H21-H26=127.0478 C1-H26-H25= 66.4861 C2-H26-H25= 97.0668
C4-H25-H26= 96.6579 C6-H26-H25= 96.9338 C7-H25-H26= 66.362
C8-H25-H26= 96.3434 H25-C11-H26=109.3415 H17-H26-H25= 70.8061
H18-H26-H25=114.7713 H20-H25-H26=115.9318 H21-H26-H25=114.9186
H22-H25-H26= 71.089 H23-H25-H26=115.9326 C3-C12-H27=126.6498
C5-C12-H27= 99.0379 C8-C12-H27=112.8131 C9-C12-H27=143.3047
C10-C12-H27=157.1722 C5-N13-H27=118.9797 C8-N13-H27=170.6459
C9-N13-H27=148.6996 C12-N13-H27=112.7345 O14-C12-H27=136.0153
C9-O15-H27= 83.9096 C10-O15-H27=110.5366 O15-C12-H27=101.4771
O15-N13-H27= 88.0429 H23-C12-H27= 96.6504 H23-N13-H27=160.7774
H24-C12-H27=165.3142 H24-O15-H27=132.5482 C3-C9-H28=138.8416
C4-C9-H28=164.5358 C5-C9-H28=159.2366 C6-C9-H28=115.0219
C7-C9-H28=115.7521 C8-C9-H28=130.4351 C2-C10-H28=150.1565
C3-C10-H28=144.8555 C4-C10-H28=104.3296 C5-C10-H28=114.8487
C6-C10-H28=113.7122 C7-C10-H28= 88.8042 C8-C10-H28= 75.2495
C10-C9-H28=107.4923 C3-C12-H28=101.3964 C5-C12-H28=124.1676
C8-C12-H28= 78.454 C12-C9-H28= 88.9245 C10-C12-H28= 69.3854
N13-C9-H28=100.0876 N13-C12-H28=121.8651 C7-O14-H28=165.239
C8-O14-H28=144.9935 C9-O14-H28=111.6022 C10-O14-H28=108.94
C12-O14-H28= 80.9383 O15-C9-H28= 79.5312 C10-O15-H28= 61.3613
O15-C12-H28= 90.4468 N13-O15-H28= 80.8039 O14-H28-O15= 97.9024
H19-C10-H28=141.5202 H21-C10-H28=108.6233 H22-C9-H28= 95.1653

H22-O14-H28=163.9989 H23-C9-H28=109.5441 H23-C12-H28= 77.8407
H23-O14-H28=138.3624 C3-H24-H28=114.588 C6-H24-H28= 94.8987
H24-C9-H28= 83.4814 C10-H24-H28= 82.4008 C12-H28-H24= 65.996
H24-O14-H28= 88.3816 O15-H24-H28= 61.7177 H19-H24-H28=132.6389
H21-H24-H28=101.184 H27-C12-H28=130.6818 H27-O15-H28= 97.7531
C1-C3-H29=104.9494 C2-C3-H29=134.4739 C4-C3-H29= 81.246
C1-C5-H29=148.4693 C2-C5-H29=132.1097 C3-C5-H29=101.2188
C4-C5-H29=149.6394 C6-C3-H29=156.3361 C8-C3-H29=101.863
C8-C5-H29=149.743 C9-C3-H29=100.0472 C9-C5-H29=121.8912
C10-C3-H29=127.6086 C10-C5-H29=118.4532 C12-C3-H29= 70.8111
C12-C5-H29= 90.5529 N13-C5-H29= 88.6015 C3-O16-H29= 90.5678
C4-O16-H29=147.5953 C5-O16-H29=117.7867 H17-C5-H29=128.0111
H18-C3-H29=129.5108 C2-H19-H29=108.5829 C3-H19-H29= 85.3267
H19-C5-H29= 75.3452 C10-H19-H29=105.8793 O16-H29-H19= 90.074
H18-H19-H29=120.9405 H20-C5-H29=122.437 H20-O16-H29=168.1967
H24-C3-H29=121.5237 H24-H19-H29=116.8704

Stoichiometry C12H13NO3
Framework group C1[X(C12H13NO3)]
Deg. of freedom 81
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.042804	0.978405	-0.358996
2	6	0	-1.701809	0.620879	1.125211
3	6	0	-0.148231	0.901024	1.340689
4	6	0	-0.625327	0.914389	-1.020541
5	6	0	0.204644	1.519671	0.044121
6	6	0	-1.421209	-0.920993	1.072759
7	6	0	-1.617740	-1.256917	-0.431809
8	6	0	-0.329272	-0.658215	-1.047447
9	6	0	0.761909	-1.010435	-0.041235
10	6	0	0.102750	-0.657952	1.284497
11	6	0	-2.731991	-0.295471	-0.870936
12	6	0	2.094497	-0.276934	-0.229958
13	7	0	2.288639	0.174239	-1.425578
14	8	0	0.919465	-2.450932	-0.096024
15	8	0	2.811896	-0.156136	0.837348
16	8	0	0.917230	2.583228	-0.120512
17	1	0	-2.561578	1.915611	-0.500641
18	1	0	-2.373140	1.013366	1.871398
19	1	0	0.198822	1.420037	2.218048
20	1	0	-0.508755	1.383123	-1.980952
21	1	0	-1.941771	-1.558244	1.768693
22	1	0	-1.750857	-2.303362	-0.650579
23	1	0	-0.081612	-0.975436	-2.044524
24	1	0	0.609210	-1.049911	2.146784
25	1	0	-2.889837	-0.287596	-1.943126
26	1	0	-3.676567	-0.477691	-0.370137
27	1	0	3.187511	0.629754	-1.531049

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   28          1             0        1.788694   -2.727099    0.229198
   29          1             0        1.518172    2.843784    0.601313
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9404643      0.6630259      0.5395908
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,N-
14,O-16,
 O-16,O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1
 Standard basis: 3-21+G* (6D, 7F)
 There are   234 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    131072 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
   234 basis functions      343 primitive gaussians
    58 alpha electrons       58 beta electrons
       nuclear repulsion energy      1231.4501668083 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   234 RedAO= T  NBF=   234
 NBsUse=   234 1.00D-04 NBFU=   234
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -736.887954090     A.U. after   18 cycles
            Convg  =    0.5326D-08             -V/T =  2.0022
            S**2   =   0.0000
 Range of M.O.s used for correlation:     1   234
 NBasis=   234 NAE=    58 NBE=    58 NFC=     0 NFV=     0
 NROrb=    234 NOA=    58 NOB=    58 NVA=   176 NVB=   176

 **** Warning!!: The largest alpha MO coefficient is  0.12282836D+03

          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   3 vectors were produced by pass 12.
   3 vectors were produced by pass 13.
 Inv2:  IOpt= 1 Iter= 1 AM= 6.70D-16 Conv= 1.00D-12.
```

```
 Inverted reduced A of dimension  42 with in-core refinement.
 PrsmSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 G2DrvN: will do   10 atoms at a time, making    3 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  45 IRICut=      45 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
          There are  90 degrees of freedom in the 1st order CPHF.
  87 vectors were produced by pass  0.
 AX will form  44 AO Fock derivatives at one time.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  1.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  3.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  4.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  5.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  87 vectors were produced by pass  6.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  45 vectors were produced by pass  7.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
   3 vectors were produced by pass  8.
 Inv2:  IOpt= 1 Iter= 1 AM= 5.22D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 657 with in-core refinement.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.

 ******************************************************************

           Population analysis using the SCF density.

 ******************************************************************

 Alpha  occ. eigenvalues --  -20.63015 -20.47649 -20.37476 -15.41736 -
11.40613
 Alpha  occ. eigenvalues --  -11.24089 -11.24077 -11.23882 -11.23422 -
11.23241
```

```
 Alpha  occ. eigenvalues --  -11.22784 -11.20885 -11.20270 -11.20232 -
11.19610
 Alpha  occ. eigenvalues --  -11.19314  -1.55087  -1.36944  -1.30055  -
1.27744
 Alpha  occ. eigenvalues --   -1.13652  -1.13105  -1.11286  -1.07501  -
0.96769
 Alpha  occ. eigenvalues --   -0.95937  -0.93073  -0.89412  -0.82709  -
0.81862
 Alpha  occ. eigenvalues --   -0.77017  -0.76636  -0.74971  -0.71725  -
0.70363
 Alpha  occ. eigenvalues --   -0.68707  -0.66894  -0.65705  -0.63621  -
0.62913
 Alpha  occ. eigenvalues --   -0.59456  -0.57824  -0.56767  -0.56075  -
0.53429
 Alpha  occ. eigenvalues --   -0.52600  -0.51563  -0.50789  -0.49820  -
0.49160
 Alpha  occ. eigenvalues --   -0.48322  -0.47481  -0.46702  -0.45694  -
0.42570
 Alpha  occ. eigenvalues --   -0.37878  -0.35226  -0.31013
 Alpha virt. eigenvalues --    0.02537   0.04322   0.05499   0.06471
0.07139
 Alpha virt. eigenvalues --    0.08229   0.08658   0.09478   0.10407
0.10642
 Alpha virt. eigenvalues --    0.11850   0.12189   0.13656   0.13813
0.14615
 Alpha virt. eigenvalues --    0.14995   0.15289   0.16962   0.17316
0.17703
 Alpha virt. eigenvalues --    0.17952   0.18497   0.19168   0.19216
0.19750
 Alpha virt. eigenvalues --    0.20354   0.20633   0.22675   0.22923
0.23325
 Alpha virt. eigenvalues --    0.23429   0.23948   0.24252   0.24708
0.25005
 Alpha virt. eigenvalues --    0.25637   0.25963   0.26332   0.27033
0.27196
 Alpha virt. eigenvalues --    0.27463   0.28065   0.28377   0.29571
0.29759
 Alpha virt. eigenvalues --    0.30531   0.31073   0.31615   0.31921
0.33415
 Alpha virt. eigenvalues --    0.33944   0.34547   0.34869   0.35543
0.36619
 Alpha virt. eigenvalues --    0.37266   0.37821   0.39426   0.40075
0.40624
 Alpha virt. eigenvalues --    0.41469   0.42226   0.42962   0.43294
0.43978
 Alpha virt. eigenvalues --    0.44323   0.45054   0.46083   0.46881
0.47378
 Alpha virt. eigenvalues --    0.47784   0.48734   0.48997   0.49614
0.51354
 Alpha virt. eigenvalues --    0.51744   0.52226   0.52458   0.53038
0.54386
 Alpha virt. eigenvalues --    0.55048   0.55794   0.57416   0.57637
0.58822
```

```
 Alpha virt. eigenvalues --    0.58883   0.60327   0.60766   0.61113
0.63270
 Alpha virt. eigenvalues --    0.63533   0.64642   0.65706   0.66354
0.66869
 Alpha virt. eigenvalues --    0.71444   0.74284   0.78397   0.87534
1.07688
 Alpha virt. eigenvalues --    1.08798   1.10111   1.10662   1.12485
1.12568
 Alpha virt. eigenvalues --    1.13568   1.14334   1.15567   1.17335
1.17422
 Alpha virt. eigenvalues --    1.18181   1.19213   1.19490   1.20367
1.21090
 Alpha virt. eigenvalues --    1.22688   1.23188   1.25050   1.26416
1.26685
 Alpha virt. eigenvalues --    1.29918   1.32424   1.33126   1.36408
1.37026
 Alpha virt. eigenvalues --    1.39139   1.43383   1.44461   1.45510
1.47840
 Alpha virt. eigenvalues --    1.48878   1.50591   1.52303   1.52605
1.53345
 Alpha virt. eigenvalues --    1.56128   1.57459   1.58170   1.59010
1.62505
 Alpha virt. eigenvalues --    1.65215   1.68378   1.71683   1.73380
1.76036
 Alpha virt. eigenvalues --    1.78973   1.82511   1.86204   1.87873
1.97248
 Alpha virt. eigenvalues --    1.99420   2.04534   2.12055   2.13230
2.19282
 Alpha virt. eigenvalues --    2.21956   2.22837   2.26503   2.28304
2.29885
 Alpha virt. eigenvalues --    2.34930   2.36214   2.40952   2.46247
2.52008
 Alpha virt. eigenvalues --    2.54809   2.71519   2.88947   3.05948
3.15119
 Alpha virt. eigenvalues --    3.22300   3.37953   3.75164   3.82039
3.85082
 Alpha virt. eigenvalues --    3.95674
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   14.045331  -7.740504   5.035899  -4.369225  -1.874281   4.929754
  2  C   -7.740504  23.051568 -16.078978   0.462245   8.629063 -13.360665
  3  C    5.035899 -16.078978  41.652920  10.945717 -32.163903  11.396668
  4  C   -4.369225   0.462245  10.945717  27.618532 -23.641753  -0.904482
  5  C   -1.874281   8.629063 -32.163903 -23.641753  53.617491  -4.992549
  6  C    4.929754 -13.360665  11.396668  -0.904482  -4.992549  23.385336
  7  C   -1.940846   4.258595  -2.064755   2.469968   0.231531  -7.532558
  8  C    2.105210  -2.119559  -3.837872  -9.215656   7.195174   2.010121
  9  C    1.006465  -1.957589   6.880867   6.426960 -10.780990   6.557459
 10  C   -3.227666  10.791461 -17.555672  -5.035868  14.315298 -14.869650
 11  C   -1.761362  -0.113630   0.311205  -0.356178   0.515268   0.100528
 12  C   -0.432518  -0.136490   0.883648   0.066979  -3.958888  -0.704189
 13  N   -0.029519   0.009600   0.178753   0.440862  -0.189859  -0.076806
 14  O    0.040190  -0.083493   0.020252  -0.127491   0.119659   0.034618
 15  O    0.057498  -0.134487   0.276837   0.047186   0.005659   0.014847
```

16	O	-0.087792	-0.106498	0.990670	0.836771	-1.397569	0.037545
17	H	0.514248	-0.145039	0.027146	-0.126241	0.005011	0.027951
18	H	-0.094429	0.546702	-0.107186	0.022419	-0.000334	-0.102069
19	H	0.031420	-0.061381	0.512674	-0.017014	-0.132148	0.046486
20	H	-0.009190	-0.028384	0.056685	0.569357	-0.185639	0.007807
21	H	-0.017019	-0.080696	0.049737	0.005700	0.013699	0.548532
22	H	-0.027874	0.033144	-0.005922	0.055698	0.006165	-0.104666
23	H	0.032414	-0.006331	0.014147	-0.096828	0.019057	-0.030074
24	H	-0.006758	0.037648	-0.033436	0.010484	-0.018827	-0.108126
25	H	-0.085407	0.018613	0.016002	0.072671	-0.033142	0.027453
26	H	-0.079311	0.004570	-0.006709	0.020205	0.006011	0.055340
27	H	0.002903	-0.003903	0.022137	-0.008422	-0.058434	0.005556
28	H	-0.004305	0.009719	-0.008791	0.006961	-0.012988	-0.028943
29	H	0.027878	-0.049115	0.125508	0.042934	-0.116258	0.020956

		7	8	9	10	11	12
1	C	-1.940846	2.105210	1.006465	-3.227666	-1.761362	-0.432518
2	C	4.258595	-2.119559	-1.957589	10.791461	-0.113630	-0.136490
3	C	-2.064755	-3.837872	6.880867	-17.555672	0.311205	0.883648
4	C	2.469968	-9.215656	6.426960	-5.035868	-0.356178	0.066979
5	C	0.231531	7.195174	-10.780990	14.315298	0.515268	-3.958888
6	C	-7.532558	2.010121	6.557459	-14.869650	0.100528	-0.704189
7	C	17.028251	-8.010952	1.607865	4.233106	-3.846593	-1.124778
8	C	-8.010952	33.778352	-35.631144	11.341510	1.162687	7.104929
9	C	1.607865	-35.631144	88.772206	-35.413919	-0.883094	-19.062078
10	C	4.233106	11.341510	-35.413919	38.479832	0.470988	1.283594
11	C	-3.846593	1.162687	-0.883094	0.470988	12.115420	-0.798162
12	C	-1.124778	7.104929	-19.062078	1.283594	-0.798162	23.121745
13	N	0.096680	0.168702	-1.354678	0.836428	-0.038055	-1.063777
14	O	-0.032299	1.250722	-3.548526	1.283856	-0.033062	0.490960
15	O	0.037291	0.060806	-0.801796	0.465953	0.005902	-0.323021
16	O	-0.004077	-0.044577	-0.204790	-0.159214	-0.017440	0.183480
17	H	0.018867	0.044852	0.002069	-0.002106	-0.022784	0.003905
18	H	-0.000367	0.006462	-0.003145	0.069949	0.024345	0.000797
19	H	-0.007625	0.032208	-0.050691	-0.013357	-0.005361	0.010279
20	H	0.029587	-0.086238	-0.005689	-0.008902	-0.006391	0.007759
21	H	-0.102823	0.042380	-0.037414	-0.099655	0.046891	-0.007773
22	H	0.567524	-0.182219	-0.001040	0.034812	-0.025651	-0.003330
23	H	-0.046165	0.650744	-0.386984	0.139509	0.028938	-0.005296
24	H	0.013116	0.103615	-0.350604	0.648653	0.002273	0.042999
25	H	-0.116620	0.037125	-0.024103	0.001584	0.397386	0.005793
26	H	-0.171314	0.060104	-0.007289	-0.017870	0.454107	0.000001
27	H	-0.004219	0.038339	0.039078	-0.043435	0.000465	0.083319
28	H	0.017837	-0.027740	0.158814	-0.097422	0.000150	0.026089
29	H	-0.002708	-0.006101	0.034843	-0.046289	0.002742	-0.046950

		13	14	15	16	17	18
1	C	-0.029519	0.040190	0.057498	-0.087792	0.514248	-0.094429
2	C	0.009600	-0.083493	-0.134487	-0.106498	-0.145039	0.546702
3	C	0.178753	0.020252	0.276837	0.990670	0.027146	-0.107186
4	C	0.440862	-0.127491	0.047186	0.836771	-0.126241	0.022419
5	C	-0.189859	0.119659	0.005659	-1.397569	0.005011	-0.000334
6	C	-0.076806	0.034618	0.014847	0.037545	0.027951	-0.102069
7	C	0.096680	-0.032299	0.037291	-0.004077	0.018867	-0.000367
8	C	0.168702	1.250722	0.060806	-0.044577	0.044852	0.006462
9	C	-1.354678	-3.548526	-0.801796	-0.204790	0.002069	-0.003145

10	C	0.836428	1.283856	0.465953	-0.159214	-0.002106	0.069949
11	C	-0.038055	-0.033062	0.005902	-0.017440	-0.022784	0.024345
12	C	-1.063777	0.490960	-0.323021	0.183480	0.003905	0.000797
13	N	8.852464	0.131389	-0.050067	0.045942	0.000141	-0.000037
14	O	0.131389	8.961027	0.080513	0.002595	0.000056	0.000034
15	O	-0.050067	0.080513	9.142675	0.002073	0.000002	0.000050
16	O	0.045942	0.002595	0.002073	8.338603	0.000418	0.000446
17	H	0.000141	0.000056	0.000002	0.000418	0.370782	-0.000393
18	H	-0.000037	0.000034	0.000050	0.000446	-0.000393	0.354950
19	H	0.002185	0.000606	0.001410	0.002329	-0.000027	0.000031
20	H	0.005069	0.000429	0.000191	0.004789	-0.000042	-0.000014
21	H	0.000003	0.003380	0.000011	-0.000048	-0.000005	-0.000469
22	H	0.000562	0.004996	-0.000024	-0.000024	-0.000013	-0.000008
23	H	0.020385	0.019273	0.001353	0.000816	-0.000003	0.000000
24	H	0.002849	0.009136	0.000401	0.001109	0.000000	-0.000038
25	H	0.000106	-0.000058	0.000001	0.000236	-0.000162	-0.000021
26	H	-0.000055	-0.000129	-0.000005	-0.000040	-0.000425	0.000179
27	H	0.212311	-0.003767	-0.026988	-0.002057	0.000000	0.000000
28	H	-0.001698	0.184584	-0.001617	0.000102	0.000000	0.000000
29	H	-0.002720	-0.000027	0.004402	0.238307	-0.000002	0.000003

		19	20	21	22	23	24
1	C	0.031420	-0.009190	-0.017019	-0.027874	0.032414	-0.006758
2	C	-0.061381	-0.028384	-0.080696	0.033144	-0.006331	0.037648
3	C	0.512674	0.056685	0.049737	-0.005922	0.014147	-0.033436
4	C	-0.017014	0.569357	0.005700	0.055698	-0.096828	0.010484
5	C	-0.132148	-0.185639	0.013699	0.006165	0.019057	-0.018827
6	C	0.046486	0.007807	0.548532	-0.104666	-0.030074	-0.108126
7	C	-0.007625	0.029587	-0.102823	0.567524	-0.046165	0.013116
8	C	0.032208	-0.086238	0.042380	-0.182219	0.650744	0.103615
9	C	-0.050691	-0.005689	-0.037414	-0.001040	-0.386984	-0.350604
10	C	-0.013357	-0.008902	-0.099655	0.034812	0.139509	0.648653
11	C	-0.005361	-0.006391	0.046891	-0.025651	0.028938	0.002273
12	C	0.010279	0.007759	-0.007773	-0.003330	-0.005296	0.042999
13	N	0.002185	0.005069	0.000003	0.000562	0.020385	0.002849
14	O	0.000606	0.000429	0.003380	0.004996	0.019273	0.009136
15	O	0.001410	0.000191	0.000011	-0.000024	0.001353	0.000401
16	O	0.002329	0.004789	-0.000048	-0.000024	0.000816	0.001109
17	H	-0.000027	-0.000042	-0.000005	-0.000013	-0.000003	0.000000
18	H	0.000031	-0.000014	-0.000469	-0.000008	0.000000	-0.000038
19	H	0.348943	-0.000011	-0.000071	0.000000	-0.000001	-0.000287
20	H	-0.000011	0.327540	0.000000	-0.000008	0.000297	-0.000001
21	H	-0.000071	0.000000	0.361474	-0.000359	-0.000005	-0.000219
22	H	0.000000	-0.000008	-0.000359	0.347753	0.000330	0.000010
23	H	-0.000001	0.000297	-0.000005	0.000330	0.329184	-0.000001
24	H	-0.000287	-0.000001	-0.000219	0.000010	-0.000001	0.336951
25	H	0.000000	0.000078	-0.000030	-0.000334	0.000139	0.000000
26	H	0.000000	-0.000021	0.000018	-0.000352	-0.000060	0.000000
27	H	-0.000001	0.000015	0.000000	0.000000	-0.000132	-0.000002
28	H	0.000000	0.000000	0.000008	-0.000047	-0.000010	0.000527
29	H	-0.000481	0.000014	0.000000	0.000000	0.000000	0.000004

		25	26	27	28	29
1	C	-0.085407	-0.079311	0.002903	-0.004305	0.027878
2	C	0.018613	0.004570	-0.003903	0.009719	-0.049115
3	C	0.016002	-0.006709	0.022137	-0.008791	0.125508

4	C	0.072671	0.020205	-0.008422	0.006961	0.042934
5	C	-0.033142	0.006011	-0.058434	-0.012988	-0.116258
6	C	0.027453	0.055340	0.005556	-0.028943	0.020956
7	C	-0.116620	-0.171314	-0.004219	0.017837	-0.002708
8	C	0.037125	0.060104	0.038339	-0.027740	-0.006101
9	C	-0.024103	-0.007289	0.039078	0.158814	0.034843
10	C	0.001584	-0.017870	-0.043435	-0.097422	-0.046289
11	C	0.397386	0.454107	0.000465	0.000150	0.002742
12	C	0.005793	0.000001	0.083319	0.026089	-0.046950
13	N	0.000106	-0.000055	0.212311	-0.001698	-0.002720
14	O	-0.000058	-0.000129	-0.003767	0.184584	-0.000027
15	O	0.000001	-0.000005	-0.026988	-0.001617	0.004402
16	O	0.000236	-0.000040	-0.002057	0.000102	0.238307
17	H	-0.000162	-0.000425	0.000000	0.000000	-0.000002
18	H	-0.000021	0.000179	0.000000	0.000000	0.000003
19	H	0.000000	0.000000	-0.000001	0.000000	-0.000481
20	H	0.000078	-0.000021	0.000015	0.000000	0.000014
21	H	-0.000030	0.000018	0.000000	0.000008	0.000000
22	H	-0.000334	-0.000352	0.000000	-0.000047	0.000000
23	H	0.000139	-0.000060	-0.000132	-0.000010	0.000000
24	H	0.000000	0.000000	-0.000002	0.000527	0.000004
25	H	0.421248	-0.015489	0.000000	0.000000	0.000000
26	H	-0.015489	0.426190	0.000000	0.000000	0.000000
27	H	0.000000	0.000000	0.388895	0.000014	0.000125
28	H	0.000000	0.000000	0.000014	0.310560	0.000000
29	H	0.000000	0.000000	0.000125	0.000000	0.238592

Total atomic charges:

		1
1	C	-0.041205
2	C	0.353812
3	C	-1.534247
4	C	-0.222492
5	C	0.878476
6	C	-0.392182
7	C	0.398482
8	C	-2.031984
9	C	5.018936
10	C	-1.805509
11	C	-1.731531
12	C	0.350972
13	N	-1.197160
14	O	-0.809424
15	O	-0.867056
16	O	-0.662105
17	H	0.281795
18	H	0.282142
19	H	0.299885
20	H	0.320911
21	H	0.274755
22	H	0.300878
23	H	0.315305
24	H	0.308525
25	H	0.276933
26	H	0.272344

```
27  H    0.358204
28  H    0.468198
29  H    0.534345
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
                1
 1  C    0.240590
 2  C    0.635954
 3  C   -1.234362
 4  C    0.098419
 5  C    0.878476
 6  C   -0.117426
 7  C    0.699359
 8  C   -1.716679
 9  C    5.018936
10  C   -1.496985
11  C   -1.182254
12  C    0.350972
13  N   -0.838956
14  O   -0.341227
15  O   -0.867056
16  O   -0.127760
17  H    0.000000
18  H    0.000000
19  H    0.000000
20  H    0.000000
21  H    0.000000
22  H    0.000000
23  H    0.000000
24  H    0.000000
25  H    0.000000
26  H    0.000000
27  H    0.000000
28  H    0.000000
29  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  2434.6352
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=    -7.8876    Y=     4.7115    Z=     2.5710  Tot=     9.5406
Quadrupole moment (Debye-Ang):
  XX=  -108.0503   YY=   -88.7652   ZZ=   -97.3657
  XY=     3.0096   XZ=    -0.0228   YZ=     3.1192
Octapole moment (Debye-Ang**2):
 XXX=   -49.1446  YYY=    29.8320  ZZZ=    14.5569  XYY=    25.5377
 XXY=     6.4836  XXZ=   -15.7327  XZZ=   -19.5251  YZZ=     6.0414
 YYZ=    22.5322  XYZ=     3.1878
Hexadecapole moment (Debye-Ang**3):
XXXX= -1783.2947 YYYY=  -930.2932 ZZZZ=  -610.7134 XXXY=    23.0568
XXXZ=   -86.3270 YYYX=    19.4506 YYYZ=    27.2670 ZZZX=    27.6867
ZZZY=     0.1017 XXYY=  -357.4977 XXZZ=  -411.6028 YYZZ=  -248.1672
XXYZ=    -1.1795 YYXZ=    34.6339 ZZXY=    10.9408
N-N= 1.231450166808D+03 E-N=-4.186413676724D+03  KE= 7.353044688646D+02
 Exact polarizability: 132.784   5.248 119.007   0.415  -1.687 118.492
```

```
 Approx polarizability: 113.101   5.295 113.882   2.179  -2.656 119.128
 Full mass-weighted force constant matrix:
 Low frequencies --- -115.8477   -1.7300   -1.4585   -1.1768   -0.0008
0.0002
 Low frequencies ---    0.0007  125.1852  156.6928
 ******    1 imaginary frequencies (negative Signs) ******
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                      1                      2                      3
                     ?A                     ?A                     ?A
 Frequencies --  -115.8477               125.1852               156.6928
 Red. masses --     8.0705                 6.1906                 6.1014
 Frc consts  --     0.0638                 0.0572                 0.0883
 IR Inten    --     3.3450                18.7971                 1.8852
 Raman Activ --     2.5321                 0.6922                 0.4132
 Depolar     --     0.5751                 0.6344                 0.7077
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.03   0.00   0.04     0.13   0.05  -0.01    -0.06  -0.01
0.08
   2   6    -0.04  -0.05   0.03     0.13   0.06  -0.01     0.06  -0.01
0.06
   3   6    -0.07  -0.01   0.05     0.18  -0.12  -0.04     0.08   0.01  -
0.06
   4   6    -0.03   0.06   0.06     0.10  -0.10  -0.05    -0.09   0.03  -
0.02
   5   6    -0.03  -0.01   0.08     0.15  -0.11  -0.07    -0.05   0.04  -
0.08
   6   6    -0.01  -0.04  -0.02    -0.03   0.02   0.02     0.07  -0.01
0.02
   7   6     0.01   0.01  -0.03    -0.08   0.01   0.03     0.01   0.01
0.02
   8   6     0.00   0.04   0.00    -0.03  -0.11   0.00    -0.03   0.06  -
0.04
   9   6     0.00   0.03  -0.01    -0.02  -0.13  -0.01     0.01   0.02  -
0.08
  10   6    -0.01  -0.01   0.00     0.00  -0.13  -0.01     0.06   0.00  -
0.06
  11   6    -0.01   0.00  -0.01     0.00   0.11   0.03    -0.05  -0.03
0.12
  12   6     0.00   0.05  -0.06    -0.11   0.06   0.06     0.06  -0.04
0.09
  13   7     0.15  -0.33  -0.16    -0.14   0.12   0.07     0.30  -0.09
0.11
  14   8    -0.02   0.02  -0.03     0.07  -0.11  -0.10    -0.08   0.01  -
0.20
  15   8    -0.16   0.44   0.03    -0.20   0.24   0.10    -0.12  -0.06
0.22
  16   8     0.20  -0.17   0.06    -0.04   0.03  -0.03    -0.13   0.08  -
0.17
  17   1    -0.05  -0.01   0.07     0.21   0.10  -0.02    -0.09  -0.02
0.12
```

18	1	-0.07	-0.09	0.03	0.19	0.14	0.00	0.11	-0.03	0.11
19	1	-0.07	-0.04	0.07	0.25	-0.13	-0.07	0.14	0.00	-0.08
20	1	-0.02	0.09	0.07	0.11	-0.13	-0.06	-0.19	0.05	-0.02
21	1	0.01	-0.08	-0.04	-0.09	0.10	0.04	0.11	-0.03	0.03
22	1	0.03	0.01	-0.07	-0.18	0.02	0.06	0.03	0.01	0.02
23	1	0.01	0.09	-0.01	-0.07	-0.17	0.01	-0.06	0.06	-0.05
24	1	0.00	-0.02	-0.01	-0.03	-0.17	-0.01	0.11	0.02	-0.08
25	1	0.00	0.03	-0.01	-0.03	0.10	0.04	-0.15	-0.02	0.13
26	1	-0.01	-0.03	-0.02	-0.01	0.20	0.06	0.00	-0.06	0.20
27	1	0.14	-0.32	-0.18	-0.22	0.30	0.13	0.35	-0.15	0.26
28	1	0.04	-0.01	-0.23	0.06	-0.09	-0.04	-0.10	-0.09	-0.23
29	1	0.31	-0.33	0.04	-0.06	0.07	-0.03	-0.09	0.15	-0.23

	4			5			6		
	?A			?A			?A		
Frequencies --	181.7961			263.1047			303.3941		
Red. masses --	5.2200			5.2574			2.9227		
Frc consts --	0.1016			0.2144			0.1585		
IR Inten --	7.4112			24.1521			14.4429		
Raman Activ --	1.0321			1.2058			1.6675		
Depolar --	0.5275			0.6977			0.6251		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.08	-0.03	0.02	-0.01	0.06	0.01	-0.01	0.00	-0.05
2 6	-0.03	-0.01	0.01	-0.04	0.05	0.01	-0.03	0.05	-0.02
3 6	-0.04	0.03	-0.04	-0.03	-0.02	0.02	-0.02	0.00	0.00
4 6	-0.10	0.03	-0.01	-0.02	-0.03	0.01	0.00	0.00	0.00
5 6	0.01	-0.03	-0.07	-0.03	-0.04	0.02	-0.01	-0.01	-0.01
6 6	0.00	-0.01	0.01	-0.09	0.03	0.00	-0.06	0.04	0.05
7 6	-0.01	-0.02	0.02	-0.12	0.04	0.01	0.01	0.00	0.06
8 6	-0.04	0.02	-0.01	-0.07	-0.05	0.00	0.02	0.03	0.09
9 6	-0.01	0.04	-0.02	-0.01	0.03	-0.02	0.00	0.00	0.09
10 6	-0.01	0.02	-0.01	-0.07	-0.02	-0.01	-0.05	-0.03	0.10

11	6	-0.05	-0.06	0.05	-0.09	0.11	0.02	0.03	-0.03	-0.04
12	6	-0.02	0.07	0.05	-0.02	0.03	-0.02	0.02	0.00	0.09
13	7	-0.04	0.24	0.12	0.11	-0.10	-0.04	-0.09	-0.08	0.04
14	8	0.06	0.05	-0.06	0.43	0.08	-0.01	0.02	0.02	-0.21
15	8	-0.02	-0.05	0.07	-0.03	-0.12	0.00	0.15	0.02	0.00
16	8	0.30	-0.24	-0.12	-0.04	-0.04	-0.01	-0.01	0.00	-0.03
17	1	-0.12	-0.05	0.04	0.05	0.10	0.00	-0.03	-0.02	-0.09
18	1	-0.02	-0.02	0.02	-0.03	0.06	0.01	-0.03	0.09	-0.04
19	1	-0.03	0.05	-0.06	-0.01	-0.03	0.02	-0.04	0.04	-0.01
20	1	-0.14	0.01	-0.03	0.01	-0.03	0.01	0.03	-0.03	-0.02
21	1	0.02	-0.02	0.02	-0.10	0.06	0.01	-0.12	0.08	0.05
22	1	0.02	-0.02	0.02	-0.20	0.04	0.02	0.06	0.00	0.08
23	1	-0.04	0.03	-0.01	-0.11	-0.06	-0.01	0.05	-0.01	0.11
24	1	0.01	0.05	-0.01	-0.09	-0.05	-0.01	-0.09	-0.01	0.13
25	1	-0.09	-0.07	0.05	-0.11	0.12	0.02	0.11	-0.07	-0.05
26	1	-0.03	-0.09	0.08	-0.08	0.15	0.04	-0.01	-0.02	-0.10
27	1	-0.06	0.30	0.17	0.19	-0.27	-0.05	-0.09	-0.12	-0.09
28	1	0.03	0.09	0.04	0.47	0.41	0.17	0.21	-0.05	-0.80
29	1	0.48	-0.46	-0.19	-0.07	0.01	0.00	0.01	0.00	-0.06

	7	8	9
	?A	?A	?A
Frequencies --	328.1560	346.7573	372.5388
Red. masses --	3.3920	1.5313	5.2323
Frc consts --	0.2152	0.1085	0.4278
IR Inten --	40.2629	89.9021	29.9585
Raman Activ --	0.3965	1.1620	2.7831
Depolar --	0.6522	0.7499	0.3526

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.05	0.11	-0.01	-0.01	-0.03	-0.01	0.04	-0.05
2	6	0.00	-0.07	0.06	0.01	0.02	-0.03	-0.02	0.05	-0.04
3	6	0.01	-0.05	0.03	0.00	0.01	-0.04	-0.03	-0.07	-0.04

4	6	-0.04	0.03	0.06	0.00	0.00	-0.04	-0.01	-0.08	-0.08
5	6	-0.02	-0.02	0.00	0.00	0.01	-0.02	-0.02	-0.12	-0.04
6	6	-0.01	-0.07	-0.08	0.02	0.02	0.00	-0.08	0.02	-0.02
7	6	-0.02	0.05	-0.12	-0.01	-0.01	0.02	-0.11	0.01	0.01
8	6	0.02	0.04	-0.02	-0.02	-0.01	-0.03	-0.05	-0.06	-0.02
9	6	0.02	-0.02	0.03	-0.01	-0.01	-0.03	0.04	0.00	0.00
10	6	-0.02	-0.06	-0.01	0.02	0.02	-0.03	-0.05	-0.03	-0.01
11	6	-0.01	0.13	-0.05	-0.03	-0.03	0.04	-0.14	0.06	0.10
12	6	0.03	0.00	0.05	-0.01	0.00	-0.02	0.18	0.06	0.02
13	7	-0.03	0.01	0.04	0.03	0.03	0.00	0.20	0.09	0.03
14	8	0.00	-0.04	0.18	-0.01	-0.02	0.10	-0.09	-0.02	0.01
15	8	0.09	0.04	0.00	-0.05	-0.03	0.00	0.28	0.14	-0.05
16	8	-0.05	-0.03	-0.20	0.03	0.01	0.09	-0.06	-0.09	0.10
17	1	0.03	0.08	0.19	-0.02	-0.02	-0.05	0.06	0.08	-0.08
18	1	0.02	-0.14	0.12	0.01	0.04	-0.03	-0.01	0.09	-0.06
19	1	0.05	-0.08	0.03	0.00	0.01	-0.04	0.00	-0.03	-0.07
20	1	-0.09	0.07	0.07	0.00	-0.01	-0.04	0.02	-0.08	-0.07
21	1	-0.02	-0.13	-0.14	0.03	0.03	0.02	-0.11	0.06	0.00
22	1	-0.07	0.07	-0.20	0.00	-0.02	0.04	-0.19	0.02	0.02
23	1	0.07	0.11	-0.03	-0.05	-0.03	-0.03	-0.06	-0.13	0.00
24	1	-0.05	-0.11	-0.01	0.05	0.02	-0.06	-0.10	-0.06	0.01
25	1	0.04	0.27	-0.05	-0.11	-0.08	0.05	-0.38	0.00	0.14
26	1	-0.03	0.06	-0.11	0.01	-0.01	0.12	-0.04	0.13	0.33
27	1	-0.05	0.05	0.01	0.03	0.06	0.06	0.21	0.11	0.11
28	1	0.29	0.02	-0.54	0.37	0.05	-0.85	-0.21	-0.15	0.22
29	1	0.06	0.06	-0.33	-0.03	-0.04	0.16	-0.11	-0.15	0.16
			10			11			12	
			?A			?A			?A	

Frequencies --	394.8983			451.7730			474.8894		
Red. masses --	3.7777			2.4424			5.8314		
Frc consts --	0.3471			0.2937			0.7748		
IR Inten --	3.8047			9.0448			20.1431		
Raman Activ --	1.8565			2.1668			5.3853		
Depolar --	0.6800			0.1383			0.3414		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.07	-0.01	-0.01	0.10	0.00	-0.06	0.03	-0.01	0.01
2 6	-0.06	0.02	0.04	-0.01	-0.02	-0.05	0.12	-0.03	0.00
3 6	-0.06	0.05	0.13	-0.06	0.02	0.09	0.15	-0.16	-0.04
4 6	0.09	-0.11	0.09	0.12	-0.06	0.01	-0.03	-0.03	-0.10
5 6	-0.01	-0.05	0.12	0.03	-0.04	0.08	0.07	-0.20	-0.10
6 6	-0.02	0.03	0.08	0.02	-0.03	-0.06	0.01	-0.05	0.03
7 6	-0.04	-0.03	0.09	0.05	-0.01	-0.07	0.01	-0.02	0.02
8 6	-0.04	-0.08	0.04	0.05	0.02	-0.04	-0.04	0.06	0.00
9 6	-0.01	0.01	-0.05	-0.02	0.06	0.01	-0.09	0.22	0.04
10 6	0.01	0.04	0.02	-0.02	0.02	0.02	0.01	-0.03	0.06
11 6	0.08	0.03	-0.11	-0.04	0.00	0.15	0.07	-0.01	-0.07
12 6	0.02	0.04	-0.11	-0.03	0.03	0.01	-0.07	0.14	0.03
13 7	0.16	0.14	-0.05	-0.05	-0.02	-0.01	0.00	-0.04	-0.03
14 8	-0.07	0.01	-0.04	-0.03	0.08	-0.02	-0.11	0.31	0.08
15 8	-0.07	-0.02	-0.05	-0.03	-0.03	0.01	-0.02	-0.06	0.01
16 8	-0.04	-0.09	-0.10	-0.01	-0.04	-0.08	-0.08	-0.10	0.06
17 1	0.14	0.02	-0.07	0.15	0.02	-0.09	0.02	-0.02	0.05
18 1	-0.13	0.03	-0.03	-0.12	-0.06	-0.12	0.20	0.04	0.05
19 1	-0.09	0.02	0.16	-0.13	0.02	0.12	0.23	-0.04	-0.14
20 1	0.19	-0.09	0.12	0.22	0.00	0.05	-0.07	0.01	-0.08
21 1	0.02	0.04	0.12	-0.01	-0.05	-0.10	-0.04	0.00	0.03
22 1	-0.09	-0.03	0.14	0.04	0.00	-0.10	0.04	-0.02	-0.02
23 1	-0.12	-0.11	0.03	0.14	0.00	-0.01	0.05	-0.07	0.06

24	1	0.05	0.00	-0.02	-0.02	-0.03	0.00	0.08	-0.15	-0.04
25	1	0.38	0.04	-0.15	-0.47	-0.07	0.22	0.28	0.03	-0.11
26	1	-0.06	0.10	-0.36	0.16	0.05	0.55	-0.04	0.00	-0.27
27	1	0.18	0.15	0.14	-0.04	-0.06	-0.07	0.11	-0.28	-0.13
28	1	0.02	-0.04	-0.33	-0.01	0.05	-0.11	-0.05	0.29	-0.10
29	1	-0.11	0.17	-0.14	-0.11	0.20	-0.09	-0.08	-0.19	0.09

		13			14			15		
		?A			?A			?A		
Frequencies --		529.7009			540.3569			597.7943		
Red. masses --		3.0659			6.5916			5.0515		
Frc consts --		0.5068			1.1340			1.0636		
IR Inten --		9.2959			0.7868			5.4655		
Raman Activ --		2.0791			8.3240			2.1655		
Depolar --		0.3880			0.1704			0.5697		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.07	0.00	-0.09	0.06	-0.09	0.01	0.05	0.07	-0.03
2	6	0.01	0.10	-0.05	0.00	-0.19	-0.05	0.00	-0.10	-0.05
3	6	0.13	-0.11	0.07	-0.02	-0.01	-0.03	-0.13	-0.07	-0.10
4	6	-0.02	0.10	0.07	0.06	0.00	0.02	0.01	0.11	-0.11
5	6	0.06	-0.01	0.09	0.20	0.19	-0.02	-0.08	0.02	-0.14
6	6	-0.09	0.07	-0.02	-0.10	-0.20	0.04	-0.03	-0.13	0.07
7	6	0.05	0.01	0.00	-0.18	-0.15	0.03	0.07	0.07	0.04
8	6	0.00	0.09	0.03	-0.12	-0.06	0.07	0.08	0.09	0.18
9	6	-0.03	-0.02	0.01	-0.09	0.05	0.02	0.03	-0.04	0.16
10	6	-0.07	-0.11	0.04	-0.07	-0.08	0.00	0.03	-0.08	0.21
11	6	-0.02	-0.16	0.00	-0.09	-0.02	-0.02	0.06	0.12	0.06
12	6	-0.02	0.01	-0.05	-0.05	0.09	0.03	-0.03	-0.01	-0.11
13	7	0.08	0.05	-0.03	0.09	0.00	0.02	0.11	0.09	-0.07
14	8	0.01	-0.03	0.05	-0.04	0.08	0.01	0.01	-0.06	-0.01
15	8	-0.02	0.00	-0.06	0.07	0.02	-0.05	-0.13	-0.04	-0.08
16	8	-0.02	0.04	-0.05	0.21	0.29	-0.05	-0.03	0.00	0.00

17	1	-0.18	-0.08	-0.17	0.06	-0.07	0.14	0.05	0.08	0.10
18	1	0.07	0.16	-0.03	-0.02	-0.16	-0.08	-0.02	-0.06	-0.10
19	1	0.14	-0.18	0.11	-0.16	-0.11	0.08	-0.24	0.11	-0.16
20	1	0.09	0.14	0.10	-0.01	-0.11	-0.05	0.00	-0.02	-0.17
21	1	-0.24	0.14	-0.06	-0.06	-0.15	0.12	-0.15	-0.13	-0.01
22	1	0.20	-0.02	0.05	-0.21	-0.12	-0.09	0.08	0.11	-0.16
23	1	-0.01	0.16	0.00	-0.12	-0.09	0.08	0.19	0.03	0.23
24	1	-0.15	-0.25	0.02	-0.01	-0.05	-0.02	-0.01	0.07	0.30
25	1	-0.13	-0.23	0.02	-0.04	-0.04	-0.03	-0.07	0.04	0.08
26	1	0.05	-0.20	0.12	-0.14	0.15	-0.05	0.12	0.17	0.19
27	1	0.13	-0.01	0.10	0.18	-0.16	0.09	0.15	0.06	0.14
28	1	0.02	0.03	0.08	-0.02	0.10	-0.03	0.00	-0.11	0.00
29	1	0.35	-0.08	-0.32	0.21	0.33	-0.07	0.10	-0.24	-0.02

	16			17			18		
	?A			?A			?A		
Frequencies --	634.2395			671.6170			692.9981		
Red. masses --	3.3723			2.4085			2.2366		
Frc consts --	0.7992			0.6401			0.6329		
IR Inten --	14.7849			87.2673			59.7763		
Raman Activ --	3.2469			1.5992			6.4526		
Depolar --	0.6269			0.4830			0.0663		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.03	-0.05	0.18	0.03	0.02	0.02	0.10	-0.01	0.03
2 6	-0.03	0.08	0.12	-0.05	0.01	0.04	-0.03	0.01	0.05
3 6	0.01	0.06	-0.03	-0.09	-0.08	-0.04	-0.05	0.00	-0.01
4 6	-0.02	-0.12	0.02	0.05	0.09	-0.05	0.03	0.00	-0.03
5 6	0.08	-0.02	-0.10	0.03	-0.01	-0.03	-0.06	0.02	-0.01
6 6	-0.10	0.07	-0.07	-0.07	-0.03	0.08	-0.02	-0.01	0.03
7 6	0.08	-0.01	-0.13	0.06	0.05	0.10	0.05	-0.01	0.03
8 6	0.10	-0.07	-0.02	-0.03	0.09	-0.05	0.01	-0.04	-0.08
9 6	-0.02	-0.01	0.07	-0.03	-0.01	-0.08	-0.06	0.00	-0.05

10	6	-0.14	0.03	0.04	-0.07	-0.06	-0.08	-0.07	0.03	-0.07
11	6	0.05	-0.05	0.03	0.11	-0.04	0.06	0.13	0.02	0.06
12	6	-0.05	0.03	-0.03	0.01	0.00	0.02	-0.10	-0.02	0.03
13	7	0.07	0.03	-0.02	-0.01	-0.01	0.01	0.01	-0.02	0.08
14	8	-0.01	0.00	-0.03	0.01	-0.02	0.03	0.00	0.01	0.00
15	8	-0.03	-0.01	-0.07	0.03	0.02	0.00	0.04	0.02	-0.07
16	8	0.06	0.03	0.02	0.04	-0.04	-0.05	-0.06	0.03	0.03
17	1	0.00	-0.05	0.07	-0.06	-0.03	0.02	0.10	-0.02	0.00
18	1	0.05	0.07	0.20	-0.04	0.10	0.00	-0.07	0.07	-0.02
19	1	0.14	0.07	-0.09	-0.05	-0.18	0.00	0.01	-0.04	-0.02
20	1	-0.27	-0.15	-0.03	0.03	0.16	-0.02	-0.02	0.04	-0.01
21	1	-0.18	0.00	-0.19	-0.06	-0.08	0.04	0.03	-0.06	0.01
22	1	0.07	-0.03	-0.04	0.14	0.04	0.07	0.00	-0.01	0.04
23	1	0.29	-0.05	0.02	-0.21	0.04	-0.08	-0.04	-0.06	-0.09
24	1	-0.28	0.02	0.13	0.02	-0.04	-0.13	-0.01	0.03	-0.11
25	1	-0.02	0.19	0.04	0.15	-0.12	0.05	0.11	0.02	0.07
26	1	0.10	-0.26	0.04	0.09	-0.02	0.03	0.13	0.04	0.07
27	1	0.12	-0.02	0.14	-0.03	0.04	0.02	0.09	-0.13	0.26
28	1	-0.01	-0.04	-0.07	0.02	0.08	0.09	0.02	0.08	0.00
29	1	-0.30	0.19	0.26	-0.58	0.47	0.27	0.59	-0.50	-0.31

	19			20			21		
	?A			?A			?A		
Frequencies --	708.2940			792.9973			813.7938		
Red. masses --	3.1611			5.3356			4.3616		
Frc consts --	0.9344			1.9769			1.7019		
IR Inten --	97.8415			33.4204			45.0093		
Raman Activ --	2.1461			5.9241			24.8149		
Depolar --	0.4271			0.5959			0.1777		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.04	-0.01	0.03	0.08	0.00	-0.01	-0.10	0.07	0.04
2 6	-0.05	0.03	0.04	0.21	0.01	-0.09	-0.10	-0.03	-0.02

3	6	-0.03	-0.06	-0.03	0.04	0.08	0.03	-0.09	0.02	0.07
4	6	0.01	-0.03	0.00	-0.10	0.07	-0.01	0.01	0.02	-0.06
5	6	-0.03	0.04	-0.02	-0.23	0.16	0.07	0.23	-0.17	-0.05
6	6	-0.10	0.00	0.01	0.01	0.05	-0.08	0.10	0.02	0.01
7	6	0.01	-0.01	0.04	-0.01	-0.09	-0.01	0.06	0.07	0.01
8	6	0.06	-0.06	0.01	-0.02	-0.10	0.00	-0.07	-0.01	-0.14
9	6	0.08	0.03	-0.03	-0.03	0.00	0.02	-0.04	-0.01	-0.02
10	6	-0.08	-0.04	-0.07	-0.01	-0.11	0.00	0.04	0.05	0.12
11	6	0.06	0.01	0.04	0.10	0.01	0.05	0.00	-0.01	0.01
12	6	0.19	0.11	-0.03	-0.14	0.32	0.07	-0.06	0.22	0.05
13	7	-0.05	0.03	-0.16	0.02	-0.01	-0.02	0.01	0.00	-0.04
14	8	-0.03	0.01	0.02	-0.02	-0.13	0.00	0.00	-0.17	-0.01
15	8	-0.03	-0.06	0.17	0.04	-0.05	0.00	0.03	-0.04	0.03
16	8	0.00	0.06	0.00	0.03	-0.09	-0.02	-0.03	0.07	0.02
17	1	0.05	-0.01	-0.02	-0.03	-0.05	0.06	-0.13	0.06	0.05
18	1	-0.03	0.12	0.02	0.17	-0.06	-0.10	-0.15	-0.19	0.03
19	1	0.04	-0.14	-0.01	-0.01	0.07	0.06	-0.29	0.24	0.03
20	1	-0.07	-0.06	-0.03	-0.08	0.06	-0.01	0.01	0.15	-0.01
21	1	-0.10	-0.02	-0.01	-0.14	0.25	-0.02	0.08	-0.05	-0.07
22	1	-0.04	-0.01	0.07	-0.13	-0.08	0.03	0.05	0.06	0.06
23	1	0.01	-0.07	0.00	0.05	-0.04	0.00	-0.16	-0.11	-0.13
24	1	-0.13	-0.06	-0.04	-0.05	-0.15	0.00	0.09	-0.01	0.07
25	1	0.03	0.03	0.05	0.11	0.05	0.05	0.10	-0.04	0.00
26	1	0.06	0.02	0.06	0.09	0.08	0.03	-0.03	-0.12	-0.08
27	1	-0.13	0.04	-0.68	0.19	-0.38	-0.14	0.17	-0.36	-0.26
28	1	-0.04	-0.11	-0.06	-0.03	-0.12	0.06	0.02	-0.12	0.01
29	1	0.35	-0.26	-0.16	-0.33	0.14	0.20	0.25	-0.05	-0.17

		22			23			24		
		?A			?A			?A		
Frequencies --		816.9410			829.1904			845.6030		
Red. masses --		3.4611			4.9447			4.5099		
Frc consts --		1.3610			2.0031			1.9000		
IR Inten --		0.4976			3.0902			5.9438		
Raman Activ --		3.0036			7.2594			4.7906		
Depolar --		0.2689			0.0847			0.0850		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.04	-0.04	-0.09	0.14	-0.19	0.02	-0.10	0.06	-0.07
2	6	-0.10	0.00	0.17	0.13	-0.03	0.13	-0.02	0.04	0.14
3	6	0.07	-0.03	-0.06	0.03	0.15	0.09	-0.04	-0.10	0.21
4	6	0.13	-0.06	0.00	0.09	0.09	-0.15	-0.02	-0.02	-0.23
5	6	-0.07	0.05	0.00	-0.05	0.00	-0.01	-0.10	0.11	-0.01
6	6	0.02	-0.05	0.10	-0.12	-0.01	0.17	0.05	0.04	0.02
7	6	0.00	0.11	-0.02	-0.08	-0.01	-0.10	0.03	0.08	0.03
8	6	0.09	0.06	0.07	0.00	0.10	-0.20	0.08	-0.17	-0.13
9	6	0.01	-0.01	0.02	-0.06	0.00	-0.02	0.03	0.02	0.01
10	6	0.02	0.02	-0.11	-0.04	0.00	0.16	0.09	-0.17	0.09
11	6	-0.13	-0.01	-0.09	-0.12	-0.07	-0.08	-0.04	0.02	-0.02
12	6	-0.11	0.17	0.05	0.08	-0.04	-0.02	-0.01	-0.06	-0.01
13	7	0.01	-0.01	0.01	-0.01	0.03	-0.04	-0.01	-0.01	0.03
14	8	-0.01	-0.06	0.00	0.02	-0.06	0.00	-0.02	0.10	0.01
15	8	0.01	-0.03	-0.03	0.01	0.01	0.04	-0.01	0.01	-0.03
16	8	0.01	-0.02	0.00	-0.03	-0.03	0.01	0.09	0.07	-0.03
17	1	0.10	0.03	-0.16	0.15	-0.15	0.20	-0.11	0.05	-0.13
18	1	-0.03	0.15	0.16	0.08	0.21	-0.04	-0.09	-0.06	0.14
19	1	0.39	-0.23	-0.07	0.04	0.35	-0.03	-0.04	-0.10	0.22
20	1	0.24	-0.14	-0.02	0.04	0.36	-0.04	-0.02	0.00	-0.23
21	1	0.24	-0.28	0.05	-0.22	0.01	0.13	-0.04	-0.03	-0.12
22	1	0.12	0.10	-0.04	0.10	-0.04	-0.10	-0.14	0.06	0.20

23	1	0.12	0.04	0.09	0.06	0.04	-0.17	0.18	-0.40	-0.04
24	1	0.09	0.15	-0.09	0.06	0.03	0.12	0.12	-0.41	-0.03
25	1	-0.24	-0.09	-0.08	-0.13	0.06	-0.08	0.02	-0.04	-0.03
26	1	-0.07	-0.02	0.03	-0.13	0.03	-0.07	-0.05	-0.08	-0.07
27	1	0.14	-0.27	-0.01	-0.04	0.07	-0.15	-0.05	0.11	0.14
28	1	-0.02	-0.08	0.02	0.06	0.08	0.04	-0.06	-0.01	0.00
29	1	0.00	-0.05	0.02	0.05	-0.12	-0.03	-0.01	0.08	0.05

	25			26			27		
	?A			?A			?A		
Frequencies --	872.9939			885.8721			904.9953		
Red. masses --	3.0898			2.4254			2.6379		
Frc consts --	1.3874			1.1214			1.2729		
IR Inten --	3.7915			20.2304			8.2435		
Raman Activ --	10.6509			2.8103			2.0588		
Depolar --	0.0132			0.4887			0.4647		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.01	0.08	-0.10	-0.01	-0.02	0.02	-0.13	0.08	0.06
2 6	-0.13	0.07	0.05	0.02	0.15	-0.05	0.12	0.01	0.04
3 6	0.13	0.01	0.05	-0.11	-0.11	-0.05	-0.07	-0.01	-0.10
4 6	-0.06	0.14	-0.02	-0.07	-0.03	0.08	0.18	0.13	-0.02
5 6	0.01	-0.02	0.00	0.03	0.00	0.03	0.00	-0.02	0.05
6 6	0.03	-0.15	0.05	-0.03	-0.03	0.14	-0.03	-0.02	-0.03
7 6	-0.06	-0.16	-0.07	0.00	-0.07	-0.09	-0.06	-0.05	-0.01
8 6	-0.02	-0.09	-0.04	0.07	-0.01	-0.05	0.04	-0.11	0.00
9 6	-0.01	0.00	0.05	0.01	0.00	-0.03	0.02	-0.01	0.04
10 6	-0.04	0.11	0.05	0.13	-0.01	0.02	-0.01	0.05	-0.04
11 6	0.12	0.03	0.03	-0.01	0.04	-0.02	-0.02	-0.06	0.02
12 6	0.02	-0.01	-0.01	-0.03	0.03	0.01	-0.01	0.00	0.00
13 7	0.01	0.01	-0.02	0.00	-0.01	0.01	0.00	0.01	0.00
14 8	0.01	-0.02	-0.02	-0.01	0.00	0.00	-0.01	0.04	-0.01
15 8	0.00	0.00	0.01	0.00	0.00	-0.01	-0.01	0.00	-0.01

```
  16   8     0.00  -0.02   0.00     0.01   0.01  -0.01    -0.04  -0.03
0.00
  17   1    -0.21  -0.05  -0.23     0.01  -0.03  -0.10    -0.29   0.01
0.13
  18   1    -0.17   0.13  -0.01     0.16   0.47  -0.08     0.37   0.00
0.27
  19   1     0.44  -0.06  -0.03    -0.36  -0.13   0.07    -0.21  -0.01  -
0.04
  20   1    -0.01   0.21   0.01    -0.19   0.01   0.08     0.53   0.17
0.04
  21   1     0.24  -0.24   0.13    -0.09   0.05   0.17    -0.04   0.03
0.01
  22   1    -0.28  -0.10  -0.24    -0.06  -0.05  -0.14    -0.18  -0.05
0.02
  23   1     0.12  -0.02  -0.02     0.21   0.12  -0.06     0.12  -0.12
0.02
  24   1    -0.08   0.13   0.08     0.44   0.12  -0.10    -0.02   0.18
0.03
  25   1    -0.01  -0.03   0.05    -0.10   0.19  -0.01     0.06  -0.02
0.01
  26   1     0.14   0.15   0.12     0.01   0.01   0.02    -0.05  -0.18  -
0.08
  27   1    -0.01   0.04  -0.02     0.02  -0.05   0.02     0.02  -0.04
0.01
  28   1     0.01  -0.03  -0.03    -0.01  -0.02   0.01    -0.03  -0.07  -
0.05
  29   1    -0.14   0.11   0.06     0.01   0.09  -0.04     0.07   0.02  -
0.12
                     28                    29                    30
                     ?A                    ?A                    ?A
 Frequencies --    913.5264              954.7830              967.7336
 Red. masses --      2.5746                1.4335                3.0343
 Frc consts  --      1.2659                0.7700                1.6742
 IR Inten    --      6.5254               58.2952               13.5257
 Raman Activ --      2.0835                2.9153                2.8478
 Depolar     --      0.5747                0.2946                0.7031
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.05  -0.10   0.05    -0.01   0.00   0.00     0.10  -0.01
0.04
   2   6    -0.07  -0.07  -0.08    -0.01  -0.03  -0.01     0.06   0.17
0.08
   3   6     0.01  -0.09  -0.01     0.02   0.02  -0.02    -0.13  -0.07
0.09
   4   6    -0.01   0.12  -0.01     0.01   0.01   0.02     0.01   0.01  -
0.08
   5   6     0.03  -0.03   0.01     0.00  -0.02   0.00     0.01  -0.01  -
0.06
   6   6     0.04   0.13   0.02    -0.02   0.00   0.02     0.13  -0.02  -
0.12
   7   6    -0.04  -0.04   0.09     0.01   0.01   0.00    -0.09  -0.08  -
0.02
   8   6     0.16  -0.03  -0.06     0.01  -0.02  -0.01    -0.06   0.11
0.08
```

```
    9   6     0.06   0.00   0.06     0.01  -0.02  -0.02     0.02   0.02
0.05
   10   6    -0.04   0.05  -0.05     0.00  -0.01   0.01    -0.02   0.02  -
0.04
   11   6    -0.10   0.03   0.00     0.00   0.01  -0.01    -0.06  -0.08
0.02
   12   6    -0.03   0.01   0.00    -0.05   0.10   0.02    -0.02   0.03
0.01
   13   7     0.00   0.00   0.00     0.04  -0.11  -0.04     0.02  -0.03  -
0.02
   14   8     0.00   0.01  -0.01    -0.01   0.02   0.00     0.01  -0.04
0.00
   15   8    -0.03  -0.01  -0.03     0.02  -0.04   0.00     0.00  -0.02
0.00
   16   8    -0.01  -0.02  -0.01    -0.01   0.01   0.00     0.00   0.02
0.00
   17   1     0.07  -0.06   0.24    -0.01   0.00   0.03     0.11  -0.02  -
0.10
   18   1    -0.23  -0.11  -0.21    -0.01  -0.02  -0.01     0.00   0.24  -
0.01
   19   1     0.10  -0.22   0.03     0.02   0.06  -0.04    -0.16  -0.08
0.11
   20   1    -0.18   0.32   0.06     0.02   0.04   0.03    -0.06  -0.06  -
0.12
   21   1     0.17   0.21   0.18    -0.06   0.02   0.01     0.46  -0.14
0.01
   22   1    -0.06  -0.08   0.31    -0.01   0.01   0.01     0.08  -0.10  -
0.07
   23   1     0.34  -0.02  -0.02    -0.02   0.00  -0.02     0.04   0.14
0.11
   24   1    -0.21   0.01   0.03     0.04   0.02   0.01    -0.33  -0.19
0.04
   25   1     0.00   0.08  -0.02    -0.04   0.00   0.00     0.20   0.01  -
0.02
   26   1    -0.17   0.18  -0.08     0.03   0.00   0.03    -0.20   0.04  -
0.21
   27   1     0.04  -0.06   0.05    -0.40   0.84   0.26    -0.12   0.28
0.10
   28   1    -0.04  -0.13  -0.03    -0.02   0.00   0.02     0.01  -0.04
0.01
   29   1    -0.05   0.10  -0.02     0.05  -0.04  -0.02     0.04  -0.08
0.00
                      31                     32                     33
                      ?A                     ?A                     ?A
 Frequencies --    990.2835               1000.0286              1011.2033
 Red. masses --      3.0487                  2.5237                 2.6679
 Frc consts  --      1.7615                  1.4870                 1.6073
 IR Inten    --      4.2578                 25.4794                 7.1123
 Raman Activ --      4.5665                  6.3473                 7.8995
 Depolar     --      0.4022                  0.1486                 0.2703
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.13   0.02  -0.03    -0.02  -0.08  -0.04     0.07   0.21  -
0.02
```

2	6	-0.01	0.03	-0.07	0.10	0.00	-0.07	0.05	0.00	0.03
3	6	0.04	0.15	-0.02	0.02	-0.05	-0.02	-0.01	0.04	-0.01
4	6	0.02	-0.10	0.00	-0.07	-0.06	-0.03	-0.08	0.01	0.04
5	6	0.01	-0.02	0.02	0.00	0.03	0.11	0.01	0.00	0.01
6	6	0.04	-0.09	0.06	0.04	-0.10	0.00	-0.02	-0.10	0.01
7	6	-0.01	-0.07	0.06	0.04	0.17	0.04	0.14	-0.11	0.09
8	6	0.15	0.12	-0.08	-0.01	-0.03	-0.07	0.03	-0.05	-0.05
9	6	0.02	0.01	-0.04	-0.03	0.00	0.06	0.03	0.01	-0.02
10	6	-0.10	-0.16	-0.03	-0.11	0.11	0.02	-0.08	0.01	0.00
11	6	-0.03	0.07	0.12	-0.02	0.03	0.05	-0.13	-0.02	-0.10
12	6	0.00	0.00	0.01	0.01	-0.01	-0.01	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.01	0.01	-0.02	0.00	0.00	0.01
14	8	0.00	0.00	0.01	0.01	-0.01	-0.02	0.00	0.00	0.00
15	8	-0.02	0.00	-0.02	0.00	0.00	0.01	-0.01	0.00	-0.01
16	8	-0.01	0.00	0.01	0.01	-0.01	0.00	0.00	0.00	0.00
17	1	-0.14	-0.01	-0.16	-0.03	-0.08	0.02	0.41	0.43	0.12
18	1	0.06	0.03	0.00	0.27	0.32	-0.08	0.18	0.04	0.12
19	1	-0.05	0.30	-0.06	-0.09	-0.24	0.13	-0.03	0.06	-0.01
20	1	0.13	-0.10	0.01	-0.09	0.06	0.03	-0.17	0.07	0.06
21	1	0.14	-0.01	0.21	0.12	-0.34	-0.17	-0.02	-0.16	-0.05
22	1	-0.10	-0.03	-0.10	-0.04	0.20	-0.03	0.40	-0.18	0.22
23	1	0.30	0.20	-0.06	-0.07	-0.24	-0.02	-0.05	-0.04	-0.07
24	1	-0.17	-0.27	-0.04	-0.21	0.28	0.16	-0.09	0.05	0.03
25	1	0.39	0.10	0.06	0.24	-0.03	0.01	-0.18	-0.21	-0.09
26	1	-0.24	0.12	-0.28	-0.09	-0.06	-0.14	-0.11	0.06	-0.02
27	1	0.01	-0.02	0.00	-0.03	0.09	0.00	0.01	-0.02	0.02
28	1	0.00	0.03	0.03	0.01	0.00	-0.02	-0.02	-0.06	-0.01

```
  29   1     0.04  -0.03  -0.01     0.06   0.21  -0.11    -0.01   0.02  -
0.01
                     34                    35                    36
                     ?A                    ?A                    ?A
 Frequencies --  1014.2370             1033.4872             1042.5796
 Red. masses --     2.2347                1.9990                2.1859
 Frc consts  --     1.3544                1.2580                1.3999
 IR Inten    --    38.3450                0.8942               58.3176
 Raman Activ --     3.9108                5.2596                5.4595
 Depolar     --     0.6630                0.6270                0.5978
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.05  -0.08  -0.09    -0.04   0.00   0.00     0.02  -0.06
0.08
   2   6     0.03   0.00   0.10     0.05  -0.03  -0.01    -0.06   0.09  -
0.08
   3   6    -0.06   0.06  -0.07    -0.03   0.01   0.01     0.04   0.10
0.02
   4   6    -0.05   0.06   0.12    -0.02   0.01  -0.02     0.02   0.08  -
0.02
   5   6     0.05  -0.05  -0.03     0.02  -0.01   0.01     0.01  -0.02
0.00
   6   6     0.04   0.01  -0.04     0.11   0.06   0.13    -0.02  -0.09  -
0.02
   7   6    -0.08   0.09   0.04     0.06   0.00  -0.06     0.04   0.05
0.00
   8   6     0.02  -0.04  -0.03    -0.03  -0.05   0.06    -0.03  -0.08
0.07
   9   6     0.06  -0.03   0.00    -0.05  -0.01   0.00     0.12  -0.03  -
0.03
  10   6     0.00  -0.09   0.01    -0.12  -0.05  -0.05     0.03  -0.08  -
0.03
  11   6     0.04  -0.01  -0.05     0.03   0.05  -0.10    -0.05   0.00  -
0.01
  12   6    -0.01   0.01   0.01     0.02  -0.01  -0.01    -0.02   0.02
0.01
  13   7     0.00   0.00   0.01     0.01   0.01  -0.02    -0.01  -0.01
0.03
  14   8    -0.01   0.05   0.01     0.00   0.01   0.00     0.00   0.06
0.01
  15   8    -0.01   0.00  -0.02     0.01   0.01   0.01    -0.02   0.00  -
0.02
  16   8    -0.01   0.01   0.00     0.00   0.00   0.00    -0.02  -0.01
0.01
  17   1     0.01  -0.12  -0.27    -0.13  -0.02   0.18    -0.05  -0.07
0.25
  18   1     0.18   0.07   0.21     0.08   0.05  -0.03    -0.20   0.39  -
0.36
  19   1    -0.21   0.27  -0.13    -0.16   0.02   0.06     0.07   0.20  -
0.04
  20   1    -0.22   0.17   0.16     0.08  -0.08  -0.05     0.05   0.12
0.00
  21   1     0.15  -0.19  -0.14     0.43   0.09   0.39     0.03  -0.23  -
0.10
```

```
  22   1    -0.29   0.09   0.16     0.11   0.00  -0.11     0.13   0.06  -
0.09
  23   1     0.00   0.09  -0.08    -0.05  -0.10   0.07    -0.33  -0.23
0.05
  24   1    -0.18  -0.14   0.10    -0.28  -0.22  -0.04     0.01  -0.14  -
0.04
  25   1    -0.13  -0.29  -0.02    -0.36   0.16  -0.04    -0.03   0.19  -
0.01
  26   1     0.12   0.20   0.17     0.23  -0.10   0.23    -0.04  -0.16  -
0.04
  27   1     0.04  -0.08   0.00    -0.01   0.03  -0.04     0.05  -0.13
0.04
  28   1    -0.05  -0.11  -0.02     0.03   0.11   0.01    -0.09  -0.25  -
0.04
  29   1    -0.03   0.00   0.02     0.01   0.02  -0.02    -0.02  -0.01
0.00
                     37                    38                    39
                     ?A                    ?A                    ?A
 Frequencies --  1046.9878             1067.7250             1100.4441
 Red. masses --     4.5128                1.6973                1.9709
 Frc consts  --     2.9146                1.1400                1.4062
 IR Inten    --    16.2419                1.3471               57.9150
 Raman Activ --     2.2417                5.1905                8.3012
 Depolar     --     0.7353                0.7447                0.6873
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.03   0.01   0.07    -0.05  -0.11  -0.04    -0.01   0.03  -
0.01
   2   6    -0.14   0.08  -0.05     0.01   0.01   0.06     0.02  -0.03
0.00
   3   6     0.02  -0.08  -0.19    -0.01  -0.02  -0.01     0.00  -0.05
0.00
   4   6     0.15   0.01   0.14     0.01   0.01  -0.02     0.01  -0.06  -
0.01
   5   6    -0.12   0.10   0.00     0.01  -0.01   0.01    -0.03   0.02
0.01
   6   6     0.20   0.05   0.00    -0.02   0.01  -0.05    -0.01   0.03
0.06
   7   6     0.06  -0.03  -0.04     0.09  -0.10   0.03    -0.02  -0.02  -
0.04
   8   6    -0.12  -0.06  -0.12    -0.04   0.01   0.01    -0.06   0.07  -
0.08
   9   6    -0.14  -0.08   0.03     0.03   0.01  -0.02     0.18  -0.07  -
0.01
  10   6    -0.01  -0.13   0.18     0.00   0.02   0.02    -0.02   0.03
0.05
  11   6    -0.07  -0.02   0.03    -0.02   0.13   0.00     0.03  -0.02
0.01
  12   6     0.02  -0.01  -0.02    -0.01   0.00   0.00    -0.02   0.03
0.02
  13   7     0.01   0.03  -0.04     0.00  -0.01   0.01    -0.01  -0.01
0.02
  14   8    -0.01   0.06   0.00     0.00   0.00   0.00     0.01   0.07
0.02
```

15	8	0.04	0.01	0.05	0.00	0.00	-0.01	-0.03	-0.01	-0.03
16	8	0.02	0.00	-0.02	0.00	0.00	0.00	0.02	0.01	-0.01
17	1	0.18	0.07	-0.05	-0.29	-0.27	-0.23	0.06	0.07	-0.02
18	1	-0.13	0.09	-0.05	0.12	-0.03	0.18	0.02	-0.11	0.05
19	1	0.11	-0.05	-0.25	-0.02	-0.01	-0.01	0.03	-0.12	0.03
20	1	0.20	0.08	0.18	0.11	0.00	-0.02	0.03	-0.06	-0.01
21	1	0.17	-0.07	-0.14	-0.10	-0.03	-0.15	0.02	0.22	0.26
22	1	0.17	-0.08	0.15	0.41	-0.17	0.20	-0.05	0.02	-0.24
23	1	-0.10	0.14	-0.18	-0.22	-0.03	-0.02	-0.41	0.15	-0.20
24	1	-0.12	0.01	0.32	-0.04	0.05	0.06	-0.31	0.13	0.27
25	1	0.12	0.10	0.00	-0.11	0.39	0.01	0.02	-0.01	0.01
26	1	-0.16	-0.01	-0.15	-0.05	0.41	0.03	0.04	-0.09	0.00
27	1	0.01	0.03	-0.10	0.00	-0.01	0.02	0.04	-0.10	0.05
28	1	0.03	0.25	0.03	-0.01	-0.06	-0.01	-0.14	-0.48	-0.07
29	1	-0.07	-0.10	0.09	0.02	0.05	-0.03	0.00	-0.01	0.02

	40	41	42
	?A	?A	?A
Frequencies --	1138.4223	1165.0874	1192.5663
Red. masses --	2.0294	1.9829	2.1432
Frc consts --	1.5497	1.5859	1.7959
IR Inten --	39.8595	60.0816	52.2787
Raman Activ --	2.8169	2.4035	3.6333
Depolar --	0.6742	0.7080	0.6086

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.05	-0.02	0.02	0.03	-0.02	-0.07	0.01	-0.02	0.02
2	6	0.03	0.00	-0.05	0.06	-0.01	0.02	-0.06	0.00	-0.02
3	6	0.06	-0.08	0.10	-0.04	0.00	0.05	0.06	-0.06	-0.05
4	6	0.05	0.01	0.10	-0.01	0.08	0.07	0.06	0.00	0.02
5	6	-0.05	0.02	-0.12	0.02	-0.03	-0.07	-0.03	0.03	0.01
6	6	-0.02	-0.05	-0.01	0.00	0.00	0.05	-0.01	-0.01	0.00
7	6	0.00	0.02	0.06	0.06	0.05	-0.06	0.00	0.02	-0.01

```
    8   6     0.05  -0.02  -0.03     0.02  -0.09   0.04    -0.02  -0.03
0.00
    9   6     0.00   0.02  -0.07    -0.03  -0.09   0.00     0.03   0.21
0.00
   10   6    -0.04   0.11   0.05    -0.04   0.03  -0.04    -0.02   0.01
0.02
   11   6     0.00   0.01  -0.04    -0.08  -0.01   0.10    -0.01  -0.01
0.01
   12   6     0.00   0.00   0.01    -0.01   0.00   0.00     0.06   0.00
0.01
   13   7     0.00  -0.01   0.02     0.01   0.01  -0.02     0.00  -0.03
0.08
   14   8     0.00  -0.02   0.00     0.00   0.04   0.00     0.01  -0.09  -
0.01
   15   8     0.00   0.00  -0.01     0.02   0.00   0.02    -0.05   0.00  -
0.07
   16   8     0.01   0.03  -0.04     0.00   0.02  -0.02     0.01  -0.01  -
0.01
   17   1    -0.13  -0.04   0.14     0.08  -0.03  -0.37     0.19   0.04  -
0.31
   18   1     0.04   0.16  -0.12    -0.08  -0.31   0.05     0.16  -0.13
0.25
   19   1    -0.24   0.14   0.09     0.03  -0.04   0.05    -0.26   0.23  -
0.09
   20   1     0.21  -0.20   0.02    -0.04   0.10   0.08    -0.20   0.29
0.14
   21   1     0.02  -0.15  -0.07    -0.11   0.19   0.14     0.05   0.15
0.19
   22   1    -0.13   0.01   0.15     0.24   0.09  -0.38     0.05   0.06  -
0.25
   23   1    -0.06   0.29  -0.15    -0.07  -0.06   0.01    -0.17  -0.34
0.07
   24   1    -0.11  -0.19  -0.05     0.10  -0.01  -0.15    -0.05  -0.23  -
0.07
   25   1    -0.10  -0.05  -0.02     0.28   0.08   0.04     0.02   0.07
0.01
   26   1     0.05   0.04   0.07    -0.25  -0.01  -0.24     0.00  -0.12  -
0.02
   27   1    -0.01  -0.02  -0.03     0.03  -0.03  -0.02    -0.11   0.11  -
0.12
   28   1     0.02   0.04   0.00    -0.02  -0.02  -0.02     0.02  -0.03
0.02
   29   1    -0.24  -0.46   0.36    -0.13  -0.25   0.19    -0.02  -0.01
0.02
                     43                    44                    45
                     ?A                    ?A                    ?A
 Frequencies --  1213.1786             1218.9843             1228.6649
 Red. masses --     2.0490                2.0338                2.0220
 Frc consts  --     1.7768                1.7806                1.7984
 IR Inten    --    19.4963               37.6874               86.9939
 Raman Activ --     8.1087                3.4135                3.8866
 Depolar     --     0.6679                0.3105                0.4343
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
```

1	6	-0.02	-0.01	-0.02	0.05	0.02	-0.07	0.01	0.02	-0.02
2	6	0.08	0.02	0.00	-0.03	-0.09	0.06	-0.03	-0.07	0.01
3	6	-0.11	0.06	0.00	0.02	-0.03	-0.03	0.05	0.01	-0.01
4	6	-0.01	-0.01	0.06	-0.08	0.04	0.00	-0.01	-0.02	0.02
5	6	0.02	-0.03	-0.03	0.01	-0.01	0.02	0.00	0.00	0.00
6	6	0.04	-0.01	0.02	-0.02	0.10	0.04	-0.04	0.05	0.02
7	6	0.01	0.02	0.00	0.03	-0.01	-0.09	0.00	0.00	-0.04
8	6	-0.05	-0.02	-0.05	-0.04	-0.05	0.03	-0.08	0.00	-0.06
9	6	0.01	0.14	0.07	0.01	0.00	-0.05	0.01	0.09	0.15
10	6	-0.03	-0.08	0.00	0.01	0.02	0.00	0.01	-0.02	-0.07
11	6	0.00	0.01	-0.02	-0.02	-0.01	0.09	0.02	-0.01	0.04
12	6	0.06	0.00	0.02	0.06	0.03	0.03	-0.04	-0.04	-0.03
13	7	0.01	-0.02	0.06	0.02	-0.02	0.09	-0.02	0.02	-0.10
14	8	0.02	-0.04	0.00	0.00	0.00	0.00	0.04	-0.01	0.00
15	8	-0.05	-0.01	-0.07	-0.04	0.00	-0.07	0.03	0.00	0.07
16	8	0.00	0.03	-0.01	0.01	0.00	0.01	0.00	0.01	-0.02
17	1	-0.13	-0.04	0.12	0.03	0.04	0.17	-0.02	0.02	0.07
18	1	-0.17	-0.05	-0.19	0.00	0.27	-0.11	0.09	0.21	-0.02
19	1	0.54	-0.45	0.05	-0.17	0.18	-0.07	-0.26	0.11	0.05
20	1	0.22	-0.03	0.09	0.34	-0.33	-0.14	0.17	0.02	0.06
21	1	-0.11	0.03	-0.06	0.05	-0.19	-0.17	0.12	-0.13	-0.03
22	1	-0.04	0.01	0.09	0.01	-0.04	0.09	0.17	-0.05	0.10
23	1	0.05	0.05	-0.04	0.18	0.27	-0.01	0.11	0.01	-0.01
24	1	0.18	0.16	-0.02	-0.10	-0.07	0.02	0.17	-0.16	-0.23
25	1	-0.03	-0.03	-0.01	0.24	0.03	0.04	0.10	-0.01	0.03
26	1	0.02	0.03	0.02	-0.14	-0.03	-0.16	-0.03	0.08	-0.03
27	1	-0.09	0.11	-0.18	-0.10	0.06	-0.33	0.10	-0.04	0.43

```
  28   1    -0.03  -0.21  -0.01     0.00   0.01   0.00    -0.11  -0.52  -
0.05
  29   1    -0.05  -0.22   0.12     0.05   0.19  -0.10    -0.07  -0.16
0.12
                     46                     47                     48
                     ?A                     ?A                     ?A
 Frequencies --  1253.8286              1267.0963              1277.1836
 Red. masses --     1.9240                 1.0849                 1.4231
 Frc consts  --     1.7821                 1.0262                 1.3677
 IR Inten    --    23.8337                 9.2374                23.1705
 Raman Activ --     5.3654                11.5875                 0.9272
 Depolar     --     0.5726                 0.7431                 0.4644
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01  -0.04  -0.04     0.00   0.01  -0.02    -0.03  -0.01  -
0.04
   2   6     0.03   0.01   0.03     0.02  -0.03  -0.02    -0.01  -0.06
0.02
   3   6    -0.05  -0.03  -0.03     0.01   0.02   0.01    -0.03   0.03
0.00
   4   6    -0.03   0.05   0.03     0.00   0.01  -0.02    -0.01  -0.02
0.00
   5   6     0.01   0.00  -0.01     0.00  -0.01   0.00     0.01  -0.04
0.01
   6   6     0.01   0.00   0.01    -0.02  -0.01   0.02    -0.05   0.05  -
0.02
   7   6     0.04  -0.01   0.01    -0.01   0.00   0.01     0.01  -0.04  -
0.01
   8   6     0.03  -0.04   0.03    -0.02   0.03   0.01     0.00   0.01
0.01
   9   6     0.06   0.14  -0.10     0.00  -0.03   0.02     0.03   0.01  -
0.03
  10   6    -0.03   0.01   0.06     0.00  -0.01  -0.02     0.09  -0.02
0.00
  11   6    -0.04   0.02   0.01     0.01  -0.01   0.01     0.01   0.03
0.03
  12   6    -0.05  -0.03  -0.03     0.00   0.00   0.00    -0.01   0.00  -
0.01
  13   7    -0.04   0.00  -0.07     0.01   0.00   0.01    -0.01   0.00
0.00
  14   8    -0.01  -0.05   0.00     0.00   0.01   0.00    -0.03  -0.02
0.00
  15   8     0.04   0.01   0.07    -0.01   0.00  -0.01     0.01   0.00
0.01
  16   8     0.00  -0.01   0.02     0.00   0.01  -0.01     0.01   0.04  -
0.03
  17   1     0.16   0.04  -0.04     0.17   0.06  -0.35     0.12   0.11
0.14
  18   1    -0.11  -0.07  -0.06     0.00  -0.07  -0.01     0.13   0.32  -
0.05
  19   1     0.26   0.03  -0.19    -0.05  -0.04   0.07     0.08  -0.19
0.09
  20   1     0.19  -0.22  -0.07    -0.03   0.15   0.04     0.07   0.30
0.17
```

21	1	-0.07	0.05	-0.01	0.08	-0.16	-0.05	0.10	0.00	0.04
22	1	-0.33	0.04	-0.02	-0.14	-0.07	0.42	0.01	-0.01	-0.14
23	1	-0.15	0.15	-0.07	0.04	0.09	0.01	0.00	-0.24	0.09
24	1	-0.12	-0.11	0.06	0.01	0.09	0.02	-0.32	0.06	0.28
25	1	0.02	0.15	0.00	-0.07	0.52	0.02	0.08	-0.06	0.02
26	1	-0.01	-0.33	-0.07	0.09	-0.48	-0.02	0.00	-0.06	-0.02
27	1	0.10	-0.09	0.49	-0.01	0.01	-0.06	0.03	-0.05	0.09
28	1	0.03	0.06	0.01	-0.01	-0.01	0.00	0.09	0.38	0.04
29	1	0.08	0.24	-0.14	-0.04	-0.10	0.07	-0.12	-0.31	0.21

	49			50			51		
	?A			?A			?A		
Frequencies --	1302.5874			1316.9085			1332.2537		
Red. masses --	1.6300			2.1502			1.5192		
Frc consts --	1.6294			2.1970			1.5887		
IR Inten --	30.5450			10.9065			12.3676		
Raman Activ --	0.9372			1.3967			1.3772		
Depolar --	0.7490			0.7381			0.7486		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	0.08	0.01	-0.08	-0.08	-0.05	0.05	-0.01	0.00
2	6	0.06	-0.01	0.00	0.04	0.02	0.05	-0.01	0.05	0.05
3	6	-0.02	-0.02	-0.01	-0.03	-0.03	0.00	0.05	-0.02	-0.03
4	6	-0.02	-0.03	0.06	0.01	-0.01	0.02	-0.11	0.01	0.00
5	6	-0.01	0.01	-0.02	-0.01	0.00	-0.03	0.00	-0.03	0.03
6	6	-0.09	-0.04	0.00	-0.07	-0.02	-0.07	-0.01	0.01	-0.06
7	6	-0.06	0.07	0.01	0.09	-0.05	0.07	-0.02	-0.01	0.02
8	6	0.03	-0.03	-0.07	-0.02	0.02	-0.05	0.08	0.03	-0.02
9	6	0.00	0.02	0.03	-0.07	-0.06	0.15	0.00	0.00	0.05
10	6	0.09	0.01	-0.01	0.07	0.05	-0.05	-0.05	-0.05	0.01
11	6	0.01	-0.06	0.00	0.00	0.09	0.00	0.00	-0.02	-0.01
12	6	0.00	0.00	0.00	0.01	0.00	0.01	0.01	0.00	0.01
13	7	0.00	0.00	0.00	0.03	0.01	0.00	0.00	0.00	-0.01

```
  14   8    -0.01  -0.01  -0.01     0.01   0.01  -0.01    -0.01  -0.01  -
0.01
  15   8     0.00   0.00   0.00    -0.01   0.00  -0.02    -0.01   0.00  -
0.01
  16   8     0.00  -0.01   0.02     0.01   0.00   0.02     0.01   0.03  -
0.02
  17   1    -0.33  -0.15  -0.17     0.32   0.17   0.16     0.01  -0.02
0.12
  18   1    -0.25  -0.09  -0.24    -0.16   0.04  -0.14    -0.19  -0.18
0.01
  19   1     0.12   0.12  -0.15     0.10   0.20  -0.18    -0.28   0.12
0.02
  20   1     0.05  -0.11   0.03     0.10   0.11   0.09     0.47  -0.11
0.01
  21   1     0.24  -0.03   0.26     0.10   0.10   0.17     0.19   0.04
0.11
  22   1     0.43   0.00   0.06    -0.20   0.04  -0.16    -0.08   0.01  -
0.06
  23   1     0.03  -0.06  -0.07    -0.19   0.14  -0.13    -0.35  -0.21  -
0.05
  24   1    -0.28  -0.12   0.15    -0.01  -0.35  -0.18     0.30   0.38
0.01
  25   1    -0.04   0.23   0.01     0.01  -0.11   0.00    -0.03   0.09
0.00
  26   1    -0.01   0.07   0.00     0.08  -0.28   0.02     0.01  -0.02
0.01
  27   1     0.00   0.00   0.03    -0.04   0.07  -0.22     0.01   0.00
0.01
  28   1     0.05   0.19   0.02    -0.01  -0.02   0.00     0.04   0.18
0.02
  29   1     0.07   0.15  -0.10     0.08   0.22  -0.13    -0.06  -0.11
0.10
                     52                    53                    54
                     ?A                    ?A                    ?A
 Frequencies --  1345.0554             1354.3916             1367.3325
 Red. masses --     1.4501                1.5526                1.6285
 Frc consts  --     1.5457                1.6781                1.7939
 IR Inten    --     6.3516                5.0947               43.5000
 Raman Activ --     2.3028                1.2068                3.8084
 Depolar     --     0.7481                0.3646                0.3853
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01  -0.03   0.02     0.07  -0.01   0.04     0.00   0.00
0.01
   2   6     0.01   0.07   0.03    -0.10  -0.02  -0.03     0.01   0.03
0.00
   3   6     0.04  -0.02  -0.02    -0.02   0.06   0.01     0.06   0.05
0.00
   4   6    -0.04  -0.01  -0.01    -0.05   0.05  -0.01     0.06   0.03
0.00
   5   6    -0.01  -0.02   0.02     0.02   0.00   0.01     0.05   0.05  -
0.03
   6   6     0.03  -0.07   0.04     0.03  -0.07  -0.02    -0.05   0.03
0.05
```

7	6	0.03	0.02	0.04	0.01	0.04	0.03	0.07	-0.02	-0.01
8	6	-0.10	0.00	-0.01	0.01	-0.01	-0.05	-0.03	-0.03	-0.02
9	6	0.01	0.00	-0.03	-0.02	-0.01	0.07	0.03	0.04	0.08
10	6	0.03	0.01	-0.07	0.06	0.01	-0.03	0.04	-0.05	-0.05
11	6	0.00	0.02	-0.03	-0.02	-0.03	-0.02	-0.03	0.02	0.00
12	6	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.01	0.00
13	7	0.00	0.00	0.00	0.01	0.00	0.00	-0.01	0.00	-0.01
14	8	0.00	0.00	0.01	-0.01	0.00	-0.01	-0.03	-0.02	-0.01
15	8	0.00	0.00	0.01	0.00	0.00	0.00	-0.01	0.00	-0.01
16	8	0.01	0.02	-0.01	-0.01	-0.01	0.00	-0.04	-0.06	0.02
17	1	0.06	-0.01	-0.01	0.03	-0.07	-0.12	-0.07	-0.05	-0.07
18	1	-0.27	-0.25	-0.05	0.41	0.18	0.32	-0.16	-0.23	-0.02
19	1	-0.26	0.12	0.01	0.08	-0.20	0.13	-0.34	-0.26	0.33
20	1	0.30	0.10	0.08	0.26	-0.36	-0.17	-0.28	-0.21	-0.16
21	1	-0.35	0.16	-0.03	-0.23	0.33	0.15	0.06	-0.21	-0.09
22	1	-0.01	0.05	-0.05	-0.06	0.06	0.00	-0.21	0.03	-0.07
23	1	0.54	0.01	0.13	-0.07	0.07	-0.09	-0.17	0.23	-0.14
24	1	-0.34	0.09	0.18	-0.17	-0.22	0.00	-0.14	0.16	0.15
25	1	-0.03	-0.06	-0.02	-0.04	0.15	-0.01	0.02	-0.16	-0.01
26	1	0.05	-0.04	0.04	0.00	-0.03	0.01	-0.06	0.03	-0.04
27	1	0.01	-0.01	0.04	0.00	0.02	-0.03	0.01	-0.01	0.10
28	1	-0.01	-0.06	-0.01	0.02	0.09	0.01	0.07	0.30	0.03
29	1	-0.02	-0.04	0.05	-0.03	-0.05	0.03	0.01	-0.02	-0.05

	55	56	57
	?A	?A	?A
Frequencies --	1379.2292	1392.1764	1401.0854
Red. masses --	1.5023	1.3500	1.6367
Frc consts --	1.6838	1.5416	1.8930
IR Inten --	29.4728	1.6741	11.1102
Raman Activ --	2.5806	1.6515	2.8155
Depolar --	0.7320	0.7491	0.4250

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.05	0.00	0.00	0.00	0.00	0.05	0.00	0.00
2	6	0.01	-0.06	0.06	-0.01	-0.04	0.05	-0.02	0.03	-0.06
3	6	0.01	-0.02	0.00	0.02	-0.01	0.03	-0.03	-0.04	0.05
4	6	0.01	-0.03	0.01	0.04	0.02	0.00	0.01	-0.05	-0.05
5	6	-0.01	0.00	-0.02	0.00	0.00	0.00	-0.05	-0.06	0.03
6	6	0.11	-0.02	0.03	0.00	-0.04	-0.10	-0.03	-0.01	0.02
7	6	-0.01	-0.02	-0.04	0.01	0.02	0.01	0.06	0.03	-0.03
8	6	0.03	0.03	0.01	-0.03	-0.03	0.00	-0.05	-0.04	0.03
9	6	0.03	-0.01	0.07	0.00	0.02	-0.02	0.07	-0.01	0.06
10	6	-0.03	0.02	-0.06	-0.03	-0.05	0.00	-0.01	-0.01	-0.04
11	6	0.00	-0.02	0.00	-0.02	0.07	0.00	-0.02	-0.01	0.00
12	6	0.02	0.01	0.01	0.00	0.00	-0.01	0.03	0.02	0.00
13	7	-0.01	0.00	-0.01	0.00	0.00	0.00	-0.02	0.00	0.00
14	8	-0.02	-0.01	-0.01	0.00	0.00	0.00	-0.03	-0.01	-0.01
15	8	-0.01	0.00	-0.01	0.00	0.00	0.00	-0.01	0.00	-0.01
16	8	0.00	0.00	0.01	0.00	0.00	0.00	0.04	0.05	-0.01
17	1	-0.15	-0.04	-0.11	-0.09	-0.07	-0.11	-0.19	-0.11	0.17
18	1	-0.17	0.33	-0.31	-0.01	0.33	-0.14	0.23	-0.15	0.25
19	1	-0.10	0.14	-0.05	-0.07	0.12	-0.01	0.22	0.30	-0.25
20	1	-0.08	0.15	0.09	-0.22	-0.12	-0.10	-0.03	0.26	0.10
21	1	-0.51	0.25	-0.19	0.10	0.40	0.38	0.09	-0.03	0.09
22	1	-0.13	-0.05	0.15	0.14	-0.01	0.13	-0.14	0.03	0.13
23	1	-0.31	-0.09	-0.03	0.15	0.19	-0.03	0.02	0.44	-0.10
24	1	-0.05	-0.04	-0.09	0.14	0.42	0.12	0.10	0.10	-0.06
25	1	-0.04	0.04	0.00	0.06	-0.21	-0.01	0.04	-0.03	-0.01
26	1	-0.04	0.06	-0.04	0.04	-0.25	0.00	-0.05	0.09	-0.01

```
  27   1     0.02  -0.02   0.09     0.00   0.00   0.00     0.04  -0.06
0.15
  28   1     0.06   0.26   0.03    -0.01  -0.05  -0.01     0.07   0.34
0.04
  29   1     0.03   0.06  -0.04    -0.01  -0.02   0.01     0.01   0.01
0.03
                     58                     59                     60
                     ?A                     ?A                     ?A
 Frequencies --  1408.4924              1423.2275              1434.3840
 Red. masses --     1.6150                 1.4534                 1.4315
 Frc consts  --     1.8877                 1.7346                 1.7353
 IR Inten    --    12.7678                 2.3721                 1.6167
 Raman Activ --     5.3700                 1.2281                 1.3117
 Depolar     --     0.6360                 0.7483                 0.7469
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.10  -0.07   0.00    -0.05  -0.01   0.14     0.02   0.03
0.07
   2   6     0.00   0.03  -0.03     0.03  -0.04  -0.04     0.00  -0.05
0.01
   3   6     0.01   0.01   0.03    -0.01   0.00   0.02     0.02   0.03  -
0.03
   4   6    -0.01   0.03  -0.01    -0.03   0.03  -0.01    -0.04  -0.05  -
0.06
   5   6    -0.01  -0.02  -0.03    -0.02  -0.02  -0.01    -0.02  -0.02  -
0.02
   6   6     0.03  -0.02   0.02    -0.04   0.01   0.00     0.01   0.05  -
0.02
   7   6    -0.12   0.03  -0.04     0.07   0.01  -0.06    -0.03  -0.01
0.09
   8   6     0.01  -0.05   0.00    -0.02   0.02   0.01     0.02  -0.06
0.03
   9   6     0.04   0.01   0.03     0.01  -0.01  -0.01     0.00   0.00  -
0.01
  10   6    -0.01  -0.01  -0.02     0.00   0.00   0.00    -0.02   0.00
0.04
  11   6     0.08   0.01   0.02    -0.01  -0.01  -0.02    -0.01   0.01  -
0.03
  12   6     0.03   0.01   0.01     0.00   0.00   0.00     0.01   0.00
0.00
  13   7    -0.02  -0.01   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   8    -0.02  -0.01  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
  15   8    -0.01   0.00  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
  16   8     0.01   0.00   0.01     0.01   0.01   0.00     0.01   0.01
0.01
  17   1     0.54   0.30   0.05     0.25   0.04  -0.60    -0.07  -0.09  -
0.32
  18   1     0.04  -0.05   0.05    -0.01   0.09  -0.15    -0.02   0.13  -
0.11
  19   1    -0.01  -0.02   0.06     0.10   0.04  -0.05    -0.09  -0.22
0.16
```

20	1	0.11	-0.05	-0.04	0.26	-0.04	-0.01	0.23	0.32	0.15
21	1	-0.10	0.01	-0.04	0.17	-0.04	0.11	0.03	-0.07	-0.13
22	1	0.55	-0.10	0.16	-0.26	0.00	0.18	0.17	0.07	-0.44
23	1	-0.06	0.19	-0.10	0.00	-0.16	0.07	0.03	0.46	-0.14
24	1	0.02	0.10	0.01	0.03	0.04	0.01	0.12	-0.09	-0.09
25	1	0.06	-0.07	0.03	0.01	-0.29	-0.02	-0.07	-0.04	-0.02
26	1	0.09	0.09	0.07	-0.06	0.39	0.04	0.05	-0.11	0.04
27	1	0.03	-0.04	0.15	0.00	-0.01	0.00	0.01	-0.01	0.03
28	1	0.05	0.22	0.02	0.00	0.01	0.00	0.00	0.02	0.00
29	1	0.04	0.12	-0.07	0.03	0.06	-0.03	0.05	0.10	-0.06

	61			62			63		
	?A			?A			?A		
Frequencies --	1436.7481			1455.0797			1469.6880		
Red. masses --	1.4911			1.4748			1.9825		
Frc consts --	1.8136			1.8398			2.5230		
IR Inten --	3.1989			20.8850			120.8811		
Raman Activ --	3.8007			1.6284			6.2501		
Depolar --	0.7480			0.5327			0.2801		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	0.00	-0.01	0.05	0.00	0.04	0.00	0.00	-0.03
2	6	0.00	0.03	0.03	0.00	0.00	-0.04	0.00	-0.01	0.02
3	6	0.02	0.04	-0.08	-0.02	-0.02	0.01	0.00	0.01	-0.01
4	6	-0.03	-0.04	-0.03	-0.01	0.02	0.02	0.01	0.01	0.06
5	6	0.02	0.02	0.00	0.00	0.00	0.02	0.01	0.05	-0.07
6	6	-0.02	-0.07	-0.02	0.01	0.04	0.05	-0.01	0.00	-0.05
7	6	0.00	0.03	-0.10	-0.06	-0.05	-0.01	0.02	0.00	0.04
8	6	0.02	0.00	0.04	0.00	0.04	-0.03	-0.10	0.04	-0.05
9	6	0.01	-0.01	-0.03	0.03	-0.03	0.02	0.10	-0.08	-0.01
10	6	0.00	0.05	0.07	0.00	0.01	-0.02	-0.07	0.03	0.07
11	6	-0.01	0.05	0.02	-0.03	0.13	-0.01	0.00	-0.02	-0.01
12	6	-0.01	0.00	0.00	0.03	0.02	0.01	0.11	0.06	0.04

```
  13   7     0.00   0.00   0.00    -0.01   0.00  -0.01    -0.05  -0.02  -
0.02
  14   8     0.00   0.00   0.00    -0.01   0.00   0.00    -0.02   0.00  -
0.01
  15   8     0.00   0.00   0.00    -0.01   0.00  -0.01    -0.04  -0.01  -
0.04
  16   8    -0.01  -0.01   0.00     0.00   0.01  -0.01    -0.02  -0.03
0.02
  17   1    -0.12  -0.07   0.10    -0.17  -0.17  -0.19     0.01   0.02
0.08
  18   1    -0.12  -0.15   0.02     0.07  -0.08   0.06     0.01   0.07  -
0.01
  19   1    -0.13  -0.31   0.18     0.13   0.11  -0.12    -0.03  -0.16
0.11
  20   1     0.12   0.25   0.12     0.06  -0.19  -0.07     0.04  -0.06
0.03
  21   1     0.06   0.14   0.25    -0.05  -0.20  -0.21     0.14   0.06
0.11
  22   1     0.04  -0.10   0.51     0.22  -0.09   0.00    -0.07   0.05  -
0.08
  23   1    -0.12   0.07  -0.01     0.00  -0.26   0.06     0.42  -0.29
0.17
  24   1     0.02  -0.39  -0.13     0.00  -0.06  -0.05     0.32  -0.17  -
0.24
  25   1     0.13  -0.30   0.00     0.08  -0.48  -0.03    -0.01   0.20
0.00
  26   1     0.00  -0.07  -0.02     0.10  -0.52   0.01     0.01   0.00
0.02
  27   1     0.00   0.00  -0.02     0.02  -0.03   0.09     0.09  -0.12
0.40
  28   1     0.00   0.01   0.01     0.02   0.10   0.01     0.06   0.29
0.04
  29   1     0.00  -0.03   0.00    -0.03  -0.06   0.04     0.05   0.09  -
0.09
                     64                     65                     66
                     ?A                     ?A                     ?A
 Frequencies --  1500.9972              1504.2997              1632.2237
 Red. masses --     2.1943                 2.6581                 2.8652
 Frc consts  --     2.9128                 3.5440                 4.4975
 IR Inten    --   115.7158               122.3256               211.0092
 Raman Activ --     1.8171                 5.6091                12.0195
 Depolar     --     0.6652                 0.7284                 0.1861
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.04   0.00   0.02     0.02   0.00   0.00    -0.02   0.00
0.02
   2   6     0.04   0.00   0.04    -0.02   0.01  -0.02    -0.01  -0.01
0.00
   3   6    -0.01   0.01  -0.10     0.00   0.00   0.04    -0.05  -0.06
0.03
   4   6     0.02   0.04  -0.07    -0.01  -0.02   0.01    -0.06  -0.05  -
0.06
   5   6     0.02  -0.06   0.22    -0.02   0.00  -0.07     0.22   0.26
0.04
```

```
   6   6     0.00  -0.01  -0.01     0.00  -0.01   0.00     0.01   0.01
0.00
   7   6     0.00   0.01   0.02     0.02  -0.01  -0.02     0.00   0.00
0.00
   8   6     0.01  -0.02   0.01     0.07   0.00   0.04     0.00  -0.03
0.02
   9   6    -0.04  -0.02   0.01    -0.21   0.00  -0.06     0.00   0.00
0.00
  10   6     0.01   0.05   0.03     0.07  -0.02  -0.03    -0.01  -0.01  -
0.01
  11   6     0.02  -0.02  -0.01    -0.01   0.01   0.01    -0.04  -0.01  -
0.03
  12   6     0.10   0.05   0.01     0.21   0.07   0.09     0.01   0.01
0.02
  13   7    -0.04  -0.02   0.00    -0.07  -0.02  -0.04     0.00   0.00  -
0.01
  14   8     0.00   0.00   0.00     0.04   0.02   0.02     0.00   0.00
0.00
  15   8    -0.03  -0.01  -0.03    -0.06  -0.01  -0.06    -0.01   0.00  -
0.01
  16   8     0.01   0.05  -0.07     0.01   0.00   0.02    -0.10  -0.11  -
0.01
  17   1     0.11   0.07  -0.11    -0.07  -0.04   0.05     0.05   0.03  -
0.05
  18   1    -0.23  -0.03  -0.19     0.08   0.00   0.08     0.02   0.03
0.00
  19   1     0.03   0.01  -0.13    -0.01   0.00   0.05     0.22   0.28  -
0.25
  20   1    -0.33  -0.28  -0.27     0.08   0.18   0.11     0.21   0.20
0.07
  21   1     0.00   0.00   0.00     0.00   0.01   0.02    -0.01   0.01  -
0.01
  22   1     0.03   0.02  -0.07    -0.07  -0.02   0.08     0.03   0.01  -
0.03
  23   1    -0.02   0.18  -0.07    -0.20   0.01  -0.02    -0.02   0.15  -
0.05
  24   1     0.01  -0.29  -0.12    -0.22   0.21   0.24     0.01   0.07
0.02
  25   1    -0.07   0.04   0.01     0.02  -0.05   0.00     0.39   0.07  -
0.08
  26   1    -0.01   0.11  -0.01    -0.02  -0.02  -0.02     0.18   0.09
0.39
  27   1     0.05  -0.07   0.29     0.10  -0.10   0.59     0.00   0.02
0.03
  28   1    -0.01  -0.02   0.00    -0.09  -0.40  -0.04     0.00   0.02
0.00
  29   1    -0.16  -0.39   0.26     0.06   0.12  -0.08    -0.14  -0.34
0.12
                     67                    68                    69
                     ?A                    ?A                    ?A
 Frequencies --  1637.4047             1662.8118             3215.1174
 Red. masses --     1.2178                9.6469                1.0589
 Frc consts  --     1.9238               15.7154                6.4489
 IR Inten    --    18.6216              395.9156               32.3348
```

Raman Activ --		7.6466			57.2665			140.6170		
Depolar --		0.7490			0.2112			0.1931		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.01	-0.01	-0.01	0.00	0.00	0.00	-0.01	0.00
2	6	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
3	6	0.01	0.01	-0.01	0.00	0.00	-0.02	0.00	0.00	0.00
4	6	0.02	0.01	0.01	0.02	0.01	-0.01	0.00	0.00	0.00
5	6	-0.05	-0.07	0.00	-0.04	-0.02	0.05	0.00	0.00	0.00
6	6	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00	0.00
7	6	0.00	-0.01	0.00	-0.01	0.01	-0.01	0.00	0.00	0.00
8	6	0.01	0.01	0.00	-0.03	-0.03	0.01	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.07	0.05	-0.06	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.02	0.01	0.01	0.00	0.00	0.00
11	6	-0.08	-0.02	-0.04	0.00	-0.01	0.00	-0.06	-0.01	-0.02
12	6	0.00	0.00	-0.01	-0.10	-0.24	0.69	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.10	0.15	-0.37	0.00	0.00	0.00
14	8	0.00	0.00	0.00	-0.01	-0.01	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	-0.06	0.01	-0.13	0.00	0.00	0.00
16	8	0.02	0.03	0.00	0.02	0.01	-0.01	0.00	0.00	0.00
17	1	-0.03	0.00	0.01	0.01	0.01	-0.01	-0.06	0.10	-0.02
18	1	-0.03	-0.01	-0.02	-0.02	0.00	-0.02	0.00	0.00	0.00
19	1	-0.06	-0.07	0.06	0.02	-0.02	-0.01	0.00	0.00	0.00
20	1	-0.08	-0.06	-0.03	-0.11	-0.02	-0.03	0.00	0.00	0.00
21	1	-0.02	-0.01	-0.01	0.00	0.00	0.00	-0.01	-0.01	0.01
22	1	-0.02	-0.01	0.00	0.02	0.00	0.00	-0.01	-0.05	-0.01
23	1	-0.03	-0.04	0.00	0.01	0.02	0.01	0.00	0.00	-0.01
24	1	-0.01	-0.02	0.00	0.02	-0.02	0.00	0.00	0.00	0.00
25	1	0.66	0.14	-0.13	0.03	0.00	0.00	0.07	-0.01	0.61

```
  26   1     0.28   0.04   0.62     0.01   0.04   0.03     0.67   0.13  -
0.37
  27   1     0.00   0.00   0.00     0.14   0.19  -0.39     0.00   0.00
0.00
  28   1     0.00  -0.01   0.00     0.03   0.14   0.05     0.00   0.00
0.00
  29   1     0.03   0.08  -0.03    -0.03  -0.04   0.04     0.00   0.00
0.00
                     70                    71                    72
                     ?A                    ?A                    ?A
 Frequencies --  3262.3094             3275.7462             3298.9675
 Red. masses --     1.1063                1.0881                1.0892
 Frc consts  --     6.9368                6.8789                6.9840
 IR Inten    --    18.3315               24.0634               11.4791
 Raman Activ --    89.6400              106.7152               66.3128
 Depolar     --     0.7497                0.3485                0.7409
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.04  -0.07   0.01    -0.01   0.01
0.00
   2   6     0.00   0.00   0.00    -0.01   0.01   0.01    -0.03   0.02
0.04
   3   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.01  -
0.01
   4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.03   0.04  -
0.04
   7   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.01
0.00
   8   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.01
  11   6    -0.04  -0.01   0.09     0.01   0.00   0.01     0.00   0.00
0.00
  12   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  17   1     0.02  -0.04   0.01    -0.46   0.83  -0.13     0.08  -0.15
0.02
  18   1    -0.01   0.00   0.01     0.14  -0.08  -0.15     0.36  -0.21  -
0.40
```

```
  19   1     0.00   0.00   0.00     0.00   0.01   0.01     0.04   0.07
0.12
  20   1     0.00   0.00   0.00     0.00  -0.03   0.06     0.00   0.01  -
0.01
  21   1     0.00   0.00   0.00    -0.01  -0.02   0.02    -0.37  -0.45
0.49
  22   1     0.00   0.01   0.00     0.01   0.05   0.01     0.02   0.16
0.03
  23   1     0.00   0.00   0.01     0.00   0.00   0.00     0.00   0.00  -
0.01
  24   1     0.00   0.00   0.00     0.00   0.00   0.00    -0.04   0.03  -
0.07
  25   1    -0.12   0.00  -0.77    -0.01   0.00  -0.10     0.00   0.00
0.02
  26   1     0.55   0.11  -0.28    -0.05  -0.01   0.03     0.01   0.00  -
0.01
  27   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  29   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     73                     74                     75
                     ?A                     ?A                     ?A
 Frequencies --  3310.0098              3322.0934              3325.4866
 Red. masses --     1.0891                 1.0891                 1.0902
 Frc consts  --     7.0302                 7.0816                 7.1036
 IR Inten    --    23.8084                15.4895                12.3803
 Raman Activ --   116.6861                69.5632               205.1777
 Depolar     --     0.4906                 0.3943                 0.1101
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01  -0.01   0.00     0.00   0.00   0.00     0.00   0.01
0.00
   2   6     0.04  -0.02  -0.04     0.02  -0.01  -0.02    -0.01   0.01
0.02
   3   6     0.01   0.02   0.03    -0.02  -0.03  -0.06     0.01   0.01
0.02
   4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.02   0.03  -0.03     0.00   0.00   0.00    -0.01  -0.02
0.02
   7   6     0.00  -0.03  -0.01     0.00  -0.03  -0.01    -0.01  -0.07  -
0.01
   8   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.01
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00     0.00   0.00   0.01     0.00   0.00  -
0.01
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	1	-0.06	0.11	-0.02	-0.02	0.03	-0.01	0.04	-0.07	0.01
18	1	-0.41	0.24	0.46	-0.19	0.11	0.21	0.17	-0.10	-0.19
19	1	-0.12	-0.18	-0.32	0.27	0.40	0.70	-0.09	-0.13	-0.22
20	1	0.00	-0.01	0.02	0.00	-0.02	0.03	0.00	0.01	-0.02
21	1	-0.25	-0.32	0.34	0.01	0.01	-0.02	0.16	0.20	-0.22
22	1	0.04	0.32	0.06	0.05	0.38	0.08	0.10	0.80	0.17
23	1	0.01	-0.01	-0.03	0.01	-0.02	-0.05	0.03	-0.05	-0.14
24	1	-0.01	0.01	-0.03	-0.06	0.04	-0.10	0.05	-0.04	0.10
25	1	0.00	0.00	0.00	0.00	0.00	0.02	0.01	0.00	0.05
26	1	-0.01	0.00	0.00	0.01	0.00	0.00	0.04	0.01	-0.02
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	1	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00

	76			77			78	
	?A			?A			?A	
Frequencies --	3348.7809			3359.3647			3362.8888	
Red. masses --	1.0888			1.0881			1.0910	
Frc consts --	7.1939			7.2353			7.2698	
IR Inten --	2.0389			1.3299			1.9453	
Raman Activ --	33.3186			37.5265			219.9819	
Depolar --	0.7050			0.3263			0.0887	
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	-0.01
4 6	0.01	0.03	-0.06	0.00	0.02	-0.04	0.00	-0.01	0.02

```
    5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
    6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.01  -
0.01
    7   6     0.00   0.01   0.00     0.00  -0.01   0.00     0.00   0.01
0.00
    8   6    -0.01   0.01   0.05     0.01  -0.02  -0.05    -0.01   0.01
0.04
    9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   10   6     0.00   0.00   0.00    -0.02   0.02  -0.04    -0.03   0.03  -
0.06
   11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   12   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   13   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   14   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   16   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   17   1     0.03  -0.04   0.01     0.02  -0.03   0.00    -0.02   0.03
0.00
   18   1     0.01   0.00  -0.01     0.00   0.00   0.00    -0.03   0.02
0.04
   19   1    -0.01  -0.01  -0.02     0.02   0.03   0.05     0.04   0.06
0.10
   20   1    -0.08  -0.33   0.70    -0.05  -0.23   0.48     0.03   0.13  -
0.28
   21   1     0.00  -0.01   0.01    -0.02  -0.02   0.03    -0.06  -0.07
0.08
   22   1    -0.01  -0.10  -0.02     0.01   0.08   0.02    -0.01  -0.09  -
0.02
   23   1     0.14  -0.18  -0.57    -0.14   0.19   0.59     0.10  -0.13  -
0.40
   24   1    -0.01   0.01  -0.03     0.25  -0.20   0.43     0.38  -0.30
0.66
   25   1     0.00   0.00   0.00     0.00   0.00   0.02     0.00   0.00  -
0.01
   26   1     0.00   0.00   0.00     0.01   0.00   0.00    -0.01   0.00
0.00
   27   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   29   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                      79                     80                     81
                      ?A                     ?A                     ?A
 Frequencies --   3610.3805              3769.0879              3856.2784
 Red. masses --      1.0732                 1.0668                 1.0673
```

Frc consts	--	8.2420			8.9290			9.3515		
IR Inten	--	5.9526			286.3085			94.9552		
Raman Activ	--	216.4919			92.7319			102.1771		
Depolar	--	0.3230			0.3286			0.2487		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	7	-0.06	-0.03	0.01	0.00	0.00	0.00	0.00	0.00	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	-0.06	0.02	-0.02
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.04	0.02	0.05	0.00	0.00	0.00
17	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
18	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
22	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
23	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  25   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  27   1     0.88   0.46  -0.15     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.01   0.00   0.00     0.89  -0.30
0.33
  29   1     0.00   0.00   0.00    -0.62  -0.29  -0.73     0.00   0.00
0.01

 -------------------
 - Thermochemistry -
 -------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Atom  1 has atomic number  6 and mass  12.00000
 Atom  2 has atomic number  6 and mass  12.00000
 Atom  3 has atomic number  6 and mass  12.00000
 Atom  4 has atomic number  6 and mass  12.00000
 Atom  5 has atomic number  6 and mass  12.00000
 Atom  6 has atomic number  6 and mass  12.00000
 Atom  7 has atomic number  6 and mass  12.00000
 Atom  8 has atomic number  6 and mass  12.00000
 Atom  9 has atomic number  6 and mass  12.00000
 Atom 10 has atomic number  6 and mass  12.00000
 Atom 11 has atomic number  6 and mass  12.00000
 Atom 12 has atomic number  6 and mass  12.00000
 Atom 13 has atomic number  7 and mass  14.00307
 Atom 14 has atomic number  8 and mass  15.99491
 Atom 15 has atomic number  8 and mass  15.99491
 Atom 16 has atomic number  8 and mass  15.99491
 Atom 17 has atomic number  1 and mass   1.00783
 Atom 18 has atomic number  1 and mass   1.00783
 Atom 19 has atomic number  1 and mass   1.00783
 Atom 20 has atomic number  1 and mass   1.00783
 Atom 21 has atomic number  1 and mass   1.00783
 Atom 22 has atomic number  1 and mass   1.00783
 Atom 23 has atomic number  1 and mass   1.00783
 Atom 24 has atomic number  1 and mass   1.00783
 Atom 25 has atomic number  1 and mass   1.00783
 Atom 26 has atomic number  1 and mass   1.00783
 Atom 27 has atomic number  1 and mass   1.00783
 Atom 28 has atomic number  1 and mass   1.00783
 Atom 29 has atomic number  1 and mass   1.00783
 Molecular mass:   219.08954 amu.
 Principal axes and moments of inertia in atomic units:
                           1         2         3
     EIGENVALUES --  1918.98957 2721.97674 3344.64803
           X            0.99992   0.01235   0.00230
           Y           -0.01236   0.99992   0.00394
           Z           -0.00226  -0.00397   0.99999
 THIS MOLECULE IS AN ASYMMETRIC TOP.
 ROTATIONAL SYMMETRY NUMBER  1.
 WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
```

MAY CAUSE SIGNIFICANT ERROR

ROTATIONAL TEMPERATURES (KELVIN) 0.04513 0.03182 0.02590

ROTATIONAL CONSTANTS (GHZ) 0.94046 0.66303 0.53959

1 IMAGINARY FREQUENCIES IGNORED.

Zero-point vibrational energy 662177.9 (Joules/Mol)

158.26433 (Kcal/Mol)

WARNING-- EXPLICIT CONSIDERATION OF 14 DEGREES OF FREEDOM AS VIBRATIONS MAY CAUSE SIGNIFICANT ERROR

VIBRATIONAL TEMPERATURES:	180.11	225.44	261.56	378.55	436.51
(KELVIN)	472.14	498.90	536.00	568.17	650.00
	683.26	762.12	777.45	860.09	912.52
	966.30	997.06	1019.07	1140.94	1170.86
	1175.39	1193.01	1216.63	1256.04	1274.57
	1302.08	1314.35	1373.71	1392.34	1424.79
	1438.81	1454.89	1459.25	1486.95	1500.03
	1506.37	1536.21	1583.28	1637.93	1676.29
	1715.83	1745.48	1753.84	1767.76	1803.97
	1823.06	1837.57	1874.12	1894.73	1916.80
	1935.22	1948.66	1967.28	1984.39	2003.02
	2015.84	2026.49	2047.70	2063.75	2067.15
	2093.52	2114.54	2159.59	2164.34	2348.39
	2355.85	2392.40	4625.81	4693.71	4713.04
	4746.45	4762.34	4779.72	4784.61	4818.12
	4833.35	4838.42	5194.50	5422.85	5548.29

Zero-point correction= 0.252210

(Hartree/Particle)

Thermal correction to Energy= 0.262041

Thermal correction to Enthalpy= 0.262985

Thermal correction to Gibbs Free Energy= 0.217185

Sum of electronic and zero-point Energies= -736.635744

Sum of electronic and thermal Energies= -736.625913

Sum of electronic and thermal Enthalpies= -736.624969

Sum of electronic and thermal Free Energies= -736.670769

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	164.433	43.588	96.394
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	42.056
ROTATIONAL	0.889	2.981	31.236
VIBRATIONAL	162.656	37.627	23.102
VIBRATION 1	0.610	1.928	3.019
VIBRATION 2	0.620	1.895	2.589
VIBRATION 3	0.630	1.865	2.310
VIBRATION 4	0.670	1.740	1.641
VIBRATION 5	0.695	1.667	1.398
VIBRATION 6	0.711	1.619	1.269
VIBRATION 7	0.725	1.582	1.181
VIBRATION 8	0.744	1.529	1.069
VIBRATION 9	0.762	1.481	0.982
VIBRATION 10	0.810	1.357	0.790
VIBRATION 11	0.832	1.306	0.724
VIBRATION 12	0.885	1.184	0.588

VIBRATION 13	0.895	1.161	0.565
VIBRATION 14	0.956	1.036	0.453

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.126608D-99	-99.897539	-230.022584
TOTAL V=0	0.128926D+17	16.110340	37.095429
VIB (BOT)	0.663842-114	-114.177935	-262.904411
VIB (BOT) 1	0.163045D+01	0.212307	0.488855
VIB (BOT) 2	0.129151D+01	0.111097	0.255811
VIB (BOT) 3	0.110413D+01	0.043021	0.099059
VIB (BOT) 4	0.737101D+00	-0.132473	-0.305030
VIB (BOT) 5	0.625632D+00	-0.203681	-0.468994
VIB (BOT) 6	0.570030D+00	-0.244102	-0.562067
VIB (BOT) 7	0.533190D+00	-0.273118	-0.628877
VIB (BOT) 8	0.487852D+00	-0.311712	-0.717742
VIB (BOT) 9	0.453029D+00	-0.343874	-0.791799
VIB (BOT) 10	0.379043D+00	-0.421312	-0.970106
VIB (BOT) 11	0.353722D+00	-0.451338	-1.039243
VIB (BOT) 12	0.302009D+00	-0.519980	-1.197297
VIB (BOT) 13	0.293107D+00	-0.532973	-1.227217
VIB (BOT) 14	0.250353D+00	-0.601447	-1.384884
VIB (V=0)	0.675996D+02	1.829944	4.213602
VIB (V=0) 1	0.220539D+01	0.343486	0.790905
VIB (V=0) 2	0.188492D+01	0.275292	0.633884
VIB (V=0) 3	0.171207D+01	0.233521	0.537701
VIB (V=0) 4	0.139068D+01	0.143228	0.329796
VIB (V=0) 5	0.130088D+01	0.114239	0.263044
VIB (V=0) 6	0.125824D+01	0.099765	0.229717
VIB (V=0) 7	0.123095D+01	0.090241	0.207788
VIB (V=0) 8	0.119857D+01	0.078663	0.181129
VIB (V=0) 9	0.117471D+01	0.069931	0.161022
VIB (V=0) 10	0.112743D+01	0.052091	0.119944
VIB (V=0) 11	0.111247D+01	0.046288	0.106583
VIB (V=0) 12	0.108413D+01	0.035082	0.080779
VIB (V=0) 13	0.107958D+01	0.033254	0.076571
VIB (V=0) 14	0.105917D+01	0.024968	0.057490
ELECTRONIC	0.100000D+01	0.000000	0.000000
TRANSLATIONAL	0.127466D+09	8.105393	18.663357
ROTATIONAL	0.149625D+07	6.175003	14.218470

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000004145	0.000004831	-0.000008854
2	6	-0.000003043	0.000010864	-0.000004537
3	6	-0.000014549	-0.000003545	0.000002264
4	6	0.000003883	0.000018782	-0.000004532
5	6	0.000011588	-0.000007170	0.000008177
6	6	-0.000008218	-0.000007194	0.000005016
7	6	0.000001117	-0.000003525	-0.000004221
8	6	-0.000011420	-0.000020943	0.000011897
9	6	0.000008764	-0.000005986	-0.000000675
10	6	0.000007794	0.000004930	-0.000010795
11	6	-0.000004911	0.000004665	0.000005353

12	6	-0.000029249	-0.000011501	-0.000069185
13	7	0.000009835	-0.000003679	0.000020331
14	8	-0.000000174	0.000000433	0.000015304
15	8	0.000027309	0.000002717	0.000045842
16	8	-0.000007118	0.000013986	-0.000003432
17	1	-0.000002087	0.000002103	0.000000889
18	1	-0.000000681	0.000000769	-0.000001070
19	1	0.000001927	-0.000002204	-0.000004060
20	1	-0.000000085	-0.000002950	-0.000000091
21	1	-0.000000119	-0.000000869	-0.000001210
22	1	-0.000001779	0.000000119	0.000002596
23	1	0.000004612	0.000007130	0.000003050
24	1	0.000000883	-0.000001462	-0.000001671
25	1	0.000000884	0.000001043	-0.000000046
26	1	-0.000000505	-0.000001383	-0.000000283
27	1	0.000000231	0.000005029	-0.000004626
28	1	0.000000880	-0.000002657	-0.000003803
29	1	0.000008376	-0.000002335	0.000002371

Cartesian Forces: Max 0.000069185 RMS 0.000011918

Internal Coordinate Forces (Hartree/Bohr or radian)

Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	C		-0.000004(1)		0.000005(30)		-0.000009(59)	
2	C		-0.000003(2)		0.000011(31)		-0.000005(60)	
3	C		-0.000015(3)		-0.000004(32)		0.000002(61)	
4	C		0.000004(4)		0.000019(33)		-0.000005(62)	
5	C		0.000012(5)		-0.000007(34)		0.000008(63)	
6	C		-0.000008(6)		-0.000007(35)		0.000005(64)	
7	C		0.000001(7)		-0.000004(36)		-0.000004(65)	
8	C		-0.000011(8)		-0.000021(37)		0.000012(66)	
9	C		0.000009(9)		-0.000006(38)		-0.000001(67)	
10	C		0.000008(10)		0.000005(39)		-0.000011(68)	
11	C		-0.000005(11)		0.000005(40)		0.000005(69)	
12	C		-0.000029(12)		-0.000012(41)		-0.000069(70)	
13	N		0.000010(13)		-0.000004(42)		0.000020(71)	
14	O		0.000000(14)		0.000000(43)		0.000015(72)	
15	O		0.000027(15)		0.000003(44)		0.000046(73)	
16	O		-0.000007(16)		0.000014(45)		-0.000003(74)	
17	H		-0.000002(17)		0.000002(46)		0.000001(75)	
18	H		-0.000001(18)		0.000001(47)		-0.000001(76)	
19	H		0.000002(19)		-0.000002(48)		-0.000004(77)	
20	H		0.000000(20)		-0.000003(49)		0.000000(78)	
21	H		0.000000(21)		-0.000001(50)		-0.000001(79)	
22	H		-0.000002(22)		0.000000(51)		0.000003(80)	
23	H		0.000005(23)		0.000007(52)		0.000003(81)	
24	H		0.000001(24)		-0.000001(53)		-0.000002(82)	
25	H		0.000001(25)		0.000001(54)		0.000000(83)	
26	H		-0.000001(26)		-0.000001(55)		0.000000(84)	
27	H		0.000000(27)		0.000005(56)		-0.000005(85)	
28	H		0.000001(28)		-0.000003(57)		-0.000004(86)	
29	H		0.000008(29)		-0.000002(58)		0.000002(87)	

```
Internal  Forces:  Max     0.000069185 RMS     0.000011918

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   1 out of a maximum of  97
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
    Eigenvalues ---   -0.00501   0.00374   0.00455   0.00569   0.00624
    Eigenvalues ---    0.01155   0.01290   0.01805   0.02374   0.02563
    Eigenvalues ---    0.03422   0.04217   0.04246   0.04557   0.04651
    Eigenvalues ---    0.04733   0.04897   0.04934   0.05075   0.05118
    Eigenvalues ---    0.05180   0.05341   0.05453   0.05581   0.05794
    Eigenvalues ---    0.05897   0.06050   0.06895   0.07619   0.07848
    Eigenvalues ---    0.08741   0.10165   0.10501   0.11114   0.13765
    Eigenvalues ---    0.14815   0.15963   0.17255   0.18801   0.19024
    Eigenvalues ---    0.19899   0.21038   0.24800   0.26558   0.28713
    Eigenvalues ---    0.31252   0.33356   0.34621   0.37097   0.38960
    Eigenvalues ---    0.40439   0.43639   0.43691   0.49071   0.50117
    Eigenvalues ---    0.50563   0.53511   0.55745   0.57627   0.58155
    Eigenvalues ---    0.63274   0.66498   0.69302   0.70986   0.75589
    Eigenvalues ---    0.84000   0.87881   0.89791   0.95095   0.96420
    Eigenvalues ---    0.97558   0.99390   1.02106   1.02951   1.03634
    Eigenvalues ---    1.06189   1.09183   1.12935   1.13884   1.36443
    Eigenvalues ---    1.42184
Eigenvalue   1 out of range, new value =    0.005006 Eigenvector:
                          1
          X1          -0.02160
          Y1           0.01193
          Z1           0.02913
          X2          -0.04329
          Y2          -0.01552
          Z2           0.03079
          X3          -0.06135
          Y3           0.01788
          Z3           0.04152
          X4          -0.00649
          Y4           0.04811
          Z4           0.03541
          X5          -0.02483
          Y5           0.01124
          Z5           0.07214
          X6          -0.01592
          Y6          -0.02678
          Z6          -0.00437
          X7           0.00170
          Y7           0.00044
          Z7          -0.01811
          X8           0.00328
          Y8           0.02453
          Z8          -0.00440
          X9           0.01023
          Y9           0.01790
          Z9          -0.00925
```

X10	-0.01240
Y10	-0.00746
Z10	0.00161
X11	-0.00311
Y11	0.00601
Z11	-0.00498
X12	0.00781
Y12	0.07164
Z12	-0.06818
X13	0.05502
Y13	-0.41062
Z13	-0.06957
X14	-0.00351
Y14	0.01339
Z14	-0.02767
X15	-0.05266
Y15	0.64843
Z15	-0.10935
X16	0.12446
Y16	-0.19119
Z16	0.11044
X17	-0.02941
Y17	0.01687
Z17	0.04430
X18	-0.07199
Y18	-0.03764
Z18	0.02962
X19	-0.06212
Y19	-0.00694
Z19	0.05937
X20	0.00888
Y20	0.06840
Z20	0.04224
X21	-0.01237
Y21	-0.05635
Z21	-0.01227
X22	0.01292
Y22	-0.00433
Z22	-0.04140
X23	0.02546
Y23	0.04858
Z23	-0.01583
X24	-0.01172
Y24	-0.00840
Z24	0.00066
X25	0.00778
Y25	0.02360
Z25	-0.00927
X26	-0.00809
Y26	-0.01116
Z26	-0.00863
X27	0.03796
Y27	-0.31085
Z27	-0.08284

X28	0.02138
Y28	-0.05744
Z28	-0.12944
X29	0.14912
Y29	-0.30083
Z29	0.13456

Angle between quadratic step and forces= 75.04 degrees.
Linear search not attempted -- first point.
TrRot= -0.000008 -0.000006 0.000019 -0.000003 -0.000003 -0.000003

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
X1	-3.09793	0.00000	0.00000	-0.00009	-0.00008	-3.09801
Y1	2.59142	0.00000	0.00000	0.00003	0.00004	2.59146
Z1	-1.57109	-0.00001	0.00000	-0.00006	-0.00005	-1.57113
X2	-2.86296	0.00000	0.00000	-0.00009	-0.00009	-2.86305
Y2	2.48134	0.00001	0.00000	0.00006	0.00007	2.48141
Z2	1.37356	0.00000	0.00000	-0.00005	-0.00004	1.37353
X3	0.06638	-0.00001	0.00000	-0.00009	-0.00010	0.06629
Y3	2.28581	0.00000	0.00000	0.00010	0.00009	2.28590
Z3	2.04135	0.00000	0.00000	-0.00003	-0.00001	2.04133
X4	-0.49661	0.00000	0.00000	-0.00003	-0.00003	-0.49664
Y4	1.45047	0.00002	0.00000	0.00011	0.00010	1.45057
Z4	-2.39812	0.00000	0.00000	-0.00001	0.00001	-2.39811
X5	1.20371	0.00001	0.00000	-0.00004	-0.00003	1.20368
Y5	2.59046	-0.00001	0.00000	0.00011	0.00010	2.59056
Z5	-0.49407	0.00001	0.00000	0.00000	0.00003	-0.49405
X6	-3.20309	-0.00001	0.00000	-0.00001	-0.00002	-3.20311
Y6	-0.39848	-0.00001	0.00000	0.00001	0.00002	-0.39846
Z6	1.98321	0.00001	0.00000	-0.00001	0.00000	1.98321
X7	-3.55849	0.00000	0.00000	-0.00001	-0.00002	-3.55852
Y7	-1.59136	0.00000	0.00000	-0.00001	0.00000	-1.59136
Z7	-0.67678	0.00000	0.00000	-0.00001	0.00000	-0.67678
X8	-0.82900	-0.00001	0.00000	-0.00002	-0.00003	-0.82903
Y8	-1.47936	-0.00002	0.00000	-0.00003	-0.00003	-1.47939
Z8	-1.72527	0.00001	0.00000	0.00003	0.00005	-1.72522
X9	0.82005	0.00001	0.00000	0.00003	0.00001	0.82006
Y9	-2.18396	-0.00001	0.00000	0.00000	-0.00001	-2.18397
Z9	0.53188	0.00000	0.00000	0.00001	0.00003	0.53191
X10	-0.33614	0.00001	0.00000	0.00005	0.00003	-0.33611
Y10	-0.61082	0.00000	0.00000	0.00011	0.00010	-0.61071
Z10	2.64377	-0.00001	0.00000	-0.00006	-0.00005	2.64373
X11	-4.98191	0.00000	0.00000	-0.00005	-0.00005	-4.98196
Y11	0.46132	0.00000	0.00000	-0.00002	0.00000	0.46132
Z11	-2.15452	0.00001	0.00000	0.00000	0.00000	-2.15451
X12	3.65122	-0.00003	0.00000	0.00004	0.00003	3.65125
Y12	-1.65811	-0.00001	0.00000	-0.00017	-0.00020	-1.65831
Z12	0.21897	-0.00007	0.00000	-0.00006	-0.00003	0.21894
X13	4.39739	0.00001	0.00000	0.00013	0.00012	4.39751
Y13	-1.52043	0.00000	0.00000	0.00011	0.00008	-1.52036
Z13	-2.10280	0.00002	0.00000	0.00002	0.00005	-2.10275
X14	0.31442	0.00000	0.00000	-0.00005	-0.00008	0.31434
Y14	-4.82403	0.00000	0.00000	0.00008	0.00007	-4.82396
Z14	1.06465	0.00002	0.00000	0.00038	0.00040	1.06505
X15	4.88041	0.00003	0.00000	0.00012	0.00010	4.88051

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  Y15       -1.31215   0.00000   0.00000  -0.00060  -0.00063  -1.31278
  Z15        2.29921   0.00005   0.00000   0.00009   0.00012   2.29932
  X16        3.09662  -0.00001   0.00000  -0.00004  -0.00003   3.09659
  Y16        4.02312   0.00001   0.00000   0.00015   0.00013   4.02325
  Z16       -1.05435   0.00000   0.00000   0.00001   0.00004  -1.05432
  X17       -3.49768   0.00000   0.00000  -0.00017  -0.00015  -3.49783
  Y17        4.43779   0.00000   0.00000   0.00002   0.00003   4.43782
  Z17       -2.34601   0.00000   0.00000  -0.00005  -0.00004  -2.34604
  X18       -3.94786   0.00000   0.00000  -0.00013  -0.00012  -3.94798
  Y18        3.86080   0.00000   0.00000   0.00005   0.00006   3.86086
  Z18        2.40700   0.00000   0.00000  -0.00007  -0.00006   2.40694
  X19        0.87135   0.00000   0.00000  -0.00010  -0.00010   0.87125
  Y19        3.43190   0.00000   0.00000   0.00010   0.00009   3.43199
  Z19        3.51764   0.00000   0.00000  -0.00004  -0.00002   3.51761
  X20        0.09056   0.00000   0.00000  -0.00001   0.00000   0.09056
  Y20        1.76812   0.00000   0.00000   0.00001   0.00000   1.76812
  Z20       -4.31681   0.00000   0.00000  -0.00001   0.00001  -4.31681
  X21       -4.57931   0.00000   0.00000   0.00003   0.00001  -4.57930
  Y21       -0.93081   0.00000   0.00000  -0.00005  -0.00003  -0.93084
  Z21        3.38679   0.00000   0.00000   0.00000   0.00001   3.38680
  X22       -4.35018   0.00000   0.00000  -0.00004  -0.00006  -4.35025
  Y22       -3.46697   0.00000   0.00000   0.00000   0.00001  -3.46695
  Z22       -0.67882   0.00000   0.00000   0.00005   0.00006  -0.67876
  X23       -0.43553   0.00000   0.00000   0.00007   0.00006  -0.43547
  Y23       -2.62824   0.00001   0.00000   0.00011   0.00011  -2.62813
  Z23       -3.35434   0.00000   0.00000  -0.00004  -0.00002  -3.35436
  X24        0.25442   0.00000   0.00000   0.00009   0.00006   0.25448
  Y24       -1.15552   0.00000   0.00000   0.00009   0.00008  -1.15545
  Z24        4.50774   0.00000   0.00000  -0.00009  -0.00007   4.50767
  X25       -5.13055   0.00000   0.00000  -0.00005  -0.00005  -5.13060
  Y25        0.05533   0.00000   0.00000  -0.00002   0.00000   0.05533
  Z25       -4.15640   0.00000   0.00000   0.00000   0.00000  -4.15640
  X26       -6.84705   0.00000   0.00000  -0.00006  -0.00005  -6.84711
  Y26        0.85392   0.00000   0.00000  -0.00008  -0.00005   0.85388
  Z26       -1.40121   0.00000   0.00000   0.00001   0.00001  -1.40120
  X27        6.28272   0.00000   0.00000   0.00012   0.00011   6.28284
  Y27       -1.22461   0.00001   0.00000   0.00012   0.00008  -1.22454
  Z27       -2.25782   0.00000   0.00000   0.00004   0.00008  -2.25774
  X28        1.68894   0.00000   0.00000   0.00041   0.00037   1.68931
  Y28       -5.59968   0.00000   0.00000  -0.00014  -0.00016  -5.59983
  Z28        1.99055   0.00000   0.00000  -0.00050  -0.00047   1.99008
  X29        4.23551   0.00001   0.00000   0.00018   0.00019   4.23571
  Y29        4.51301   0.00000   0.00000  -0.00012  -0.00015   4.51285
  Z29        0.30786   0.00000   0.00000  -0.00006  -0.00003   0.30783
         Item               Value     Threshold  Converged?
Maximum Force            0.000069     0.000450     YES
RMS     Force            0.000012     0.000300     YES
Maximum Displacement     0.000631     0.001800     YES
RMS     Displacement     0.000124     0.001200     YES
Predicted change in Energy=-1.616251D-08
Optimization completed.
   -- Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
```

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.00004478,0.00008614,0.00028839,-0.00016864,0.00009503,0.00035402,-0.0
0002086,-0.00004532,-0.00003823,-0.00000906,0.00006085,0.00004228,0.00
001110,0.00019695,-0.00040605,0.00007243,0.00004484,0.00003564,0.00007
501,0.21032492,0.08965371,0.29138816\\0.00000415,-0.00000483,0.0000088
5,0.00000304,-0.00001086,0.00000454,0.00001455,0.00000355,-0.00000226,
-0.00000388,-0.00001878,0.00000453,-0.00001159,0.00000717,-0.00000818,
0.00000822,0.00000719,-0.00000502,-0.00000112,0.00000352,0.00000422,0.
00001142,0.00002094,-0.00001190,-0.00000876,0.00000599,0.00000067,-0.0
0000779,-0.00000493,0.00001080,0.00000491,-0.00000466,-0.00000535,0.00
002925,0.00001150,0.00006919,-0.00000984,0.00000368,-0.00002033,0.0000
0017,-0.00000043,-0.00001530,-0.00002731,-0.00000272,-0.00004584,0.000
00712,-0.00001399,0.00000343,0.00000209,-0.00000210,-0.00000089,0.0000
0068,-0.00000077,0.00000107,-0.00000193,0.00000220,0.00000406,0.000000
09,0.00000295,0.00000009,0.00000012,0.00000087,0.00000121,0.00000178,-
0.00000012,-0.00000260,-0.00000461,-0.00000713,-0.00000305,-0.00000088
,0.00000146,0.00000167,-0.00000088,-0.00000104,0.00000005,0.00000050,0
.00000138,0.00000028,-0.00000023,-0.00000503,0.00000463,-0.00000088,0.
00000266,0.00000380,-0.00000838,0.00000233,-0.00000237\\\@

IT IS NOT EASY TO DESCRIBE
THE SEA WITH THE MOUTH

-- KOKYU

Job cpu time: 0 days 3 hours 28 minutes 48.6 seconds.
File lengths (MBytes): RWF= 322 Int=   0 D2E=   0 Chk=   7 Scr=
1
Normal termination of Gaussian 98.

```
%nproc=2
%chk=mech1s13ts2
%nosave
# opt=(gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity optcyc=100

TS2

0  1
 C
 C                  1             B1
 C                  2             B2    1             A1
 C                  1             B3    2             A2    3
D1
 C                  3             B4    2             A3    1
D2
 C                  2             B5    1             A4    4
D3
 C                  6             B6    2             A5    1
D4
 C                  7             B7    6             A6    2
D5
 C                  8             B8    7             A7    6
D6
 C                  9             B9    8             A8    7
D7
 C                  1            B10    2             A9    3
D8
 C                  9            B11    8            A10    7
D9
 N                 12            B12    9            A11    8
D10
 O                  9            B13    8            A12    7
D11
 O                 12            B14    9            A13    8
D12
 O                  5            B15    3            A14    2
D13
 H                  1            B16    2            A15    3
D14
 H                  2            B17    1            A16   11
D15
 H                  3            B18    2            A17    1
D16
 H                  4            B19    1            A18    2
D17
 H                  6            B20    2            A19    1
D18
 H                  7            B21    6            A20    2
D19
 H                  8            B22    7            A21    6
D20
 H                 10            B23    9            A22    8
D21
```

```
 H                11            B24    1             A23    2
D22
 H                11            B25    1             A24    2
D23
 H                13            B26   12             A25    9
D24
 H                14            B27    9             A26    8
D25
 H                15            B28   12             A27    9
D26
```

B1	1.540191
B2	1.549014
B3	1.493470
B4	1.489267
B5	1.507570
B6	1.556647
B7	1.556293
B8	1.461700
B9	1.566113
B10	1.551900
B11	1.540000
B12	1.293600
B13	1.430000
B14	1.258400
B15	1.258400
B16	1.070000
B17	1.070000
B18	1.070000
B19	1.070000
B20	1.070000
B21	1.070000
B22	1.070000
B23	1.070000
B24	1.070000
B25	1.070000
B26	1.000000
B27	0.960000
B28	3.698878
A1	109.288543
A2	102.169554
A3	100.119681
A4	109.231837
A5	96.449984
A6	103.607735
A7	102.114438
A8	100.057221
A9	99.892115
A10	114.219569
A11	120.000000
A12	110.164002
A13	120.000000
A14	128.325455
A15	114.846949

```
  A16          102.301841
  A17          115.817993
  A18          125.745293
  A19          114.637207
  A20          111.448807
  A21          110.173047
  A22          106.490129
  A23          114.608714
  A24          115.265473
  A25          120.000000
  A26          109.471221
  A27           86.374848
  D1            20.142728
  D2            12.568165
  D3           -75.017812
  D4            -5.394436
  D5            72.384120
  D6            45.992900
  D7           -49.017899
  D8           135.147829
  D9          -170.992787
  D10          -28.370273
  D11           67.407646
  D12          151.629727
  D13          140.621626
  D14          -98.186356
  D15          -89.715448
  D16          145.455344
  D17         -164.505643
  D18         -140.954791
  D19         -164.430862
  D20          172.085241
  D21          168.143457
  D22         -171.247093
  D23           64.642383
  D24         -179.999999
  D25         -174.788584
  D26          -88.947553

1  2 1.0  4 1.0  11 1.0  17 1.0
2  3 1.0  6 1.0  18 1.0
3  5 1.0  10 1.0  19 1.0
4  5 1.0  8 1.0  20 1.0
5  16 2.0
6  7 1.0  10 1.0  21 1.0
7  8 1.0  11 1.0  22 1.0
8  9 1.0  23 1.0
9  10 1.0  12 1.0  14 1.0
10  24 1.0
11  25 1.0  26 1.0
12  13 2.0  15 2.0
13  27 1.0
14  28 1.0
15
```

16 29 1.0
17
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1 2 1.0 4 1.0 11 1.0 17 1.0
2 3 1.0 6 1.0 18 1.0
3 5 1.0 10 1.0 19 1.0
4 5 1.0 8 1.0 20 1.0
5 16 2.0
6 7 1.0 10 1.0 21 1.0
7 8 1.0 11 1.0 22 1.0
8 9 1.0 23 1.0
9 10 1.0 12 1.0 14 1.0
10 24 1.0
11 25 1.0 26 1.0
12 13 2.0 15 2.0
13 27 1.0
14 28 1.0
15
16 29 1.0
17
18
19
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```
%chk=m1s13ts4Ntopts
# opt=(gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity optcyc=200

Std input@80.0004degrees-optcyc=200-ts search

0  1
 C                  0.000000    0.000000    0.000000
 C                  0.000000    0.000000    1.564291
 C                  1.519701    0.000000    2.043318
 C                  1.439501   -0.535325   -0.304070
 C                  2.218701    0.152764    0.748648
 C                 -0.119458   -1.520595    1.928140
 C                 -0.156320   -2.207374    0.534495
 C                  1.322917   -2.080807    0.094474
 C                  2.114895   -2.362330    1.367583
 C                  1.368045   -1.531494    2.401115
 C                 -0.903383   -1.193657   -0.344765
 C                  3.603579   -2.001562    1.311548
 N                  4.092771   -1.945796    0.116392
 O                  1.904146   -3.762821    1.679250
 O                  4.150644   -1.744295    2.453020
 O                  3.196848    0.958809    0.504477
 H                 -0.232138    0.948959   -0.461650
 H                 -0.656905    0.712200    2.036282
 H                  1.845653    0.655834    2.832749
 H                  1.821947   -0.382208   -1.297038
 H                 -0.888828   -1.820581    2.620583
 H                 -0.517115   -3.222467    0.537090
 H                  1.634681   -2.703268   -0.724953
 H                  1.614922   -1.768329    3.419265
 H                 -0.883230   -1.447187   -1.398275
 H                 -1.929712   -1.031726   -0.033857
 H                  5.083390   -1.733169    0.108272
 H                  2.610910   -4.113471    2.240617
 H                  3.722967    1.276996    1.260778

 1  2 1.0  4 1.0  11 1.0  17 1.0
 2  3 1.0  6 1.0  18 1.0
 3  5 1.0  10 1.0  19 1.0
 4  5 1.0  8 1.0  20 1.0
 5  16 1.5
 6  7 1.0  10 1.0  21 1.0
 7  8 1.0  11 1.0  22 1.0
 8  9 1.0  23 1.0
 9  10 1.0  12 1.0  14 1.0
 10  24 1.0
 11  25 1.0  26 1.0
 12  13 2.0  15 1.5
 13  27 1.0
 14  28 1.0
 15
 16  29 1.0
 17
 18
```

```
%nproc=2
%chk=m1s13ts4Ntopts
%nosave
# opt=(gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity optcyc=200

Std input@80.0004degrees-optcyc=200-ts search

0  1
 C
 C                  1             B1
 C                  2             B2    1             A1
 C                  1             B3    2             A2    3
D1
 C                  3             B4    2             A3    1
D2
 C                  2             B5    1             A4    4
D3
 C                  6             B6    2             A5    1
D4
 C                  7             B7    6             A6    2
D5
 C                  8             B8    7             A7    6
D6
 C                  9             B9    8             A8    7
D7
 C                  7            B10    6             A9    2
D8
 C                  9            B11    8            A10    7
D9
 N                 12            B12    9            A11    8
D10
 O                  9            B13    8            A12    7
D11
 O                 12            B14    9            A13    8
D12
 O                  5            B15    3            A14    2
D13
 H                  1            B16    2            A15    6
D14
 H                  2            B17    1            A16   11
D15
 H                  3            B18    2            A17    1
D16
 H                  4            B19    1            A18    2
D17
 H                  6            B20    2            A19    1
D18
 H                  7            B21    6            A20    2
D19
 H                  8            B22    7            A21    6
D20
 H                 10            B23    9            A22    8
D21
```

H	11	B24	7	A23	6
D22					
H	11	B25	7	A24	6
D23					
H	13	B26	12	A25	9
D24					
H	14	B27	9	A26	8
D25					
H	16	B28	5	A27	3
D26					

B1	1.565202
B2	1.588912
B3	1.569329
B4	1.473841
B5	1.566898
B6	1.555055
B7	1.548052
B8	1.522628
B9	1.522172
B10	1.535416
B11	1.531640
B12	1.291376
B13	1.451253
B14	1.291019
B15	1.287742
B16	1.080793
B17	1.077798
B18	1.077299
B19	1.075164
B20	1.077606
B21	1.077109
B22	1.075167
B23	1.074062
B24	1.083728
B25	1.084573
B26	1.012840
B27	0.968584
B28	0.973097
A1	107.130075
A2	101.275957
A3	101.175952
A4	103.345366
A5	102.905289
A6	101.285775
A7	104.019542
A8	102.115236
A9	103.565183
A10	116.092944
A11	114.378481
A12	106.377319
A13	114.627192
A14	126.698178
A15	115.230891

```
  A16          115.825439
  A17          120.705556
  A18          117.226616
  A19          118.335952
  A20          114.970487
  A21          116.524518
  A22          114.137112
  A23          113.110671
  A24          113.293311
  A25          112.735836
  A26          111.243152
  A27          118.553356
  D1            21.002598
  D2             5.639130
  D3           -73.703981
  D4             0.139633
  D5            74.593691
  D6            40.272459
  D7           -45.740920
  D8           -33.386055
  D9          -168.948518
  D10          -22.093835
  D11           66.525280
  D12          157.906445
  D13          140.199277
  D14          162.107801
  D15          -99.622395
  D16          135.729361
  D17         -163.170019
  D18         -129.063690
  D19         -162.788857
  D20          164.575265
  D21          166.539834
  D22          170.788872
  D23          -64.049288
  D24         -177.350306
  D25          156.583654
  D26            0.000012

1  2 1.0  4 1.0  11 1.0  17 1.0
2  3 1.0  6 1.0  18 1.0
3  5 1.0  10 1.0  19 1.0
4  5 1.0  8 1.0  20 1.0
5  16 1.5
6  7 1.0  10 1.0  21 1.0
7  8 1.0  11 1.0  22 1.0
8  9 1.0  23 1.0
9  10 1.0  12 1.0  14 1.0
10  24 1.0
11  25 1.0  26 1.0
12  13 2.0  15 1.5
13  27 1.0
14  28 1.0
15
```

16 29 1.0
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```
%mem=6MW
%nproc=1
%chk=532TSend.chk
# freq=raman rhf/3-21+g(d) geom=(connectivity,allcheck) guess=tcheck

With solvent (H3O+)-output file

0  1
 C                  0.000000    0.000000    0.000000
 C                  0.000000    0.000000    1.562280
 C                  1.497274    0.000000    2.025846
 C                  1.421932   -0.542203   -0.313535
 C                  2.265415    0.171196    0.731380
 C                 -0.131878   -1.521935    1.914941
 C                 -0.196111   -2.206124    0.516035
 C                  1.279463   -2.100119    0.054422
 C                  2.067428   -2.291132    1.306943
 C                  1.352967   -1.553453    2.391351
 C                 -0.929263   -1.169391   -0.345307
 O                  3.277500    0.816199    0.550176
 C                  1.279918   -4.429372    2.260178
 N                  1.866098   -4.954313    3.118261
 O                  3.291139   -2.643837    1.288579
 H                 -0.209523    0.955775   -0.457705
 H                 -0.671970    0.705017    2.023512
 H                  1.816339    0.637973    2.831193
 H                  1.770304   -0.393362   -1.322040
 H                 -0.883688   -1.839481    2.616512
 H                 -0.573794   -3.212274    0.523691
 H                  1.583726   -2.747325   -0.749717
 H                  1.597352   -1.832033    3.398540
 H                 -0.930445   -1.414722   -1.401018
 H                 -1.948432   -1.003790   -0.014887
 O                  4.137646   -3.549655    3.406308
 H                  4.974640   -3.677265    3.861640
 H                  3.784736   -2.918358    2.181744
 H                  3.451203   -4.256416    3.564265

 1  2 1.0  4 1.0  11 1.0  16 1.0
 2  3 1.0  6 1.0  17 1.0
 3  5 1.0  10 1.0  18 1.0
 4  5 1.0  8 1.0  19 1.0
 5  12 2.0
 6  7 1.0  10 1.0  20 1.0
 7  8 1.0  11 1.0  21 1.0
 8  9 1.0  22 1.0
 9  10 1.0  15 2.0
 10  23 1.0
 11  24 1.0  25 1.0
 12
 13  14 3.0
 14
 15
 16
```

```
17
18
19
20
21
22
23
24
25
26  27 1.0  29 1.0
27
28
29
```

```
 Entering Gaussian System, Link 0=g98
 Input=Mech1s1tsFsolvent.gjf
 Output=Mech1s1tsFsolvent.log
 Initial command:
 /usr/g98/l1.exe /usr/scratch/kruger/Gau-18306.inp -
scrdir=/usr/scratch/kruger/
 Entering Link 1 = /usr/g98/l1.exe PID=     18933.
```

```
---------------------------------------------------------------
Warning -- This program may not be used in any manner that
competes with the business of Gaussian, Inc. or will provide
assistance to any competitor of Gaussian, Inc.  The licensee
of this program is prohibited from giving any competitor of
Gaussian, Inc. access to this program.  By using this program,
the user acknowledges that Gaussian, Inc. is engaged in the
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.
---------------------------------------------------------------


Cite this work as:
Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

**********************************************
Gaussian 98:  DEC-AXP-OSF/1-G98RevA.7 11-Apr-1999
                  24-Aug-2002
**********************************************
%mem=400MB
%nproc=2
Will use up to    2 processors via shared memory.
%chk=mech1s1tsF
---------------------------------------------------------------
#N RHF/3-21+G* opt=(calcfc,ts,noeigentest,gdiis) freq optcyc=200
---------------------------------------------------------------
1/5=1,6=200,10=4,11=1,18=20,19=11,38=1/1,3;
2/9=110,17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11/1;
11/6=1,8=1,9=11,15=111,16=11/1,2,10;
10/6=1,7=6/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/10=1,18=20,25=1/1,2,3,16;
1/5=1,6=200,10=4,11=1,18=20,19=11/3(1);
```

```
 99//99;
 2/9=110/2;
 3/5=5,7=11,11=1,25=1,30=1/1,2,3;
 4/5=5,7=1,16=2/1;
 5/5=2,38=4/2;
 7//1,2,3,16;
 1/5=1,6=200,11=1,18=20,19=11/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1/1;
 99/9=1/99;
 -------------------
 With solvent (H3O+)
 -------------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                    -2.00418  -0.28299   1.23226
 C                    -1.50645   1.17185   0.97832
 C                    -1.01902   1.24175  -0.50451
 C                    -1.26656  -1.06611   0.10937
 C                    -1.33612  -0.11654  -1.07505
 C                    -0.02199   1.13756   1.48731
 C                     0.14109  -0.32634   1.99426
 C                     0.24514  -1.0942    0.66543
 C                     1.02596  -0.19366  -0.26909
 C                     0.49008   1.19801   0.01332
 C                    -1.26083  -0.67498   2.51729
 O                    -1.54559  -0.38051  -2.25555
 C                     2.84882  -0.02949   0.7687
 N                     3.89269   0.02837   1.25859
 O                     1.21818  -0.61782  -1.4871
 H                    -3.07808  -0.40624   1.22473
 H                    -2.15919   1.95352   1.33274
 H                    -1.29889   2.07761  -1.12346
 H                    -1.64865  -2.05107  -0.10558
 H                     0.30927   1.90332   2.16882
 H                     0.97572  -0.49306   2.65463
 H                     0.63682  -2.09586   0.71803
 H                     1.12265   2.00778  -0.30316
 H                    -1.36949  -1.72331   2.77124
 H                    -1.55436  -0.06824   3.36683
 O                     0.50208   0.1398   -3.5712
 H                    -0.45645   0.11269  -3.73715
 H                     0.78382  -0.11971  -2.51079
 H                     1.07491  -0.21696  -4.2619

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Initialization pass.
                        ----------------------------
                        !    Initial Parameters    !
                        ! (Angstroms and Degrees)  !
 ------------------------                           ---------------------
-----
```

```
 ! Name  Definition              Value          Derivative Info.
!
 ------------------------------------------------------------------------
-----
 ! R1    R(1,2)                  1.5585         calculate D2E/DX2
analyticall!
 ! R2    R(1,4)                  1.5551         calculate D2E/DX2
analyticall!
 ! R3    R(1,11)                 1.5354         calculate D2E/DX2
analyticall!
 ! R4    R(1,16)                 1.081          calculate D2E/DX2
analyticall!
 ! R5    R(2,3)                  1.5624         calculate D2E/DX2
analyticall!
 ! R6    R(2,6)                  1.5697         calculate D2E/DX2
analyticall!
 ! R7    R(2,17)                 1.0783         calculate D2E/DX2
analyticall!
 ! R8    R(3,5)                  1.507          calculate D2E/DX2
analyticall!
 ! R9    R(3,10)                 1.5961         calculate D2E/DX2
analyticall!
 ! R10   R(3,18)                 1.0771         calculate D2E/DX2
analyticall!
 ! R11   R(4,5)                  1.5197         calculate D2E/DX2
analyticall!
 ! R12   R(4,19)                 1.0781         calculate D2E/DX2
analyticall!
 ! R13   R(5,12)                 1.2277         calculate D2E/DX2
analyticall!
 ! R14   R(6,7)                  1.5578         calculate D2E/DX2
analyticall!
 ! R15   R(6,10)                 1.5616         calculate D2E/DX2
analyticall!
 ! R16   R(6,20)                 1.0773         calculate D2E/DX2
analyticall!
 ! R17   R(7,8)                  1.5383         calculate D2E/DX2
analyticall!
 ! R18   R(7,11)                 1.5364         calculate D2E/DX2
analyticall!
 ! R19   R(7,21)                 1.0773         calculate D2E/DX2
analyticall!
 ! R20   R(8,9)                  1.5146         calculate D2E/DX2
analyticall!
 ! R21   R(8,22)                 1.0768         calculate D2E/DX2
analyticall!
 ! R22   R(9,10)                 1.5178         calculate D2E/DX2
analyticall!
 ! R23   R(9,13)                 2.104          calculate D2E/DX2
analyticall!
 ! R24   R(9,15)                 1.304          calculate D2E/DX2
analyticall!
 ! R25   R(10,23)                1.0752         calculate D2E/DX2
analyticall!
```

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 ! R26   R(11,24)                1.0841         calculate D2E/DX2
analyticall!
 ! R27   R(11,25)                1.0844         calculate D2E/DX2
analyticall!
 ! R28   R(13,14)                1.1546         calculate D2E/DX2
analyticall!
 ! R29   R(13,21)                2.6982         calculate D2E/DX2
analyticall!
 ! R30   R(15,28)                1.2185         calculate D2E/DX2
analyticall!
 ! R31   R(26,27)                0.9732         calculate D2E/DX2
analyticall!
 ! R32   R(26,28)                1.1275         calculate D2E/DX2
analyticall!
 ! R33   R(26,29)                0.9657         calculate D2E/DX2
analyticall!
 ! A1    A(2,1,4)               101.5932         calculate D2E/DX2
analyticall!
 ! A2    A(2,1,11)              102.7136         calculate D2E/DX2
analyticall!
 ! A3    A(2,1,16)              114.998          calculate D2E/DX2
analyticall!
 ! A4    A(4,1,11)              104.2482         calculate D2E/DX2
analyticall!
 ! A5    A(4,1,16)              114.1279         calculate D2E/DX2
analyticall!
 ! A6    A(11,1,16)             117.2378         calculate D2E/DX2
analyticall!
 ! A7    A(1,2,3)               107.2197         calculate D2E/DX2
analyticall!
 ! A8    A(1,2,6)               103.2265         calculate D2E/DX2
analyticall!
 ! A9    A(1,2,17)              115.4569         calculate D2E/DX2
analyticall!
 ! A10   A(3,2,6)                90.7843         calculate D2E/DX2
analyticall!
 ! A11   A(3,2,17)              117.9281         calculate D2E/DX2
analyticall!
 ! A12   A(6,2,17)              118.7994         calculate D2E/DX2
analyticall!
 ! A13   A(2,3,5)               104.6754         calculate D2E/DX2
analyticall!
 ! A14   A(2,3,10)               89.1885         calculate D2E/DX2
analyticall!
 ! A15   A(2,3,18)              119.9361         calculate D2E/DX2
analyticall!
 ! A16   A(5,3,10)              107.2823         calculate D2E/DX2
analyticall!
 ! A17   A(5,3,18)              115.2921         calculate D2E/DX2
analyticall!
 ! A18   A(10,3,18)             116.961          calculate D2E/DX2
analyticall!
 ! A19   A(1,4,5)               103.0855         calculate D2E/DX2
analyticall!
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 ! A20   A(1,4,19)             115.8451         calculate D2E/DX2
analyticall!
 ! A21   A(5,4,19)             113.5315         calculate D2E/DX2
analyticall!
 ! A22   A(3,5,4)              104.9806         calculate D2E/DX2
analyticall!
 ! A23   A(3,5,12)             126.4246         calculate D2E/DX2
analyticall!
 ! A24   A(4,5,12)             128.5288         calculate D2E/DX2
analyticall!
 ! A25   A(2,6,7)              103.0066         calculate D2E/DX2
analyticall!
 ! A26   A(2,6,10)              90.1827         calculate D2E/DX2
analyticall!
 ! A27   A(2,6,20)             118.7113         calculate D2E/DX2
analyticall!
 ! A28   A(7,6,10)             108.0134         calculate D2E/DX2
analyticall!
 ! A29   A(7,6,20)             115.4626         calculate D2E/DX2
analyticall!
 ! A30   A(10,6,20)            117.9553         calculate D2E/DX2
analyticall!
 ! A31   A(6,7,8)              101.2474         calculate D2E/DX2
analyticall!
 ! A32   A(6,7,11)             103.2096         calculate D2E/DX2
analyticall!
 ! A33   A(6,7,21)             115.2164         calculate D2E/DX2
analyticall!
 ! A34   A(8,7,11)             104.0362         calculate D2E/DX2
analyticall!
 ! A35   A(8,7,21)             113.5712         calculate D2E/DX2
analyticall!
 ! A36   A(11,7,21)            117.5912         calculate D2E/DX2
analyticall!
 ! A37   A(7,8,9)              105.7289         calculate D2E/DX2
analyticall!
 ! A38   A(7,8,22)             116.5353         calculate D2E/DX2
analyticall!
 ! A39   A(9,8,22)             113.3103         calculate D2E/DX2
analyticall!
 ! A40   A(8,9,10)             104.38           calculate D2E/DX2
analyticall!
 ! A41   A(8,9,13)             100.8769         calculate D2E/DX2
analyticall!
 ! A42   A(8,9,15)             117.3172         calculate D2E/DX2
analyticall!
 ! A43   A(10,9,13)             98.1965         calculate D2E/DX2
analyticall!
 ! A44   A(10,9,15)            121.6073         calculate D2E/DX2
analyticall!
 ! A45   A(13,9,15)            111.0013         calculate D2E/DX2
analyticall!
 ! A46   A(3,10,6)              89.8427         calculate D2E/DX2
analyticall!
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 ! A47   A(3,10,9)             107.373          calculate D2E/DX2
analyticall!
 ! A48   A(3,10,23)            116.1127         calculate D2E/DX2
analyticall!
 ! A49   A(6,10,9)             104.8276         calculate D2E/DX2
analyticall!
 ! A50   A(6,10,23)            119.9945         calculate D2E/DX2
analyticall!
 ! A51   A(9,10,23)            115.3454         calculate D2E/DX2
analyticall!
 ! A52   A(1,11,7)              95.6768         calculate D2E/DX2
analyticall!
 ! A53   A(1,11,24)            113.2277         calculate D2E/DX2
analyticall!
 ! A54   A(1,11,25)            112.4423         calculate D2E/DX2
analyticall!
 ! A55   A(7,11,24)            112.994          calculate D2E/DX2
analyticall!
 ! A56   A(7,11,25)            112.7507         calculate D2E/DX2
analyticall!
 ! A57   A(24,11,25)           109.2926         calculate D2E/DX2
analyticall!
 ! A58   A(9,13,21)             74.3301         calculate D2E/DX2
analyticall!
 ! A59   A(14,13,21)           109.8581         calculate D2E/DX2
analyticall!
 ! A60   A(9,15,28)            126.8129         calculate D2E/DX2
analyticall!
 ! A61   A(7,21,13)             94.7495         calculate D2E/DX2
analyticall!
 ! A62   A(27,26,28)           113.5844         calculate D2E/DX2
analyticall!
 ! A63   A(27,26,29)           116.8733         calculate D2E/DX2
analyticall!
 ! A64   A(28,26,29)           116.0695         calculate D2E/DX2
analyticall!
 ! A65   L(15,28,26,29,-1)     167.5155         calculate D2E/DX2
analyticall!
 ! A66   L(9,13,14,21,-2)      177.5789         calculate D2E/DX2
analyticall!
 ! A67   L(15,28,26,29,-2)     172.1658         calculate D2E/DX2
analyticall!
 ! D1    D(4,1,2,3)             21.5597         calculate D2E/DX2
analyticall!
 ! D2    D(4,1,2,6)            -73.4639         calculate D2E/DX2
analyticall!
 ! D3    D(4,1,2,17)           155.2382         calculate D2E/DX2
analyticall!
 ! D4    D(11,1,2,3)           129.2485         calculate D2E/DX2
analyticall!
 ! D5    D(11,1,2,6)            34.2249         calculate D2E/DX2
analyticall!
 ! D6    D(11,1,2,17)          -97.0731         calculate D2E/DX2
analyticall!
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 ! D7    D(16,1,2,3)          -102.2249         calculate D2E/DX2
analyticall!
 ! D8    D(16,1,2,6)           162.7515         calculate D2E/DX2
analyticall!
 ! D9    D(16,1,2,17)           31.4536         calculate D2E/DX2
analyticall!
 ! D10   D(2,1,4,5)            -39.0313         calculate D2E/DX2
analyticall!
 ! D11   D(2,1,4,19)          -163.6453         calculate D2E/DX2
analyticall!
 ! D12   D(11,1,4,5)          -145.5236         calculate D2E/DX2
analyticall!
 ! D13   D(11,1,4,19)           89.8624         calculate D2E/DX2
analyticall!
 ! D14   D(16,1,4,5)            85.3411         calculate D2E/DX2
analyticall!
 ! D15   D(16,1,4,19)          -39.2729         calculate D2E/DX2
analyticall!
 ! D16   D(2,1,11,7)           -53.272          calculate D2E/DX2
analyticall!
 ! D17   D(2,1,11,24)          -171.2964        calculate D2E/DX2
analyticall!
 ! D18   D(2,1,11,25)            64.2138        calculate D2E/DX2
analyticall!
 ! D19   D(4,1,11,7)             52.3828        calculate D2E/DX2
analyticall!
 ! D20   D(4,1,11,24)           -65.6416        calculate D2E/DX2
analyticall!
 ! D21   D(4,1,11,25)           169.8686        calculate D2E/DX2
analyticall!
 ! D22   D(16,1,11,7)           179.6162        calculate D2E/DX2
analyticall!
 ! D23   D(16,1,11,24)           61.5918        calculate D2E/DX2
analyticall!
 ! D24   D(16,1,11,25)          -62.898          calculate D2E/DX2
analyticall!
 ! D25   D(1,2,3,5)               3.8696         calculate D2E/DX2
analyticall!
 ! D26   D(1,2,3,10)           -103.7936         calculate D2E/DX2
analyticall!
 ! D27   D(1,2,3,18)            135.2035         calculate D2E/DX2
analyticall!
 ! D28   D(6,2,3,5)             107.9807         calculate D2E/DX2
analyticall!
 ! D29   D(6,2,3,10)              0.3175         calculate D2E/DX2
analyticall!
 ! D30   D(6,2,3,18)           -120.6854         calculate D2E/DX2
analyticall!
 ! D31   D(17,2,3,5)           -128.4769         calculate D2E/DX2
analyticall!
 ! D32   D(17,2,3,10)           123.8599         calculate D2E/DX2
analyticall!
 ! D33   D(17,2,3,18)             2.857          calculate D2E/DX2
analyticall!
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 ! D34   D(1,2,6,7)             -0.9743         calculate D2E/DX2
analyticall!
 ! D35   D(1,2,6,10)            107.575         calculate D2E/DX2
analyticall!
 ! D36   D(1,2,6,20)          -129.9964         calculate D2E/DX2
analyticall!
 ! D37   D(3,2,6,7)           -108.8738         calculate D2E/DX2
analyticall!
 ! D38   D(3,2,6,10)            -0.3245         calculate D2E/DX2
analyticall!
 ! D39   D(3,2,6,20)            122.1041         calculate D2E/DX2
analyticall!
 ! D40   D(17,2,6,7)            128.3031         calculate D2E/DX2
analyticall!
 ! D41   D(17,2,6,10)         -123.1476         calculate D2E/DX2
analyticall!
 ! D42   D(17,2,6,20)            -0.719         calculate D2E/DX2
analyticall!
 ! D43   D(2,3,5,4)             -28.8087         calculate D2E/DX2
analyticall!
 ! D44   D(2,3,5,12)            153.9497         calculate D2E/DX2
analyticall!
 ! D45   D(10,3,5,4)             64.984         calculate D2E/DX2
analyticall!
 ! D46   D(10,3,5,12)          -112.2576         calculate D2E/DX2
analyticall!
 ! D47   D(18,3,5,4)           -162.7805         calculate D2E/DX2
analyticall!
 ! D48   D(18,3,5,12)            19.9779         calculate D2E/DX2
analyticall!
 ! D49   D(2,3,10,6)             -0.3191         calculate D2E/DX2
analyticall!
 ! D50   D(2,3,10,9)            105.1836         calculate D2E/DX2
analyticall!
 ! D51   D(2,3,10,23)          -124.0574         calculate D2E/DX2
analyticall!
 ! D52   D(5,3,10,6)           -105.445         calculate D2E/DX2
analyticall!
 ! D53   D(5,3,10,9)              0.0578         calculate D2E/DX2
analyticall!
 ! D54   D(5,3,10,23)           130.8167         calculate D2E/DX2
analyticall!
 ! D55   D(18,3,10,6)           123.2358         calculate D2E/DX2
analyticall!
 ! D56   D(18,3,10,9)          -131.2615         calculate D2E/DX2
analyticall!
 ! D57   D(18,3,10,23)           -0.5025         calculate D2E/DX2
analyticall!
 ! D58   D(1,4,5,3)              43.1919         calculate D2E/DX2
analyticall!
 ! D59   D(1,4,5,12)           -139.6453         calculate D2E/DX2
analyticall!
 ! D60   D(19,4,5,3)            169.3047         calculate D2E/DX2
analyticall!
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 ! D61   D(19,4,5,12)          -13.5326         calculate D2E/DX2
analyticall!
 ! D62   D(2,6,7,8)             74.8881         calculate D2E/DX2
analyticall!
 ! D63   D(2,6,7,11)           -32.6105         calculate D2E/DX2
analyticall!
 ! D64   D(2,6,7,21)          -162.1341         calculate D2E/DX2
analyticall!
 ! D65   D(10,6,7,8)           -19.6174         calculate D2E/DX2
analyticall!
 ! D66   D(10,6,7,11)         -127.116          calculate D2E/DX2
analyticall!
 ! D67   D(10,6,7,21)          103.3604         calculate D2E/DX2
analyticall!
 ! D68   D(20,6,7,8)          -154.1102         calculate D2E/DX2
analyticall!
 ! D69   D(20,6,7,11)           98.3911         calculate D2E/DX2
analyticall!
 ! D70   D(20,6,7,21)          -31.1324         calculate D2E/DX2
analyticall!
 ! D71   D(2,6,10,3)             0.3176         calculate D2E/DX2
analyticall!
 ! D72   D(2,6,10,9)          -107.6302         calculate D2E/DX2
analyticall!
 ! D73   D(2,6,10,23)          120.7564         calculate D2E/DX2
analyticall!
 ! D74   D(7,6,10,3)           104.0686         calculate D2E/DX2
analyticall!
 ! D75   D(7,6,10,9)            -3.8792         calculate D2E/DX2
analyticall!
 ! D76   D(7,6,10,23)         -135.4927         calculate D2E/DX2
analyticall!
 ! D77   D(20,6,10,3)         -122.7448         calculate D2E/DX2
analyticall!
 ! D78   D(20,6,10,9)          129.3074         calculate D2E/DX2
analyticall!
 ! D79   D(20,6,10,23)          -2.306          calculate D2E/DX2
analyticall!
 ! D80   D(6,7,8,9)             36.5443         calculate D2E/DX2
analyticall!
 ! D81   D(6,7,8,22)           163.4244         calculate D2E/DX2
analyticall!
 ! D82   D(11,7,8,9)           143.3948         calculate D2E/DX2
analyticall!
 ! D83   D(11,7,8,22)          -89.7251         calculate D2E/DX2
analyticall!
 ! D84   D(21,7,8,9)           -87.559          calculate D2E/DX2
analyticall!
 ! D85   D(21,7,8,22)           39.321          calculate D2E/DX2
analyticall!
 ! D86   D(6,7,11,1)            52.8109         calculate D2E/DX2
analyticall!
 ! D87   D(6,7,11,24)          171.0219         calculate D2E/DX2
analyticall!
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 ! D88   D(6,7,11,25)          -64.427          calculate D2E/DX2
analyticall!
 ! D89   D(8,7,11,1)           -52.5676         calculate D2E/DX2
analyticall!
 ! D90   D(8,7,11,24)           65.6434         calculate D2E/DX2
analyticall!
 ! D91   D(8,7,11,25)         -169.8055         calculate D2E/DX2
analyticall!
 ! D92   D(21,7,11,1)         -179.1326         calculate D2E/DX2
analyticall!
 ! D93   D(21,7,11,24)         -60.9216         calculate D2E/DX2
analyticall!
 ! D94   D(21,7,11,25)          63.6295         calculate D2E/DX2
analyticall!
 ! D95   D(6,7,21,13)           -67.0519        calculate D2E/DX2
analyticall!
 ! D96   D(8,7,21,13)           49.0949         calculate D2E/DX2
analyticall!
 ! D97   D(11,7,21,13)         170.8689         calculate D2E/DX2
analyticall!
 ! D98   D(7,8,9,10)            -40.4396        calculate D2E/DX2
analyticall!
 ! D99   D(7,8,9,13)            61.0469         calculate D2E/DX2
analyticall!
 ! D100  D(7,8,9,15)          -178.2891         calculate D2E/DX2
analyticall!
 ! D101  D(22,8,9,10)         -169.2488         calculate D2E/DX2
analyticall!
 ! D102  D(22,8,9,13)           -67.7623        calculate D2E/DX2
analyticall!
 ! D103  D(22,8,9,15)            52.9017        calculate D2E/DX2
analyticall!
 ! D104  D(8,9,10,3)            -68.0799        calculate D2E/DX2
analyticall!
 ! D105  D(8,9,10,6)             26.4998        calculate D2E/DX2
analyticall!
 ! D106  D(8,9,10,23)           160.7353         calculate D2E/DX2
analyticall!
 ! D107  D(13,9,10,3)         -171.5974         calculate D2E/DX2
analyticall!
 ! D108  D(13,9,10,6)           -77.0177        calculate D2E/DX2
analyticall!
 ! D109  D(13,9,10,23)           57.2178        calculate D2E/DX2
analyticall!
 ! D110  D(15,9,10,3)            67.4856        calculate D2E/DX2
analyticall!
 ! D111  D(15,9,10,6)           162.0653         calculate D2E/DX2
analyticall!
 ! D112  D(15,9,10,23)          -63.6992         calculate D2E/DX2
analyticall!
 ! D113  D(8,9,13,21)           -27.2835         calculate D2E/DX2
analyticall!
 ! D114  D(10,9,13,21)           79.1668         calculate D2E/DX2
analyticall!
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 ! D115  D(15,9,13,21)        -152.3361         calculate D2E/DX2
analyticall!
 ! D116  D(8,9,15,28)          115.1824         calculate D2E/DX2
analyticall!
 ! D117  D(10,9,15,28)         -15.0633         calculate D2E/DX2
analyticall!
 ! D118  D(13,9,15,28)        -129.6173         calculate D2E/DX2
analyticall!
 ! D119  D(9,13,21,7)          -11.8222         calculate D2E/DX2
analyticall!
 ! D120  D(14,13,21,7)         170.5989         calculate D2E/DX2
analyticall!
 ! D121  D(9,15,26,27)         -64.3827         calculate D2E/DX2
analyticall!
 ! D122  D(9,15,26,29)         159.9644         calculate D2E/DX2
analyticall!
 ---------------------------------------------------------------------
-----
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
 Number of steps in this run= 174 maximum allowed number of steps= 174.
 Search for a saddle point of order  1.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -2.004177   -0.282986    1.232261
    2          6             0       -1.506451    1.171852    0.978317
    3          6             0       -1.019024    1.241748   -0.504506
    4          6             0       -1.266560   -1.066107    0.109369
    5          6             0       -1.336116   -0.116536   -1.075047
    6          6             0       -0.021985    1.137556    1.487308
    7          6             0        0.141088   -0.326341    1.994262
    8          6             0        0.245142   -1.094199    0.665427
    9          6             0        1.025958   -0.193658   -0.269092
   10          6             0        0.490077    1.198009    0.013316
   11          6             0       -1.260825   -0.674976    2.517292
   12          8             0       -1.545587   -0.380512   -2.255545
   13          6             0        2.848819   -0.029485    0.768703
   14          7             0        3.892688    0.028367    1.258590
   15          8             0        1.218184   -0.617822   -1.487104
   16          1             0       -3.078081   -0.406241    1.224731
   17          1             0       -2.159191    1.953520    1.332742
   18          1             0       -1.298886    2.077610   -1.123459
   19          1             0       -1.648649   -2.051074   -0.105581
   20          1             0        0.309271    1.903320    2.168822
   21          1             0        0.975718   -0.493057    2.654626
   22          1             0        0.636816   -2.095865    0.718026
   23          1             0        1.122646    2.007781   -0.303163
   24          1             0       -1.369490   -1.723312    2.771236
   25          1             0       -1.554363   -0.068243    3.366829
   26          8             0        0.502082    0.139798   -3.571196
```

27	1	0	-0.456448	0.112694	-3.737150
28	1	0	0.783816	-0.119714	-2.510785
29	1	0	1.074912	-0.216960	-4.261899

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.558452	0.000000			
3	C	2.512310	1.562445	0.000000		

nuclear repulsion energy 1163.4005857738 Hartrees.
One-electron integrals computed using PRISM.
NBasis= 234 RedAO= T NBF= 234
NBsUse= 234 1.00D-04 NBFU= 234
Initial guess read from the read-write file:
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done: E(RHF) = -736.914161664 A.U. after 11 cycles
Convg = 0.8558D-08 -V/T = 2.0024
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000167	-0.000000091	0.000000058
2	6	-0.000000086	0.000000104	0.000000015
3	6	0.000000620	0.000000427	-0.000000662
4	6	-0.000000640	-0.000000199	-0.000000199
5	6	0.000000193	0.000000477	0.000000441
6	6	0.000000029	-0.000000344	-0.000000352
7	6	0.000000169	0.000000325	-0.000000334
8	6	-0.000000852	0.000000001	-0.000001148
9	6	0.000012095	0.000004177	0.000007380
10	6	-0.000002532	-0.000001755	-0.000001114
11	6	-0.000000066	0.000000135	-0.000000058
12	8	-0.000000787	0.000000170	-0.000000130
13	6	-0.000002161	-0.000006310	-0.000002061
14	7	-0.000007910	0.000003736	-0.000011273
15	8	0.000001789	0.000001194	-0.000009106
16	1	0.000000008	0.000000008	0.000000021
17	1	0.000000092	0.000000048	-0.000000011
18	1	-0.000000562	-0.000000040	0.000000163
19	1	-0.000000085	0.000000007	-0.000000032
20	1	0.000000000	-0.000000072	0.000000064
21	1	-0.000001605	0.000000607	0.000000860
22	1	0.000000210	0.000000125	0.000000048
23	1	0.000000361	0.000000448	0.000000305
24	1	0.000000001	-0.000000013	-0.000000051
25	1	-0.000000047	-0.000000007	-0.000000008
26	8	0.000009938	0.000002186	0.000014421
27	1	0.000003347	0.000001472	-0.000000944
28	1	-0.000007833	-0.000006092	0.000009419

```
  29          1          -0.000003518   -0.000000725   -0.000005713
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000014421 RMS     0.000003615

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Use GDIIS/GDPIS optimizer.
Internal  Forces:  Max     0.000035583 RMS     0.000004449
Search for a saddle point.
Step number  91 out of a maximum of 174
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Swaping is turned off.
Update second derivatives using information from points 75 76 77 78 79
                                                     80 81 82 83 84

                                                     85 86 87 88 89

                                                     90 91
    Eigenvalues ---   -0.00477   0.00111   0.00548   0.01199   0.01353
    Eigenvalues ---    0.01364   0.01826   0.01984   0.02153   0.02237
    Eigenvalues ---    0.02259   0.02357   0.02582   0.02667   0.03028
    Eigenvalues ---    0.03139   0.03416   0.03488   0.04055   0.04273
    Eigenvalues ---    0.04380   0.04519   0.04899   0.04974   0.05116
    Eigenvalues ---    0.05820   0.06165   0.06263   0.06468   0.06701
    Eigenvalues ---    0.07027   0.07354   0.07665   0.07929   0.08530
    Eigenvalues ---    0.08624   0.08869   0.09159   0.09270   0.09754
    Eigenvalues ---    0.10897   0.12955   0.13147   0.13437   0.14605
    Eigenvalues ---    0.15211   0.16072   0.17836   0.18791   0.19693
    Eigenvalues ---    0.20406   0.21922   0.22301   0.23567   0.23996
    Eigenvalues ---    0.25264   0.26611   0.27367   0.29045   0.30238
    Eigenvalues ---    0.36039   0.36833   0.36844   0.37045   0.37604
    Eigenvalues ---    0.37872   0.38382   0.38734   0.38918   0.39128
    Eigenvalues ---    0.39452   0.40049   0.40880   0.50414   0.51997
    Eigenvalues ---    0.54477   0.59839   0.80822   1.03826   1.23265
    Eigenvalues ---    1.391111000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
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    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.00000
Eigenvectors required to have negative eigenvalues:
                      R1        R2        R3        R4        R5
        1          -0.00020  -0.00482   0.00544   0.00003  -0.00127
                      R6        R7        R8        R9        R10
        1           0.00269  -0.00013   0.00145   0.00400  -0.00037
                      R11       R12       R13       R14       R15
        1           0.00699  -0.00004  -0.00043   0.00198  -0.00018
                      R16       R17       R18       R19       R20
        1          -0.00114   0.00214   0.00173   0.00753  -0.01238
                      R21       R22       R23       R24       R25
        1           0.00041  -0.01509   0.63275  -0.04670   0.00001
                      R26       R27       R28       R29       R30
        1          -0.00026   0.00000   0.00555   0.22145   0.10703
                      R31       R32       R33       A1        A2
        1          -0.00161  -0.24322   0.04537   0.00045  -0.00035
                      A3        A4        A5        A6        A7
        1           0.00120   0.00168  -0.00030  -0.00230   0.00237
                      A8        A9        A10       A11       A12
        1          -0.00045  -0.00073  -0.00035  -0.00289   0.00250
                      A13       A14       A15       A16       A17
        1           0.00801   0.00071   0.00555  -0.00982   0.00121
                      A18       A19       A20       A21       A22
        1          -0.00554   0.01344   0.00765   0.00194  -0.00226
                      A23       A24       A25       A26       A27
        1           0.00086   0.00284   0.00294   0.00081   0.00521
                      A28       A29       A30       A31       A32
        1          -0.00099  -0.00539  -0.00097  -0.00087  -0.00324
                      A33       A34       A35       A36       A37
        1          -0.00608  -0.00630   0.00582   0.00877   0.00253
                      A38       A39       A40       A41       A42
        1           0.00516   0.00184   0.01543   0.01973   0.00804
                      A43       A44       A45       A46       A47
        1          -0.10551   0.02711  -0.04461  -0.00116  -0.02344
                      A48       A49       A50       A51       A52
        1           0.00515   0.00157   0.00655   0.00628   0.00252
                      A53       A54       A55       A56       A57
        1           0.00108  -0.00386   0.00289  -0.00253   0.00002
                      A58       A59       A60       A61       A62
        1          -0.09981   0.46086   0.02190   0.07419  -0.06504
                      A63       A64       A65       A66       A67
        1           0.02211  -0.03049   0.05516   0.08241  -0.04954
                      D1        D2        D3        D4        D5
        1          -0.00500  -0.00509  -0.00749  -0.00317  -0.00326
                      D6        D7        D8        D9        D10
        1          -0.00566  -0.00561  -0.00569  -0.00810   0.01503
```

```
                    D11       D12       D13       D14       D15
          1      -0.00152   0.01478  -0.00178   0.01664   0.00008
                    D16       D17       D18       D19       D20
          1       0.00073  -0.00430  -0.00208   0.00162  -0.00340
                    D21       D22       D23       D24       D25
          1      -0.00119   0.00102  -0.00400  -0.00179  -0.00830
                    D26       D27       D28       D29       D30
          1       0.00107   0.00554  -0.00867   0.00070   0.00518
                    D31       D32       D33       D34       D35
          1      -0.00700   0.00237   0.00684   0.00216   0.00160
                    D36       D37       D38       D39       D40
          1       0.00288  -0.00015  -0.00071   0.00057   0.00263
                    D41       D42       D43       D44       D45
          1       0.00207   0.00335   0.02253   0.04039   0.02385
                    D46       D47       D48       D49       D50
          1       0.04171   0.00728   0.02514  -0.00070  -0.00103
                    D51       D52       D53       D54       D55
          1      -0.00938  -0.00882  -0.00915  -0.01750   0.00443
                    D56       D57       D58       D59       D60
          1       0.00411  -0.00425  -0.02390  -0.04161  -0.00424
                    D61       D62       D63       D64       D65
          1      -0.02196  -0.00878  -0.00087  -0.00552  -0.01040
                    D66       D67       D68       D69       D70
          1      -0.00249  -0.00714  -0.00334   0.00457  -0.00008
                    D71       D72       D73       D74       D75
          1       0.00071   0.02513   0.00845   0.00399   0.02841
                    D76       D77       D78       D79       D80
          1       0.01173  -0.00562   0.01880   0.00212  -0.01158
                    D81       D82       D83       D84       D85
          1      -0.00361  -0.01712  -0.00916  -0.00672   0.00125
                    D86       D87       D88       D89       D90
          1      -0.00115   0.00245   0.00273   0.00280   0.00639
                    D91       D92       D93       D94       D95
          1       0.00668  -0.00583  -0.00224  -0.00195   0.10185
                    D96       D97       D98       D99      D100
          1       0.10060   0.10436   0.02620  -0.07751  -0.11599
                   D101      D102      D103      D104      D105
          1       0.01648  -0.08722  -0.12570  -0.02502  -0.03215
                   D106      D107      D108      D109      D110
          1      -0.01604  -0.01344  -0.02056  -0.00445   0.12191
                   D111      D112      D113      D114      D115
          1       0.11478   0.13089   0.06018   0.04744   0.06327
                   D116      D117      D118      D119      D120
          1       0.07320  -0.09584   0.06869  -0.07084  -0.15325
                   D121      D122
          1      -0.10333   0.09224
 Cosine:  0.456 <  0.500
 Cut down GDIIS temporarily because of the cosine check. E 6
 DIIS coeff's:      1.10798     -0.01140     -0.22727      0.06004
0.06130
 DIIS coeff's:      0.04949     -0.11933      0.10447     -0.00975     -
0.04563
 DIIS coeff's:      0.00829      0.01154      0.01120     -0.00092
 Cosine:  0.616 >  0.500
```

Length: 1.630
GDIIS step was calculated using 14 of the last 17 vectors.
Iteration 1 RMS(Cart)= 0.00008400 RMS(Int)= 0.00000028
Iteration 2 RMS(Cart)= 0.00000007 RMS(Int)= 0.00000028

Variable	Old X	-DE/DX	Delta X (DIIS)	Delta X (GDIIS)	Delta X (Total)	New X
R1	2.95228	0.00000	0.00000	0.00000	0.00000	2.95228
R2	2.93619	0.00000	0.00000	0.00000	0.00000	2.93619
R3	2.89705	0.00000	0.00000	0.00000	0.00000	2.89704
R4	2.04134	0.00000	0.00000	0.00000	0.00000	2.04134
R5	2.96195	0.00000	0.00000	0.00000	0.00000	2.96195
R6	2.96274	0.00000	0.00000	0.00000	0.00000	2.96274
R7	2.03646	0.00000	0.00000	0.00000	0.00000	2.03646
R8	2.86279	0.00000	0.00000	0.00000	0.00000	2.86279
R9	3.02807	0.00000	0.00000	0.00000	0.00000	3.02807
R10	2.03301	0.00000	0.00000	0.00000	0.00000	2.03301
R11	2.87353	0.00000	0.00000	0.00000	0.00000	2.87353
R12	2.03582	0.00000	0.00000	0.00000	0.00000	2.03582
R13	2.29365	0.00000	0.00000	0.00000	0.00000	2.29365
R14	2.94529	0.00000	0.00000	0.00000	0.00000	2.94529
R15	2.94744	0.00000	-0.00001	0.00000	0.00000	2.94744
R16	2.03377	0.00000	0.00000	0.00000	0.00000	2.03377
R17	2.92855	0.00000	0.00000	0.00000	0.00000	2.92855
R18	2.89950	0.00000	0.00000	0.00000	0.00000	2.89950
R19	2.03094	0.00000	0.00000	0.00000	0.00000	2.03094
R20	2.81955	0.00000	-0.00001	0.00000	0.00000	2.81954
R21	2.03362	0.00000	0.00000	0.00000	0.00000	2.03362
R22	2.82232	0.00000	-0.00001	0.00001	0.00000	2.82232
R23	4.67096	-0.00002	0.00006	-0.00004	0.00002	4.67098
R24	2.40687	-0.00001	0.00000	0.00000	0.00001	2.40687
R25	2.02806	0.00000	0.00000	0.00000	0.00000	2.02806
R26	2.04816	0.00000	0.00000	0.00000	0.00000	2.04816
R27	2.04868	0.00000	0.00000	0.00000	0.00000	2.04868
R28	2.20011	0.00000	0.00000	0.00000	0.00000	2.20011
R29	5.32386	0.00000	0.00028	-0.00002	0.00025	5.32411
R30	1.99766	-0.00001	-0.00005	-0.00001	-0.00005	1.99761
R31	1.81667	0.00000	0.00000	0.00000	0.00000	1.81667
R32	2.68756	0.00000	0.00014	0.00000	0.00015	2.68770
R33	1.88563	-0.00001	-0.00001	0.00001	0.00000	1.88563
A1	1.77398	0.00000	0.00000	0.00000	0.00000	1.77398
A2	1.79799	0.00000	0.00000	0.00000	0.00000	1.79799
A3	2.00833	0.00000	0.00000	0.00000	0.00000	2.00833
A4	1.81634	0.00000	0.00000	0.00000	0.00000	1.81634
A5	1.98314	0.00000	0.00000	0.00000	0.00000	1.98314
A6	2.05093	0.00000	0.00000	0.00000	0.00000	2.05093
A7	1.87104	0.00000	0.00000	0.00000	0.00000	1.87104
A8	1.79768	0.00000	0.00000	0.00000	0.00000	1.79768
A9	2.01307	0.00000	0.00000	0.00000	0.00000	2.01307
A10	1.58462	0.00000	0.00000	0.00000	0.00000	1.58462
A11	2.05904	0.00000	0.00000	0.00000	0.00000	2.05904
A12	2.07870	0.00000	0.00000	0.00000	0.00000	2.07870
A13	1.80457	0.00000	-0.00001	0.00000	-0.00001	1.80456
A14	1.55223	0.00000	0.00000	0.00000	0.00000	1.55223
A15	2.09984	0.00000	0.00000	0.00000	0.00000	2.09984

A16	1.92850	0.00000	0.00001	0.00000	0.00001	1.92851
A17	2.00673	0.00000	0.00000	0.00000	0.00000	2.00673
A18	2.01624	0.00000	0.00000	0.00000	0.00000	2.01624
A19	1.77752	0.00000	-0.00001	0.00000	-0.00001	1.77751
A20	2.02264	0.00000	0.00000	0.00000	0.00000	2.02264
A21	1.98132	0.00000	0.00000	0.00000	0.00000	1.98132
A22	1.82646	0.00000	0.00000	0.00000	0.00000	1.82647
A23	2.22739	0.00000	0.00000	0.00000	0.00000	2.22739
A24	2.22593	0.00000	-0.00001	0.00000	0.00000	2.22593
A25	1.80052	0.00000	0.00000	0.00000	0.00000	1.80052
A26	1.57904	0.00000	0.00000	0.00000	0.00000	1.57904
A27	2.08497	0.00000	-0.00001	0.00000	0.00000	2.08497
A28	1.88023	0.00000	0.00000	0.00000	0.00000	1.88023
A29	2.01173	0.00000	0.00000	0.00000	0.00000	2.01173
A30	2.04874	0.00000	0.00000	0.00000	0.00000	2.04874
A31	1.77020	0.00000	0.00000	0.00000	0.00000	1.77020
A32	1.79973	0.00000	0.00000	0.00000	0.00000	1.79973
A33	2.00320	0.00000	-0.00001	0.00001	0.00000	2.00321
A34	1.81474	0.00000	0.00000	0.00000	0.00000	1.81474
A35	1.98315	0.00000	0.00002	-0.00001	0.00001	1.98316
A36	2.05855	0.00000	-0.00001	-0.00001	-0.00001	2.05854
A37	1.81732	0.00000	0.00001	0.00000	0.00001	1.81733
A38	2.03829	0.00000	0.00000	0.00000	0.00000	2.03829
A39	1.98338	0.00000	0.00000	0.00000	0.00000	1.98338
A40	1.86884	0.00000	0.00000	0.00000	0.00000	1.86884
A41	1.84047	0.00001	0.00004	0.00000	0.00004	1.84051
A42	2.13028	0.00000	-0.00001	0.00001	-0.00001	2.13027
A43	1.56564	0.00000	-0.00001	0.00000	0.00000	1.56564
A44	2.22291	0.00000	0.00000	-0.00001	-0.00001	2.22290
A45	1.64302	-0.00001	0.00001	0.00000	0.00001	1.64303
A46	1.56727	0.00000	0.00000	0.00000	0.00000	1.56727
A47	1.84434	0.00000	-0.00001	0.00001	-0.00001	1.84433
A48	2.03221	0.00000	0.00001	0.00000	0.00000	2.03221
A49	1.81689	0.00000	0.00001	0.00000	0.00000	1.81689
A50	2.10446	0.00000	-0.00001	0.00001	0.00000	2.10445
A51	2.03116	0.00000	0.00001	0.00000	0.00000	2.03116
A52	1.67028	0.00000	0.00000	0.00000	0.00000	1.67028
A53	1.97438	0.00000	0.00000	0.00000	0.00000	1.97438
A54	1.96565	0.00000	0.00000	0.00000	0.00000	1.96565
A55	1.97619	0.00000	0.00000	0.00000	0.00000	1.97619
A56	1.96201	0.00000	0.00000	0.00000	0.00000	1.96202
A57	1.90755	0.00000	0.00000	0.00000	0.00000	1.90755
A58	1.15633	0.00000	-0.00004	0.00001	-0.00003	1.15630
A59	2.94470	0.00001	-0.00005	0.00002	-0.00004	2.94466
A60	2.10399	-0.00004	-0.00003	0.00000	-0.00003	2.10396
A61	1.74994	0.00000	-0.00002	-0.00001	-0.00003	1.74991
A62	2.32238	0.00000	0.00004	0.00002	0.00007	2.32245
A63	2.01524	0.00000	-0.00001	0.00000	0.00000	2.01524
A64	1.85459	0.00000	-0.00001	-0.00002	-0.00003	1.85456
A65	2.85496	-0.00003	0.00000	-0.00002	-0.00001	2.85495
A66	3.98315	0.00000	0.00225	0.00003	0.00228	3.98542
A67	3.15559	0.00000	0.00010	-0.00004	0.00006	3.15564
D1	0.36429	0.00000	0.00000	0.00000	0.00000	0.36430
D2	-1.29294	0.00000	0.00000	0.00000	0.00000	-1.29294

D3	2.69649	0.00000	0.00000	0.00000	0.00000	2.69649
D4	2.24227	0.00000	0.00000	0.00000	0.00000	2.24227
D5	0.58504	0.00000	0.00000	0.00000	0.00000	0.58504
D6	-1.70872	0.00000	0.00000	0.00000	0.00000	-1.70872
D7	-1.78660	0.00000	0.00000	0.00000	0.00000	-1.78660
D8	2.83935	0.00000	0.00000	0.00000	0.00000	2.83935
D9	0.54560	0.00000	0.00000	0.00000	0.00000	0.54560
D10	-0.70737	0.00000	0.00000	0.00000	-0.00001	-0.70738
D11	-2.86658	0.00000	0.00000	0.00000	0.00000	-2.86658
D12	-2.57105	0.00000	-0.00001	0.00000	-0.00001	-2.57106
D13	1.55292	0.00000	0.00000	0.00000	0.00000	1.55292
D14	1.46060	0.00000	0.00000	0.00000	-0.00001	1.46060
D15	-0.69861	0.00000	0.00000	0.00000	0.00000	-0.69861
D16	-0.92465	0.00000	0.00000	0.00000	0.00000	-0.92465
D17	-2.98880	0.00000	0.00001	0.00000	0.00000	-2.98880
D18	1.12049	0.00000	0.00001	0.00000	0.00000	1.12049
D19	0.92105	0.00000	0.00000	0.00000	0.00000	0.92105
D20	-1.14310	0.00000	0.00001	0.00000	0.00000	-1.14310
D21	2.96619	0.00000	0.00001	0.00000	0.00000	2.96619
D22	3.13077	0.00000	0.00000	0.00000	0.00000	3.13077
D23	1.06662	0.00000	0.00001	0.00000	0.00000	1.06662
D24	-1.10728	0.00000	0.00001	0.00000	0.00000	-1.10727
D25	0.11643	0.00000	0.00001	0.00000	0.00001	0.11644
D26	-1.81788	0.00000	0.00000	0.00000	0.00000	-1.81787
D27	2.38435	0.00000	0.00000	0.00000	0.00000	2.38435
D28	1.92936	0.00000	0.00001	0.00000	0.00001	1.92937
D29	-0.00494	0.00000	0.00000	0.00000	0.00000	-0.00494
D30	-2.08590	0.00000	0.00000	0.00000	0.00000	-2.08590
D31	-2.19095	0.00000	0.00001	0.00000	0.00001	-2.19094
D32	2.15793	0.00000	0.00000	0.00000	0.00000	2.15793
D33	0.07698	0.00000	0.00000	0.00000	0.00000	0.07697
D34	-0.00325	0.00000	0.00000	0.00000	0.00000	-0.00325
D35	1.88766	0.00000	0.00000	0.00000	0.00000	1.88766
D36	-2.26267	0.00000	0.00000	0.00000	0.00000	-2.26267
D37	-1.88583	0.00000	0.00000	0.00000	0.00000	-1.88583
D38	0.00508	0.00000	0.00000	0.00000	0.00000	0.00508
D39	2.13794	0.00000	0.00000	0.00000	0.00000	2.13793
D40	2.25066	0.00000	0.00000	0.00000	0.00000	2.25066
D41	-2.14162	0.00000	0.00000	0.00000	0.00000	-2.14162
D42	-0.00876	0.00000	0.00000	0.00000	0.00000	-0.00876
D43	-0.57133	0.00000	-0.00001	0.00000	-0.00002	-0.57135
D44	2.48643	0.00000	-0.00005	0.00001	-0.00004	2.48639
D45	1.06815	0.00000	-0.00002	0.00000	-0.00002	1.06814
D46	-2.15727	0.00000	-0.00005	0.00001	-0.00004	-2.15731
D47	-2.89436	0.00000	-0.00001	0.00000	-0.00001	-2.89437
D48	0.16340	0.00000	-0.00004	0.00001	-0.00003	0.16336
D49	0.00497	0.00000	0.00000	0.00000	0.00000	0.00497
D50	1.83055	0.00000	0.00001	0.00000	0.00000	1.83055
D51	-2.16789	0.00000	0.00001	-0.00001	0.00000	-2.16789
D52	-1.80861	0.00000	0.00001	0.00000	0.00000	-1.80860
D53	0.01697	0.00000	0.00001	-0.00001	0.00001	0.01698
D54	2.30172	0.00000	0.00002	-0.00001	0.00001	2.30172
D55	2.15875	0.00000	0.00000	0.00000	0.00000	2.15874
D56	-2.29886	0.00000	0.00001	-0.00001	0.00000	-2.29886

D57	-0.01411	0.00000	0.00001	-0.00001	0.00000	-0.01412
D58	0.81575	0.00000	0.00001	0.00000	0.00001	0.81577
D59	-2.24210	0.00000	0.00004	-0.00001	0.00004	-2.24206
D60	3.00262	0.00000	0.00001	0.00000	0.00001	3.00263
D61	-0.05524	0.00000	0.00004	-0.00001	0.00003	-0.05520
D62	1.29642	0.00000	0.00000	0.00000	0.00000	1.29643
D63	-0.57918	0.00000	0.00000	0.00000	0.00000	-0.57917
D64	-2.84126	0.00000	0.00002	0.00000	0.00002	-2.84124
D65	-0.35812	0.00000	0.00000	0.00000	0.00000	-0.35812
D66	-2.23372	0.00000	0.00000	0.00000	0.00000	-2.23372
D67	1.78738	0.00000	0.00001	0.00000	0.00002	1.78740
D68	-2.68329	0.00000	0.00000	0.00000	0.00000	-2.68329
D69	1.72430	0.00000	0.00000	0.00000	0.00000	1.72430
D70	-0.53779	0.00000	0.00001	0.00000	0.00002	-0.53777
D71	-0.00497	0.00000	0.00000	0.00000	0.00000	-0.00497
D72	-1.85711	0.00000	0.00001	-0.00001	0.00001	-1.85710
D73	2.10688	0.00000	0.00000	0.00000	0.00000	2.10688
D74	1.80995	0.00000	0.00000	0.00000	0.00000	1.80996
D75	-0.04219	0.00000	0.00002	-0.00001	0.00001	-0.04218
D76	-2.36139	0.00000	0.00001	-0.00001	0.00000	-2.36138
D77	-2.16794	0.00000	0.00001	0.00000	0.00000	-2.16794
D78	2.26310	0.00000	0.00002	-0.00001	0.00001	2.26311
D79	-0.05610	0.00000	0.00001	0.00000	0.00001	-0.05609
D80	0.63125	0.00000	-0.00001	0.00000	-0.00001	0.63124
D81	2.83336	0.00000	0.00000	0.00000	0.00000	2.83336
D82	2.49511	0.00000	-0.00001	0.00000	-0.00001	2.49510
D83	-1.58596	0.00000	0.00000	0.00001	0.00000	-1.58596
D84	-1.52796	0.00000	-0.00001	-0.00001	-0.00002	-1.52798
D85	0.67415	0.00000	0.00000	-0.00001	-0.00001	0.67414
D86	0.92332	0.00000	0.00000	0.00000	0.00000	0.92331
D87	2.98603	0.00000	-0.00001	0.00001	0.00000	2.98602
D88	-1.12475	0.00000	-0.00001	0.00000	-0.00001	-1.12475
D89	-0.91838	0.00000	0.00000	0.00000	0.00000	-0.91838
D90	1.14433	0.00000	-0.00001	0.00000	-0.00001	1.14433
D91	-2.96644	0.00000	-0.00001	0.00000	-0.00001	-2.96644
D92	-3.13212	0.00000	-0.00002	0.00001	-0.00001	-3.13213
D93	-1.06941	0.00000	-0.00003	0.00002	-0.00001	-1.06942
D94	1.10300	0.00000	-0.00003	0.00002	-0.00001	1.10299
D95	-1.02295	0.00000	-0.00002	0.00001	-0.00002	-1.02297
D96	1.00346	0.00000	-0.00002	0.00001	-0.00001	1.00345
D97	3.13344	0.00000	-0.00001	0.00000	-0.00001	3.13343
D98	-0.69895	0.00000	0.00002	-0.00001	0.00002	-0.69894
D99	0.95125	0.00000	0.00003	0.00000	0.00003	0.95127
D100	2.78655	-0.00001	0.00006	0.00000	0.00006	2.78661
D101	-2.93519	0.00000	0.00002	-0.00001	0.00001	-2.93518
D102	-1.28499	0.00000	0.00002	0.00000	0.00002	-1.28498
D103	0.55031	0.00000	0.00005	0.00000	0.00005	0.55037
D104	-1.18379	0.00000	-0.00002	0.00001	-0.00001	-1.18381
D105	0.45375	0.00000	-0.00002	0.00001	-0.00001	0.45373
D106	2.81405	0.00000	-0.00002	0.00001	-0.00001	2.81403
D107	-3.03539	0.00000	-0.00006	0.00001	-0.00005	-3.03545
D108	-1.39785	0.00000	-0.00006	0.00001	-0.00005	-1.39791
D109	0.96244	-0.00001	-0.00006	0.00001	-0.00005	0.96239
D110	1.59002	0.00001	-0.00006	0.00000	-0.00006	1.58996

```
   D111      -3.05562   0.00001  -0.00006   0.00000  -0.00006  -3.05568
   D112      -0.69532   0.00001  -0.00006   0.00000  -0.00006  -0.69538
   D113      -0.39855   0.00000  -0.00002   0.00001  -0.00001  -0.39856
   D114       1.48034   0.00000  -0.00001   0.00001   0.00000   1.48034
   D115      -2.57840   0.00000  -0.00001   0.00000  -0.00001  -2.57841
   D116      -2.97321   0.00001  -0.00009  -0.00002  -0.00012  -2.97332
   D117       0.58593   0.00001  -0.00005  -0.00001  -0.00006   0.58587
   D118      -1.03363   0.00002  -0.00005  -0.00002  -0.00007  -1.03370
   D119      -0.32518   0.00000   0.00002  -0.00001   0.00001  -0.32517
   D120       1.97486   0.00000  -0.00223  -0.00004  -0.00227   1.97260
   D121      -2.75177   0.00000   0.00008  -0.00004   0.00005  -2.75172
   D122       0.93035   0.00000  -0.00005   0.00000  -0.00005   0.93031
         Item               Value     Threshold  Converged?
 Maximum Force            0.000036     0.000450     YES
 RMS     Force            0.000004     0.000300     YES
 Maximum Displacement     0.000518     0.001800     YES
 RMS     Displacement     0.000084     0.001200     YES
 Predicted change in Energy=-1.642989D-08
 Optimization completed.
    -- Stationary point found.
                          ----------------------------
                          !   Optimized Parameters   !
                          ! (Angstroms and Degrees)  !
 -------------------------                            --------------------
-----
 ! Name  Definition              Value          Derivative Info.
!
 ---------------------------------------------------------------------------
-----
 ! R1    R(1,2)                  1.5623         -DE/DX =    0.
!
 ! R2    R(1,4)                  1.5538         -DE/DX =    0.
!
 ! R3    R(1,11)                 1.5331         -DE/DX =    0.
!
 ! R4    R(1,16)                 1.0802         -DE/DX =    0.
!
 ! R5    R(2,3)                  1.5674         -DE/DX =    0.
!
 ! R6    R(2,6)                  1.5678         -DE/DX =    0.
!
 ! R7    R(2,17)                 1.0776         -DE/DX =    0.
!
 ! R8    R(3,5)                  1.5149         -DE/DX =    0.
!
 ! R9    R(3,10)                 1.6024         -DE/DX =    0.
!
 ! R10   R(3,18)                 1.0758         -DE/DX =    0.
!
 ! R11   R(4,5)                  1.5206         -DE/DX =    0.
!
 ! R12   R(4,19)                 1.0773         -DE/DX =    0.
!
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 ! R13   R(5,12)                1.2137         -DE/DX =    0.
!
 ! R14   R(6,7)                 1.5586         -DE/DX =    0.
!
 ! R15   R(6,10)                1.5597         -DE/DX =    0.
!
 ! R16   R(6,20)                1.0762         -DE/DX =    0.
!
 ! R17   R(7,8)                 1.5497         -DE/DX =    0.
!
 ! R18   R(7,11)                1.5344         -DE/DX =    0.
!
 ! R19   R(7,21)                1.0747         -DE/DX =    0.
!
 ! R20   R(8,9)                 1.492          -DE/DX =    0.
!
 ! R21   R(8,22)                1.0761         -DE/DX =    0.
!
 ! R22   R(9,10)                1.4935         -DE/DX =    0.
!
 ! R23   R(9,13)                2.4718         -DE/DX =    0.
!
 ! R24   R(9,15)                1.2737         -DE/DX =    0.
!
 ! R25   R(10,23)               1.0732         -DE/DX =    0.
!
 ! R26   R(11,24)               1.0838         -DE/DX =    0.
!
 ! R27   R(11,25)               1.0841         -DE/DX =    0.
!
 ! R28   R(13,14)               1.1642         -DE/DX =    0.
!
 ! R29   R(13,21)               2.8173         -DE/DX =    0.
!
 ! R30   R(15,28)               1.0571         -DE/DX =    0.
!
 ! R31   R(26,27)               0.9613         -DE/DX =    0.
!
 ! R32   R(26,28)               1.4222         -DE/DX =    0.
!
 ! R33   R(26,29)               0.9978         -DE/DX =    0.
!
 ! A1    A(2,1,4)             101.6417         -DE/DX =    0.
!
 ! A2    A(2,1,11)            103.0171         -DE/DX =    0.
!
 ! A3    A(2,1,16)            115.0691         -DE/DX =    0.
!
 ! A4    A(4,1,11)            104.0689         -DE/DX =    0.
!
 ! A5    A(4,1,16)            113.6257         -DE/DX =    0.
!
 ! A6    A(11,1,16)           117.5096         -DE/DX =    0.
!
```

```
 ! A7    A(1,2,3)              107.2029         -DE/DX =    0.
!
 ! A8    A(1,2,6)              102.9992         -DE/DX =    0.
!
 ! A9    A(1,2,17)             115.3406         -DE/DX =    0.
!
 ! A10   A(3,2,6)               90.7922         -DE/DX =    0.
!
 ! A11   A(3,2,17)             117.9741         -DE/DX =    0.
!
 ! A12   A(6,2,17)             119.1009         -DE/DX =    0.
!
 ! A13   A(2,3,5)              103.3942         -DE/DX =    0.
!
 ! A14   A(2,3,10)              88.9362         -DE/DX =    0.
!
 ! A15   A(2,3,18)             120.312          -DE/DX =    0.
!
 ! A16   A(5,3,10)             110.4949         -DE/DX =    0.
!
 ! A17   A(5,3,18)             114.9771         -DE/DX =    0.
!
 ! A18   A(10,3,18)            115.522          -DE/DX =    0.
!
 ! A19   A(1,4,5)              101.8445         -DE/DX =    0.
!
 ! A20   A(1,4,19)             115.8888         -DE/DX =    0.
!
 ! A21   A(5,4,19)             113.5212         -DE/DX =    0.
!
 ! A22   A(3,5,4)              104.6487         -DE/DX =    0.
!
 ! A23   A(3,5,12)             127.6202         -DE/DX =    0.
!
 ! A24   A(4,5,12)             127.5364         -DE/DX =    0.
!
 ! A25   A(2,6,7)              103.1622         -DE/DX =    0.
!
 ! A26   A(2,6,10)              90.4724         -DE/DX =    0.
!
 ! A27   A(2,6,20)             119.4599         -DE/DX =    0.
!
 ! A28   A(7,6,10)             107.729          -DE/DX =    0.
!
 ! A29   A(7,6,20)             115.2636         -DE/DX =    0.
!
 ! A30   A(10,6,20)            117.384          -DE/DX =    0.
!
 ! A31   A(6,7,8)              101.4249         -DE/DX =    0.
!
 ! A32   A(6,7,11)             103.117          -DE/DX =    0.
!
 ! A33   A(6,7,21)             114.7752         -DE/DX =    0.
!
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```
 ! A34   A(8,7,11)             103.9769         -DE/DX =    0.
!
 ! A35   A(8,7,21)             113.6261         -DE/DX =    0.
!
 ! A36   A(11,7,21)            117.9465         -DE/DX =    0.
!
 ! A37   A(7,8,9)              104.1249         -DE/DX =    0.
!
 ! A38   A(7,8,22)             116.7852         -DE/DX =    0.
!
 ! A39   A(9,8,22)             113.6391         -DE/DX =    0.
!
 ! A40   A(8,9,10)             107.0767         -DE/DX =    0.
!
 ! A41   A(8,9,13)             105.4513         -DE/DX =    0.
!
 ! A42   A(8,9,15)             122.0561         -DE/DX =    0.
!
 ! A43   A(10,9,13)             89.7048         -DE/DX =    0.
!
 ! A44   A(10,9,15)            127.3632         -DE/DX =    0.
!
 ! A45   A(13,9,15)             94.1383         -DE/DX =    0.
!
 ! A46   A(3,10,6)              89.7978         -DE/DX =    0.
!
 ! A47   A(3,10,9)             105.6727         -DE/DX =    0.
!
 ! A48   A(3,10,23)            116.437          -DE/DX =    0.
!
 ! A49   A(6,10,9)             104.1001         -DE/DX =    0.
!
 ! A50   A(6,10,23)            120.5764         -DE/DX =    0.
!
 ! A51   A(9,10,23)            116.3769         -DE/DX =    0.
!
 ! A52   A(1,11,7)              95.7001         -DE/DX =    0.
!
 ! A53   A(1,11,24)            113.1236         -DE/DX =    0.
!
 ! A54   A(1,11,25)            112.6234         -DE/DX =    0.
!
 ! A55   A(7,11,24)            113.2273         -DE/DX =    0.
!
 ! A56   A(7,11,25)            112.4152         -DE/DX =    0.
!
 ! A57   A(24,11,25)           109.2945         -DE/DX =    0.
!
 ! A58   A(9,13,21)             66.2527         -DE/DX =    0.
!
 ! A59   A(14,13,21)           168.7186         -DE/DX =    0.
!
 ! A60   A(9,15,28)            120.5498         -DE/DX =    0.
!
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```
 ! A61   A(7,21,13)            100.2643         -DE/DX =    0.
!
 ! A62   A(27,26,28)           133.0626         -DE/DX =    0.
!
 ! A63   A(27,26,29)           115.4647         -DE/DX =    0.
!
 ! A64   A(28,26,29)           106.2603         -DE/DX =    0.
!
 ! A65   L(15,28,26,29,-1)     163.5774         -DE/DX =    0.
!
 ! A66   L(9,13,14,21,-2)      228.2174         -DE/DX =    0.
!
 ! A67   L(15,28,26,29,-2)     180.8017         -DE/DX =    0.
!
 ! D1    D(4,1,2,3)             20.8726         -DE/DX =    0.
!
 ! D2    D(4,1,2,6)            -74.0798         -DE/DX =    0.
!
 ! D3    D(4,1,2,17)           154.4977         -DE/DX =    0.
!
 ! D4    D(11,1,2,3)           128.4726         -DE/DX =    0.
!
 ! D5    D(11,1,2,6)            33.5202         -DE/DX =    0.
!
 ! D6    D(11,1,2,17)          -97.9022         -DE/DX =    0.
!
 ! D7    D(16,1,2,3)          -102.3647         -DE/DX =    0.
!
 ! D8    D(16,1,2,6)           162.6829         -DE/DX =    0.
!
 ! D9    D(16,1,2,17)           31.2605         -DE/DX =    0.
!
 ! D10   D(2,1,4,5)            -40.5293         -DE/DX =    0.
!
 ! D11   D(2,1,4,19)          -164.2429         -DE/DX =    0.
!
 ! D12   D(11,1,4,5)          -147.3104         -DE/DX =    0.
!
 ! D13   D(11,1,4,19)           88.976          -DE/DX =    0.
!
 ! D14   D(16,1,4,5)            83.6864         -DE/DX =    0.
!
 ! D15   D(16,1,4,19)          -40.0273         -DE/DX =    0.
!
 ! D16   D(2,1,11,7)           -52.9784         -DE/DX =    0.
!
 ! D17   D(2,1,11,24)         -171.2457         -DE/DX =    0.
!
 ! D18   D(2,1,11,25)           64.1993         -DE/DX =    0.
!
 ! D19   D(4,1,11,7)            52.7724         -DE/DX =    0.
!
 ! D20   D(4,1,11,24)          -65.495          -DE/DX =    0.
!
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```
 ! D21   D(4,1,11,25)          169.9501         -DE/DX =    0.
!
 ! D22   D(16,1,11,7)          179.38           -DE/DX =    0.
!
 ! D23   D(16,1,11,24)          61.1127         -DE/DX =    0.
!
 ! D24   D(16,1,11,25)         -63.4423         -DE/DX =    0.
!
 ! D25   D(1,2,3,5)              6.6709         -DE/DX =    0.
!
 ! D26   D(1,2,3,10)          -104.1566         -DE/DX =    0.
!
 ! D27   D(1,2,3,18)           136.6133         -DE/DX =    0.
!
 ! D28   D(6,2,3,5)            110.5442         -DE/DX =    0.
!
 ! D29   D(6,2,3,10)            -0.2833         -DE/DX =    0.
!
 ! D30   D(6,2,3,18)          -119.5134         -DE/DX =    0.
!
 ! D31   D(17,2,3,5)          -125.5321         -DE/DX =    0.
!
 ! D32   D(17,2,3,10)          123.6404         -DE/DX =    0.
!
 ! D33   D(17,2,3,18)            4.4103         -DE/DX =    0.
!
 ! D34   D(1,2,6,7)             -0.1861         -DE/DX =    0.
!
 ! D35   D(1,2,6,10)           108.1548         -DE/DX =    0.
!
 ! D36   D(1,2,6,20)          -129.6415         -DE/DX =    0.
!
 ! D37   D(3,2,6,7)           -108.0499         -DE/DX =    0.
!
 ! D38   D(3,2,6,10)             0.291          -DE/DX =    0.
!
 ! D39   D(3,2,6,20)           122.4947         -DE/DX =    0.
!
 ! D40   D(17,2,6,7)           128.9535         -DE/DX =    0.
!
 ! D41   D(17,2,6,10)         -122.7056         -DE/DX =    0.
!
 ! D42   D(17,2,6,20)           -0.5019         -DE/DX =    0.
!
 ! D43   D(2,3,5,4)            -32.7348         -DE/DX =    0.
!
 ! D44   D(2,3,5,12)           142.4619         -DE/DX =    0.
!
 ! D45   D(10,3,5,4)            61.2007         -DE/DX =    0.
!
 ! D46   D(10,3,5,12)         -123.6026         -DE/DX =    0.
!
 ! D47   D(18,3,5,4)          -165.8348         -DE/DX =    0.
!
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 ! D48   D(18,3,5,12)            9.3619         -DE/DX =    0.
!
 ! D49   D(2,3,10,6)              0.2847         -DE/DX =    0.
!
 ! D50   D(2,3,10,9)            104.8827         -DE/DX =    0.
!
 ! D51   D(2,3,10,23)          -124.211          -DE/DX =    0.
!
 ! D52   D(5,3,10,6)           -103.6257         -DE/DX =    0.
!
 ! D53   D(5,3,10,9)              0.9723         -DE/DX =    0.
!
 ! D54   D(5,3,10,23)           131.8786         -DE/DX =    0.
!
 ! D55   D(18,3,10,6)           123.687          -DE/DX =    0.
!
 ! D56   D(18,3,10,9)          -131.715          -DE/DX =    0.
!
 ! D57   D(18,3,10,23)           -0.8087         -DE/DX =    0.
!
 ! D58   D(1,4,5,3)              46.7392         -DE/DX =    0.
!
 ! D59   D(1,4,5,12)           -128.4629         -DE/DX =    0.
!
 ! D60   D(19,4,5,3)            172.0374         -DE/DX =    0.
!
 ! D61   D(19,4,5,12)            -3.1647         -DE/DX =    0.
!
 ! D62   D(2,6,7,8)              74.2795         -DE/DX =    0.
!
 ! D63   D(2,6,7,11)            -33.1844         -DE/DX =    0.
!
 ! D64   D(2,6,7,21)           -162.7923         -DE/DX =    0.
!
 ! D65   D(10,6,7,8)            -20.519          -DE/DX =    0.
!
 ! D66   D(10,6,7,11)          -127.9829         -DE/DX =    0.
!
 ! D67   D(10,6,7,21)           102.4092         -DE/DX =    0.
!
 ! D68   D(20,6,7,8)           -153.7411         -DE/DX =    0.
!
 ! D69   D(20,6,7,11)            98.795          -DE/DX =    0.
!
 ! D70   D(20,6,7,21)           -30.8129         -DE/DX =    0.
!
 ! D71   D(2,6,10,3)             -0.2846         -DE/DX =    0.
!
 ! D72   D(2,6,10,9)           -106.4045         -DE/DX =    0.
!
 ! D73   D(2,6,10,23)           120.7153         -DE/DX =    0.
!
 ! D74   D(7,6,10,3)            103.7027         -DE/DX =    0.
!
```

```
 ! D75   D(7,6,10,9)            -2.4172         -DE/DX =    0.
!
 ! D76   D(7,6,10,23)         -135.2974         -DE/DX =    0.
!
 ! D77   D(20,6,10,3)         -124.214          -DE/DX =    0.
!
 ! D78   D(20,6,10,9)          129.6661         -DE/DX =    0.
!
 ! D79   D(20,6,10,23)          -3.2141         -DE/DX =    0.
!
 ! D80   D(6,7,8,9)             36.1679         -DE/DX =    0.
!
 ! D81   D(6,7,8,22)           162.3395         -DE/DX =    0.
!
 ! D82   D(11,7,8,9)           142.9595         -DE/DX =    0.
!
 ! D83   D(11,7,8,22)          -90.8688         -DE/DX =    0.
!
 ! D84   D(21,7,8,9)           -87.5459         -DE/DX =    0.
!
 ! D85   D(21,7,8,22)           38.6258         -DE/DX =    0.
!
 ! D86   D(6,7,11,1)            52.9021         -DE/DX =    0.
!
 ! D87   D(6,7,11,24)          171.0867         -DE/DX =    0.
!
 ! D88   D(6,7,11,25)          -64.4432         -DE/DX =    0.
!
 ! D89   D(8,7,11,1)           -52.6191         -DE/DX =    0.
!
 ! D90   D(8,7,11,24)           65.5656         -DE/DX =    0.
!
 ! D91   D(8,7,11,25)         -169.9643         -DE/DX =    0.
!
 ! D92   D(21,7,11,1)         -179.4573         -DE/DX =    0.
!
 ! D93   D(21,7,11,24)         -61.2726         -DE/DX =    0.
!
 ! D94   D(21,7,11,25)          63.1975         -DE/DX =    0.
!
 ! D95   D(6,7,21,13)          -58.6109         -DE/DX =    0.
!
 ! D96   D(8,7,21,13)           57.494          -DE/DX =    0.
!
 ! D97   D(11,7,21,13)         179.5326         -DE/DX =    0.
!
 ! D98   D(7,8,9,10)           -40.0471         -DE/DX =    0.
!
 ! D99   D(7,8,9,13)            54.5024         -DE/DX =    0.
!
 ! D100  D(7,8,9,15)           159.6577         -DE/DX =    0.
!
 ! D101  D(22,8,9,10)         -168.1741         -DE/DX =    0.
!
```

```
 ! D102  D(22,8,9,13)          -73.6246         -DE/DX =    0.
!
 ! D103  D(22,8,9,15)           31.5306         -DE/DX =    0.
!
 ! D104  D(8,9,10,3)           -67.8264         -DE/DX =    0.
!
 ! D105  D(8,9,10,6)            25.9979         -DE/DX =    0.
!
 ! D106  D(8,9,10,23)          161.2329         -DE/DX =    0.
!
 ! D107  D(13,9,10,3)         -173.9153         -DE/DX =    0.
!
 ! D108  D(13,9,10,6)          -80.091          -DE/DX =    0.
!
 ! D109  D(13,9,10,23)          55.144          -DE/DX =    0.
!
 ! D110  D(15,9,10,3)           91.1016         -DE/DX =    0.
!
 ! D111  D(15,9,10,6)         -175.0741         -DE/DX =    0.
!
 ! D112  D(15,9,10,23)         -39.8391         -DE/DX =    0.
!
 ! D113  D(8,9,13,21)          -22.8352         -DE/DX =    0.
!
 ! D114  D(10,9,13,21)          84.8174         -DE/DX =    0.
!
 ! D115  D(15,9,13,21)        -147.7313         -DE/DX =    0.
!
 ! D116  D(8,9,15,28)         -170.3523         -DE/DX =    0.
!
 ! D117  D(10,9,15,28)          33.5714         -DE/DX =    0.
!
 ! D118  D(13,9,15,28)         -59.2226         -DE/DX =    0.
!
 ! D119  D(9,13,21,7)          -18.6312         -DE/DX =    0.
!
 ! D120  D(14,13,21,7)         113.1514         -DE/DX =    0.
!
 ! D121  D(9,15,26,27)        -157.6647         -DE/DX =    0.
!
 ! D122  D(9,15,26,29)          53.3054         -DE/DX =    0.
!
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 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.914380   -0.271354    1.721772
    2          6             0       -1.496997    1.143876    1.208317
    3          6             0       -1.411895    1.063439   -0.354696
```

4	6	0	-1.512635	-1.171656	0.520841
5	6	0	-1.942520	-0.321340	-0.664238
6	6	0	0.066720	1.111387	1.316867
7	6	0	0.353727	-0.312416	1.882192
8	6	0	0.090102	-1.196113	0.636711
9	6	0	0.588343	-0.374517	-0.504746
10	6	0	0.185936	1.038536	-0.236583
11	6	0	-0.856107	-0.577902	2.787759
12	8	0	-2.638455	-0.655875	-1.600689
13	6	0	2.924836	0.196179	0.065110
14	7	0	3.644592	0.641005	-0.734613
15	8	0	0.891532	-0.891880	-1.628410
16	1	0	-2.951941	-0.367252	2.006674
17	1	0	-2.035529	1.969712	1.643409
18	1	0	-1.819555	1.852364	-0.961991
19	1	0	-1.934464	-2.162926	0.514274
20	1	0	0.579502	1.915537	1.815517
21	1	0	1.334775	-0.441076	2.301756
22	1	0	0.490849	-2.194653	0.656947
23	1	0	0.717053	1.796763	-0.779509
24	1	0	-0.901795	-1.597687	3.151992
25	1	0	-0.900982	0.105101	3.628473
26	8	0	2.308818	0.508124	-3.062110
27	1	0	2.531734	0.607679	-3.991932
28	1	0	1.382662	-0.318967	-2.368720
29	1	0	3.049607	0.696705	-2.420757

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.562280	0.000000			
3	C	2.519104	1.567394	0.000000		
4	C	1.553763	2.415483	2.402575	0.000000	
5	C	2.386699	2.419052	1.514923	1.520608	0.000000
6	C	2.449628	1.567816	2.232201	2.887959	3.164573
7	C	2.274145	2.449504	3.164501	2.464728	3.428868
8	C	2.459774	2.884643	2.888678	1.607107	2.566953
9	C	3.351365	3.096570	2.468033	2.470095	2.536440
10	C	3.156311	2.220607	1.602384	2.888561	2.561733
11	C	1.533050	2.422787	3.588583	2.433617	3.628002
12	O	3.422117	3.525982	2.452140	2.456499	1.213746
13	C	5.136256	4.664510	4.442478	4.665813	4.948830
14	N	6.145600	5.519402	5.088305	5.608824	5.669822
15	O	4.413832	4.230412	3.278932	3.236908	3.047457
16	H	1.080231	2.244492	3.161438	2.219542	2.855662
17	H	2.245706	1.077649	2.280937	3.376651	3.253122
18	H	3.423704	2.305697	1.075823	3.381965	2.197445
19	H	2.244214	3.407053	3.381955	1.077311	2.186411
20	H	3.318242	2.296955	3.066196	3.947656	4.184901
21	H	3.304875	3.424415	4.106641	3.437027	4.421778
22	H	3.258537	3.924451	3.906280	2.253663	3.343069
23	H	4.178272	3.046265	2.291429	3.933692	3.401907
24	H	2.197730	3.412961	4.431553	2.734518	4.156414
25	H	2.191850	2.700267	4.128569	3.414910	4.437794

26	O	6.428726	5.755429	4.634886	5.501155	4.950927
27	H	7.292945	6.600058	5.384181	6.315700	5.652926
28	H	5.254034	4.819496	3.711723	4.178443	3.736589
29	H	6.537496	5.834531	4.930325	5.740891	5.389166
		6	7	8	9	10
6	C	0.000000				
7	C	1.558582	0.000000			
8	C	2.405767	1.549723	0.000000		
9	C	2.407961	2.399245	1.492041	0.000000	
10	C	1.559720	2.518419	2.401142	1.493507	0.000000
11	C	2.422567	1.534352	2.429919	3.601165	3.584045
12	O	4.353541	4.604517	3.569711	3.419426	3.564968
13	C	3.251665	3.189209	3.209504	2.471766	2.881346
14	N	4.151025	4.311203	4.229649	3.228743	3.516869
15	O	3.656234	3.598519	2.421904	1.273659	2.482247
16	H	3.431402	3.308466	3.437708	4.340610	4.105450
17	H	2.294080	3.312653	3.943881	4.122461	3.055547
18	H	3.049635	4.183157	3.936477	3.311502	2.282658
19	H	3.920461	3.245213	2.246906	3.255974	3.912703
20	H	1.076223	2.240356	3.363252	3.260068	2.266085
21	H	2.233409	1.074729	2.211711	2.904831	3.154719
22	H	3.397835	2.250077	1.076146	2.161465	3.368216
23	H	2.299449	3.415449	3.369874	2.192377	1.073201
24	H	3.412446	2.200148	2.733453	4.133811	4.428914
25	H	2.700477	2.190459	3.409699	4.419459	4.122057
26	O	4.956448	5.379757	4.637715	3.206119	3.573733
27	H	5.874807	6.332110	5.535301	4.111197	4.448713
28	H	4.166674	4.373671	3.387139	2.026925	2.796601
29	H	4.799939	5.177013	4.657203	3.297944	3.617745
		11	12	13	14	15
11	C	0.000000				
12	O	4.737227	0.000000			
13	C	4.723087	5.869505	0.000000		
14	N	5.843726	6.473690	1.164249	0.000000	
15	O	4.759766	3.537976	2.861154	3.275355	0.000000
16	H	2.246551	3.632443	6.214791	7.214256	5.316141
17	H	3.031652	4.216799	5.499242	6.299542	5.240343
18	H	4.571111	2.714736	5.129047	5.601428	3.914713
19	H	2.973868	2.690701	5.420325	6.367701	3.767347
20	H	3.037017	5.351436	3.394216	4.185973	4.454164
21	H	2.248307	5.573309	2.817263	3.965563	3.980690
22	H	2.994751	4.154190	3.462751	4.463574	2.660943
23	H	4.565005	4.236650	2.854743	3.147742	2.824867
24	H	1.083842	5.146938	5.233536	6.386477	5.154263
25	H	1.084116	5.562556	5.229027	6.323445	5.642862
26	O	6.739227	5.288304	3.202545	2.686856	2.454426
27	H	7.671198	5.834849	4.096761	3.442338	3.244253
28	H	5.627469	4.107646	2.926979	2.950963	1.057117
29	H	6.633843	5.903900	2.538825	1.788908	2.794406
		16	17	18	19	20
16	H	0.000000				
17	H	2.536370	0.000000			
18	H	3.875818	2.616969	0.000000		
19	H	2.546951	4.285307	4.279616	0.000000	

20	H	4.209366	2.621249	3.670697	4.964587	0.000000
21	H	4.297495	4.195745	5.085441	4.104605	2.522002
22	H	4.124798	4.969671	4.933282	2.429713	4.271277
23	H	5.089921	3.671124	2.543771	4.937971	2.601381
24	H	2.651193	4.035779	5.447017	2.888505	4.040192
25	H	2.657026	2.950331	4.996905	3.988768	2.959108
26	O	7.357611	6.568981	4.822960	6.158772	5.363077
27	H	8.185625	7.380521	5.446420	6.923082	6.264835
28	H	6.159154	5.746239	4.116765	4.766043	4.811020
29	H	7.533441	6.632994	5.212704	6.452353	5.053018

		21	22	23	24	25
21	H	0.000000				
22	H	2.548066	0.000000			
23	H	3.857940	4.248056	0.000000		
24	H	2.657611	2.919089	5.440557	0.000000	
25	H	2.656520	4.006998	4.990998	1.768197	0.000000
26	O	5.533607	4.943824	3.066689	7.304625	7.431631
27	H	6.491772	5.799168	3.876422	8.227297	8.372974
28	H	4.672317	3.669903	2.728542	6.110003	6.431266
29	H	5.151439	4.937556	3.056900	7.206480	7.249161

		26	27	28	29
26	O	0.000000			
27	H	0.961338	0.000000		
28	H	1.422194	2.194050	0.000000	
29	H	0.997830	1.656716	1.952692	0.000000

Stoichiometry C12H13NO3
Framework group C1[X(C12H13NO3)]
Deg. of freedom 81
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.572698	-0.288596	-0.030360
2	6	0	-1.790011	-0.245400	1.321030
3	6	0	-0.826952	0.989702	1.259683
4	6	0	-1.648230	0.550713	-0.955076
5	6	0	-1.222888	1.679740	-0.029532
6	6	0	-0.590003	-1.221326	1.064909
7	6	0	-0.833216	-1.707155	-0.395912
8	6	0	-0.420014	-0.454193	-1.208926
9	6	0	0.728605	0.113489	-0.444335
10	6	0	0.395950	-0.014197	1.006044
11	6	0	-2.363523	-1.731371	-0.504586
12	8	0	-1.280644	2.873044	-0.243705
13	6	0	2.351103	-1.737925	-0.222082
14	7	0	3.442273	-1.538521	0.131560
15	8	0	1.568768	0.908467	-0.977574
16	1	0	-3.587345	0.079102	0.016410
17	1	0	-2.390789	-0.374473	2.206318
18	1	0	-0.723694	1.640487	2.110101

19	1	0	-2.089815	0.893086	-1.876153
20	1	0	-0.378536	-1.998856	1.778340
21	1	0	-0.294650	-2.595719	-0.670581
22	1	0	-0.211822	-0.601423	-2.254426
23	1	0	1.218921	0.052436	1.691638
24	1	0	-2.717667	-1.903059	-1.514446
25	1	0	-2.813793	-2.458687	0.161429
26	8	0	3.690858	1.134821	0.234740
27	1	0	4.418710	1.757062	0.319688
28	1	0	2.453934	1.177070	-0.465881
29	1	0	3.940049	0.171080	0.303827

Rotational constants (GHZ): 0.9148638 0.4991978 0.3975386
Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,O-16,C-12,N-14,
O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,O-16,H-1,H-1,H-1

****

Population analysis using the SCF density.

****

Alpha occ. eigenvalues -- -20.56489 -20.51970 -20.51294 -15.43460 -11.38021
Alpha occ. eigenvalues -- -11.31963 -11.23733 -11.23532 -11.23247 -11.23161
Alpha occ. eigenvalues -- -11.22032 -11.21972 -11.21642 -11.21032 -11.19886
Alpha occ. eigenvalues -- -11.13718 -1.49705 -1.44227 -1.38935 -1.28253
Alpha occ. eigenvalues -- -1.17615 -1.13551 -1.10848 -1.08434 -0.95931
Alpha occ. eigenvalues -- -0.94570 -0.92920 -0.86073 -0.83022 -0.79330
Alpha occ. eigenvalues -- -0.77394 -0.76869 -0.75561 -0.71012 -0.70343
Alpha occ. eigenvalues -- -0.67849 -0.67196 -0.65735 -0.64902 -0.62952
Alpha occ. eigenvalues -- -0.61016 -0.58607 -0.56668 -0.55996 -0.55246
Alpha occ. eigenvalues -- -0.54240 -0.53004 -0.51816 -0.51556 -0.50218
Alpha occ. eigenvalues -- -0.49396 -0.48940 -0.47483 -0.45884 -0.41706
Alpha occ. eigenvalues -- -0.41441 -0.40877 -0.39564
Alpha virt. eigenvalues -- 0.04855 0.05578 0.06524 0.07180 0.07832
Alpha virt. eigenvalues -- 0.08741 0.08965 0.09443 0.09997 0.10362
Alpha virt. eigenvalues -- 0.10847 0.12181 0.12318 0.13428 0.13631
Alpha virt. eigenvalues -- 0.14357 0.14497 0.15292 0.16896 0.17417

```
 Alpha virt. eigenvalues --    0.17773   0.17989   0.18810   0.19179
0.19346
 Alpha virt. eigenvalues --    0.19748   0.19969   0.21189   0.22317
0.23134
 Alpha virt. eigenvalues --    0.23215   0.23805   0.24155   0.24201
0.24715
 Alpha virt. eigenvalues --    0.25159   0.25743   0.26276   0.26610
0.27006
 Alpha virt. eigenvalues --    0.27593   0.27704   0.28443   0.28680
0.28920
 Alpha virt. eigenvalues --    0.29493   0.29807   0.30508   0.31065
0.31609
 Alpha virt. eigenvalues --    0.32525   0.32828   0.33094   0.34409
0.35007
 Alpha virt. eigenvalues --    0.35702   0.37002   0.37059   0.37946
0.38387
 Alpha virt. eigenvalues --    0.39300   0.40199   0.40660   0.41266
0.41520
 Alpha virt. eigenvalues --    0.42483   0.43130   0.43506   0.44873
0.45637
 Alpha virt. eigenvalues --    0.45787   0.46156   0.47230   0.47412
0.48477
 Alpha virt. eigenvalues --    0.48689   0.49239   0.50009   0.51231
0.51696
 Alpha virt. eigenvalues --    0.52915   0.53520   0.54741   0.55638
0.57229
 Alpha virt. eigenvalues --    0.57928   0.58577   0.59165   0.59885
0.60586
 Alpha virt. eigenvalues --    0.61609   0.62868   0.63262   0.64552
0.65413
 Alpha virt. eigenvalues --    0.66748   0.70551   0.77542   0.83906
1.06713
 Alpha virt. eigenvalues --    1.08273   1.10122   1.10918   1.12073
1.12968
 Alpha virt. eigenvalues --    1.14019   1.14631   1.15713   1.16168
1.17070
 Alpha virt. eigenvalues --    1.17718   1.18689   1.19034   1.19309
1.20598
 Alpha virt. eigenvalues --    1.21398   1.22897   1.24011   1.25067
1.26551
 Alpha virt. eigenvalues --    1.27977   1.31593   1.32077   1.32777
1.35616
 Alpha virt. eigenvalues --    1.37417   1.39352   1.42393   1.45279
1.47452
 Alpha virt. eigenvalues --    1.48397   1.49563   1.50823   1.51765
1.51841
 Alpha virt. eigenvalues --    1.53009   1.55286   1.56395   1.57138
1.58360
 Alpha virt. eigenvalues --    1.61908   1.64176   1.69719   1.71297
1.72429
 Alpha virt. eigenvalues --    1.75367   1.77402   1.77778   1.84383
1.92483
 Alpha virt. eigenvalues --    1.95406   1.98889   2.00518   2.05804
2.09390
```

```
 Alpha virt. eigenvalues --    2.13408   2.13908   2.17701   2.20487
2.21237
 Alpha virt. eigenvalues --    2.25370   2.29055   2.31186   2.38595
2.46589
 Alpha virt. eigenvalues --    2.54689   2.57904   2.88068   2.95819
2.99499
 Alpha virt. eigenvalues --    3.16507   3.38141   3.48570   3.74649
3.90459
 Alpha virt. eigenvalues --    4.02984
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   14.965090  -8.912957   4.403164  -5.117663  -1.852259   6.174978
  2  C   -8.912957  23.369302 -12.349188   2.954390   5.255634 -14.335569
  3  C    4.403164 -12.349188  24.247595   2.515548 -13.120176   9.443171
  4  C   -5.117663   2.954390   2.515548  18.710939 -10.713172  -3.171266
  5  C   -1.852259   5.255634 -13.120176 -10.713172  28.589011  -2.786332
  6  C    6.174978 -14.335569   9.443171  -3.171266  -2.786332  25.388425
  7  C   -2.506977   4.470267  -1.532709   4.186291  -0.525115  -8.530773
  8  C    4.725233  -3.514302  -1.278110 -12.064913   8.231926   5.332835
  9  C   -0.718769  -1.310079   5.966204   9.256136 -11.804476   0.525525
 10  C   -2.346169   9.297718 -12.863353  -2.190549   6.057521 -11.924544
 11  C   -4.092801   2.031504  -0.669865   0.556576   0.536336  -1.152977
 12  O    0.042955  -0.228167   0.501775   0.365738  -0.678651   0.114093
 13  C    0.362083  -0.630389   0.360397  -0.321679  -0.129723   0.845283
 14  N   -0.036707   0.059713  -0.029466   0.058536  -0.020967  -0.105284
 15  O    0.036404  -0.062281  -0.037770  -0.151709   0.074540   0.113323
 16  H    0.476930  -0.066045  -0.000361  -0.130783   0.030937   0.014942
 17  H   -0.079923   0.551061  -0.130490   0.004339   0.025810  -0.109070
 18  H    0.029447  -0.094420   0.486725  -0.019188  -0.017030   0.058448
 19  H   -0.025509  -0.003511   0.012706   0.474739  -0.057753   0.012361
 20  H   -0.006225  -0.090499   0.070543   0.004235   0.003399   0.498336
 21  H   -0.054137   0.056374  -0.012892   0.057033   0.005386  -0.103085
 22  H   -0.000391   0.011413  -0.026360  -0.108786   0.062056   0.004010
 23  H    0.001035   0.012017  -0.043410  -0.008309   0.019968  -0.009792
 24  H   -0.051954   0.009199   0.006466   0.010564  -0.013756   0.047410
 25  H   -0.044076  -0.016018  -0.001366   0.018417   0.001296   0.033631
 26  O    0.006636  -0.017609  -0.012834  -0.016475   0.024890   0.030706
 27  H   -0.000158   0.000527   0.000075   0.000324  -0.000197  -0.002024
 28  H   -0.000141   0.007476   0.000881  -0.002205  -0.004253  -0.027779
 29  H   -0.000135   0.000773  -0.000132   0.000754  -0.001945  -0.000127
               7          8          9         10         11         12
  1  C   -2.506977   4.725233  -0.718769  -2.346169  -4.092801   0.042955
  2  C    4.470267  -3.514302  -1.310079   9.297718   2.031504  -0.228167
  3  C   -1.532709  -1.278110   5.966204 -12.863353  -0.669865   0.501775
  4  C    4.186291 -12.064913   9.256136  -2.190549   0.556576   0.365738
  5  C   -0.525115   8.231926 -11.804476   6.057521   0.536336  -0.678651
  6  C   -8.530773   5.332835   0.525525 -11.924544  -1.152977   0.114093
  7  C   17.927011 -11.769596   7.564569   0.898814  -4.254689  -0.045372
  8  C  -11.769596  51.753746 -46.839635  10.539330  -0.982653   0.105043
  9  C    7.564569 -46.839635  70.563657 -24.085316  -0.181555  -0.213027
 10  C    0.898814  10.539330 -24.085316  30.545035   0.279139  -0.008520
 11  C   -4.254689  -0.982653  -0.181555   0.279139  16.018645   0.000169
 12  O   -0.045372   0.105043  -0.213027  -0.008520   0.000169   8.621365
 13  C   -1.011515   2.225134  -3.471371   1.006893  -0.449301   0.010975
```

14	N	0.086535	-0.239777	0.312551	-0.019188	0.034389	-0.000119
15	O	-0.346001	1.607174	-2.063626	0.591144	-0.007779	0.019457
16	H	-0.019307	0.024100	0.015309	-0.010312	0.014842	0.000122
17	H	-0.005456	0.015096	-0.011162	0.078411	0.025901	0.000373
18	H	-0.009527	0.031655	-0.062419	-0.045305	0.000598	-0.004720
19	H	0.001298	-0.061990	-0.026527	0.003741	0.020443	-0.001263
20	H	-0.083412	0.054989	-0.035460	-0.079905	0.029198	-0.000044
21	H	0.474332	-0.064930	-0.047795	0.021865	0.016709	-0.000010
22	H	-0.061348	0.653659	-0.279698	0.071349	0.015248	0.000144
23	H	-0.013463	0.100047	-0.219591	0.501983	0.001360	0.000687
24	H	-0.070445	0.067132	-0.026085	0.002630	0.332399	0.000150
25	H	-0.086033	0.066696	-0.011475	-0.000173	0.353741	-0.000036
26	O	-0.034018	-0.070292	-0.000701	-0.000230	-0.004126	-0.001147
27	H	0.000639	0.009107	0.008753	-0.001035	0.000058	0.000016
28	H	0.010839	0.037393	-0.039156	0.032502	0.001006	0.000369
29	H	0.002042	-0.013004	0.043800	-0.019330	0.000156	-0.000005

		13	14	15	16	17	18
1	C	0.362083	-0.036707	0.036404	0.476930	-0.079923	0.029447
2	C	-0.630389	0.059713	-0.062281	-0.066045	0.551061	-0.094420
3	C	0.360397	-0.029466	-0.037770	-0.000361	-0.130490	0.486725
4	C	-0.321679	0.058536	-0.151709	-0.130783	0.004339	-0.019188
5	C	-0.129723	-0.020967	0.074540	0.030937	0.025810	-0.017030
6	C	0.845283	-0.105284	0.113323	0.014942	-0.109070	0.058448
7	C	-1.011515	0.086535	-0.346001	-0.019307	-0.005456	-0.009527
8	C	2.225134	-0.239777	1.607174	0.024100	0.015096	0.031655
9	C	-3.471371	0.312551	-2.063626	0.015309	-0.011162	-0.062419
10	C	1.006893	-0.019188	0.591144	-0.010312	0.078411	-0.045305
11	C	-0.449301	0.034389	-0.007779	0.014842	0.025901	0.000598
12	O	0.010975	-0.000119	0.019457	0.000122	0.000373	-0.004720
13	C	6.974704	0.142781	0.215990	-0.000755	0.000218	-0.000314
14	N	0.142781	7.512097	-0.010540	0.000002	0.000000	0.000018
15	O	0.215990	-0.010540	8.641611	-0.000072	-0.000001	0.002754
16	H	-0.000755	0.000002	-0.000072	0.366936	-0.000735	-0.000006
17	H	0.000218	0.000000	-0.000001	-0.000735	0.354712	-0.000204
18	H	-0.000314	0.000018	0.002754	-0.000006	-0.000204	0.335132
19	H	-0.000001	-0.000002	0.002139	-0.000278	-0.000009	-0.000007
20	H	-0.001056	0.000969	0.000381	-0.000008	-0.000495	-0.000067
21	H	0.000195	-0.001516	0.000368	-0.000017	-0.000008	0.000000
22	H	0.002167	0.000199	0.008095	-0.000002	0.000000	-0.000001
23	H	0.004317	-0.002101	0.003732	0.000000	-0.000026	-0.000938
24	H	0.001746	-0.000010	0.000078	-0.000258	-0.000023	0.000000
25	H	0.001978	-0.000008	0.000023	-0.000417	0.000218	0.000000
26	O	0.041353	-0.070006	-0.066403	0.000000	0.000000	-0.000064
27	H	-0.004164	0.002824	0.002604	0.000000	0.000000	0.000000
28	H	-0.017642	-0.003738	0.161248	0.000000	0.000000	-0.000003
29	H	-0.022324	0.065342	0.001107	0.000000	0.000000	0.000000

		19	20	21	22	23	24
1	C	-0.025509	-0.006225	-0.054137	-0.000391	0.001035	-0.051954
2	C	-0.003511	-0.090499	0.056374	0.011413	0.012017	0.009199
3	C	0.012706	0.070543	-0.012892	-0.026360	-0.043410	0.006466
4	C	0.474739	0.004235	0.057033	-0.108786	-0.008309	0.010564
5	C	-0.057753	0.003399	0.005386	0.062056	0.019968	-0.013756
6	C	0.012361	0.498336	-0.103085	0.004010	-0.009792	0.047410
7	C	0.001298	-0.083412	0.474332	-0.061348	-0.013463	-0.070445

8	C	-0.061990	0.054989	-0.064930	0.653659	0.100047	0.067132
9	C	-0.026527	-0.035460	-0.047795	-0.279698	-0.219591	-0.026085
10	C	0.003741	-0.079905	0.021865	0.071349	0.501983	0.002630
11	C	0.020443	0.029198	0.016709	0.015248	0.001360	0.332399
12	O	-0.001263	-0.000044	-0.000010	0.000144	0.000687	0.000150
13	C	-0.000001	-0.001056	0.000195	0.002167	0.004317	0.001746
14	N	-0.000002	0.000969	-0.001516	0.000199	-0.002101	-0.000010
15	O	0.002139	0.000381	0.000368	0.008095	0.003732	0.000078
16	H	-0.000278	-0.000008	-0.000017	-0.000002	0.000000	-0.000258
17	H	-0.000009	-0.000495	-0.000008	0.000000	-0.000026	-0.000023
18	H	-0.000007	-0.000067	0.000000	-0.000001	-0.000938	0.000000
19	H	0.339708	0.000000	-0.000011	-0.000672	-0.000001	0.000143
20	H	0.000000	0.346349	-0.000161	-0.000007	-0.000128	-0.000026
21	H	-0.000011	-0.000161	0.323516	0.000370	0.000006	-0.000183
22	H	-0.000672	-0.000007	0.000370	0.325360	-0.000005	-0.000007
23	H	-0.000001	-0.000128	0.000006	-0.000005	0.313429	0.000000
24	H	0.000143	-0.000026	-0.000183	-0.000007	0.000000	0.425760
25	H	-0.000038	0.000114	-0.000303	-0.000028	0.000000	-0.014741
26	O	0.000002	-0.000013	0.000020	-0.000014	0.002988	0.000000
27	H	0.000000	0.000000	0.000000	0.000000	0.000002	0.000000
28	H	0.000001	0.000002	0.000000	-0.000017	-0.000308	0.000000
29	H	0.000000	0.000000	0.000000	0.000000	-0.000242	0.000000

		25	26	27	28	29
1	C	-0.044076	0.006636	-0.000158	-0.000141	-0.000135
2	C	-0.016018	-0.017609	0.000527	0.007476	0.000773
3	C	-0.001366	-0.012834	0.000075	0.000881	-0.000132
4	C	0.018417	-0.016475	0.000324	-0.002205	0.000754
5	C	0.001296	0.024890	-0.000197	-0.004253	-0.001945
6	C	0.033631	0.030706	-0.002024	-0.027779	-0.000127
7	C	-0.086033	-0.034018	0.000639	0.010839	0.002042
8	C	0.066696	-0.070292	0.009107	0.037393	-0.013004
9	C	-0.011475	-0.000701	0.008753	-0.039156	0.043800
10	C	-0.000173	-0.000230	-0.001035	0.032502	-0.019330
11	C	0.353741	-0.004126	0.000058	0.001006	0.000156
12	O	-0.000036	-0.001147	0.000016	0.000369	-0.000005
13	C	0.001978	0.041353	-0.004164	-0.017642	-0.022324
14	N	-0.000008	-0.070006	0.002824	-0.003738	0.065342
15	O	0.000023	-0.066403	0.002604	0.161248	0.001107
16	H	-0.000417	0.000000	0.000000	0.000000	0.000000
17	H	0.000218	0.000000	0.000000	0.000000	0.000000
18	H	0.000000	-0.000064	0.000000	-0.000003	0.000000
19	H	-0.000038	0.000002	0.000000	0.000001	0.000000
20	H	0.000114	-0.000013	0.000000	0.000002	0.000000
21	H	-0.000303	0.000020	0.000000	0.000000	0.000000
22	H	-0.000028	-0.000014	0.000000	-0.000017	0.000000
23	H	0.000000	0.002988	0.000002	-0.000308	-0.000242
24	H	-0.014741	0.000000	0.000000	0.000000	0.000000
25	H	0.421467	0.000000	0.000000	0.000000	0.000000
26	O	0.000000	8.777176	0.208766	0.059346	0.180534
27	H	0.000000	0.208766	0.269415	-0.000796	-0.009367
28	H	0.000000	0.059346	-0.000796	0.157274	-0.003959
29	H	0.000000	0.180534	-0.009367	-0.003959	0.205159

Total atomic charges:

	1

1	C	0.622996
2	C	-0.456335
3	C	0.093231
4	C	0.842137
5	C	-1.192906
6	C	-0.378854
7	C	1.283121
8	C	-2.681092
9	C	3.191418
10	C	-0.334145
11	C	-2.472673
12	O	-0.602352
13	C	-0.135979
14	N	-0.736528
15	O	-0.735991
16	H	0.285236
17	H	0.281463
18	H	0.309437
19	H	0.310292
20	H	0.288993
21	H	0.328875
22	H	0.323267
23	H	0.336739
24	H	0.273810
25	H	0.277130
26	O	-1.038484
27	H	0.514631
28	H	0.631659
29	H	0.570903

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.908232
2	C	-0.174872
3	C	0.402668
4	C	1.152429
5	C	-1.192906
6	C	-0.089861
7	C	1.611996
8	C	-2.357825
9	C	3.191418
10	C	0.002594
11	C	-1.921733
12	O	-0.602352
13	C	-0.135979
14	N	-0.736528
15	O	-0.104332
16	H	0.000000
17	H	0.000000
18	H	0.000000
19	H	0.000000
20	H	0.000000
21	H	0.000000
22	H	0.000000

```
 23  H    0.000000
 24  H    0.000000
 25  H    0.000000
 26  O    0.047050
 27  H    0.000000
 28  H    0.000000
 29  H    0.000000
 Sum of Mulliken charges=   0.00000
 Electronic spatial extent (au):  <R**2>=  3001.8780
 Charge=     0.0000 electrons
 Dipole moment (Debye):
    X=    -4.9089    Y=     0.9393    Z=     1.7710  Tot=     5.3025
 Quadrupole moment (Debye-Ang):
   XX=   -97.0265   YY=  -114.6810   ZZ=   -91.8287
   XY=    27.7690   XZ=     2.3305   YZ=     3.6698
 Octapole moment (Debye-Ang**2):
  XXX=    11.5678  YYY=   -10.5375  ZZZ=     1.0029  XYY=     6.4686
  XXY=    89.7237  XXZ=     6.3530  XZ=     -9.2108  YZZ=     5.7673
  YYZ=     8.8422  XYZ=     2.5233
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -2123.5316 YYYY= -1319.2522 ZZZZ=  -480.6033 XXXY=   424.4636
 XXXZ=    29.0007 YYYX=   205.2701 YYYZ=    13.1691 ZZZX=    10.3740
 ZZZY=     3.7842 XXYY=  -622.7949 XXZZ=  -482.2685 YYZZ=  -274.6840
 XXYZ=    17.5542 YYXZ=    -5.2116 ZZXY=    14.4456
 N-N= 1.163400585774D+03 E-N=-4.049095830155D+03  KE= 7.351470463674D+02
 1\1\GINC-PELICAN\FTS\RHF\3-21+G*\C12H13N1O3\KRUGER\25-Aug-2002\0\\#N R
 HF/3-21+G* OPT=(CALCFC,TS,NOEIGENTEST,GDIIS) FREQ OPTCYC=200\\With sol
 vent (H3O+)\\0,1\C,-1.9143803607,-0.271353856,1.72177189\C,-1.49699675
 6,1.1438758076,1.2083172753\C,-1.4118948906,1.0634394118,-0.3546963192
 \C,-1.5126353461,-1.1716562805,0.5208406364\C,-1.9425196109,-0.3213400
 77,-0.6642376984\C,0.0667195325,1.1113867793,1.3168669512\C,0.35372748
 73,-0.3124155445,1.8821920221\C,0.0901023639,-1.196112739,0.6367107993
 \C,0.5883428195,-0.3745170531,-0.504746123\C,0.185936039,1.0385362806,
 -0.2365833049\C,-0.8561069343,-0.5779021428,2.7877593404\O,-2.63845503
 1,-0.6558752856,-1.6006887005\C,2.9248356383,0.1961792013,0.0651099859
 \N,3.6445923365,0.6410046255,-0.7346133393\O,0.891531932,-0.8918796382
 ,-1.6284097325\H,-2.9519412553,-0.3672522196,2.0066735959\H,-2.0355291
 649,1.9697121038,1.6434088529\H,-1.819555039,1.8523636058,-0.961991188
 5\H,-1.9344642008,-2.1629257997,0.514274174\H,0.5795022626,1.915537346
 2,1.8155165658\H,1.3347754067,-0.4410764937,2.3017558807\H,0.490848777
 1,-2.1946532015,0.6569467597\H,0.7170527683,1.7967632033,-0.7795087891
 \H,-0.9017952128,-1.5976865875,3.1519924905\H,-0.9009815054,0.10510143
 05,3.6284729874\O,2.3088179032,0.5081235258,-3.0621104835\H,2.53173367
 94,0.607679278,-3.9919319157\H,1.3826616147,-0.3189674019,-2.368720055
 4\H,3.04960719,0.6967048149,-2.4207573829\\Version=DEC-AXP-OSF/1-G98Re
 vA.7\HF=-736.9141617\RMSD=8.558e-09\RMSF=3.615e-06\Dipole=-1.8730273,0
 .4511753,0.8000988\PG=C01 [X(C12H13N1O3)]\\@


 MANHOOD BEGINS BY TRYING TO SHAVE FACE,
 AND ENDS BY TRYING TO SAVE FACE.
 Job cpu time:  0 days 22 hours  7 minutes 51.7 seconds.
 File lengths (MBytes):  RWF=  216 Int=    0 D2E=    0 Chk=    8 Scr=
1
```

```
Normal termination of Gaussian 98.
Link1:  Proceeding to internal job step number  2.
--------------------------------------------
#N Geom=AllCheck Guess=TCheck RHF/3-21+G* Freq
--------------------------------------------
1/5=1,6=200,10=4,11=1,18=20,19=11,29=7,30=1,38=1/1,3;
2/9=110/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/5=101,7=1/1;
5/5=2/2;
8/6=4,11=11/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/5=1,6=200,10=4,11=1,18=20,19=11,30=1/3;
99//99;
-------------------
With solvent (H3O+)
-------------------
Redundant internal coordinates taken from checkpointfile:
mech1s1tsF.chk
Charge =  0 Multiplicity = 1
C,0,-1.9143803607,-0.271353856,1.72177189
C,0,-1.496996756,1.1438758076,1.2083172753
C,0,-1.4118948906,1.0634394118,-0.3546963192
C,0,-1.5126353461,-1.1716562805,0.5208406364
C,0,-1.9425196109,-0.321340077,-0.6642376984
C,0,0.0667195325,1.1113867793,1.3168669512
C,0,0.3537274873,-0.3124155445,1.8821920221
C,0,0.0901023639,-1.196112739,0.6367107993
C,0,0.5883428195,-0.3745170531,-0.504746123
C,0,0.185936039,1.0385362806,-0.2365833049
C,0,-0.8561069343,-0.5779021428,2.7877593404
O,0,-2.638455031,-0.6558752856,-1.6006887005
C,0,2.9248356383,0.1961792013,0.0651099859
N,0,3.6445923365,0.6410046255,-0.7346133393
O,0,0.891531932,-0.8918796382,-1.6284097325
H,0,-2.9519412553,-0.3672522196,2.0066735959
H,0,-2.0355291649,1.9697121038,1.6434088529
H,0,-1.819555039,1.8523636058,-0.9619911885
H,0,-1.9344642008,-2.1629257997,0.514274174
H,0,0.5795022626,1.9155373462,1.8155165658
H,0,1.3347754067,-0.4410764937,2.3017558807
H,0,0.4908487771,-2.1946532015,0.6569467597
H,0,0.7170527683,1.7967632033,-0.7795087891
H,0,-0.9017952128,-1.5976865875,3.1519924905
H,0,-0.9009815054,0.1051014305,3.6284729874
O,0,2.3088179032,0.5081235258,-3.0621104835
H,0,2.5317336794,0.607679278,-3.9919319157
H,0,1.3826616147,-0.3189674019,-2.3687200554
H,0,3.04960719,0.6967048149,-2.4207573829
Recover connectivity data from disk.
```

```
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Initialization pass.
                          ----------------------------
                          !    Initial Parameters    !
                          ! (Angstroms and Degrees)  !
 -------------------------                            --------------------
-----
 ! Name  Definition              Value          Derivative Info.
!
 ------------------------------------------------------------------------
-----
 ! R1    R(1,2)                  1.5623         calculate D2E/DX2
analyticall!
 ! R2    R(1,4)                  1.5538         calculate D2E/DX2
analyticall!
 ! R3    R(1,11)                 1.5331         calculate D2E/DX2
analyticall!
 ! R4    R(1,16)                 1.0802         calculate D2E/DX2
analyticall!
 ! R5    R(2,3)                  1.5674         calculate D2E/DX2
analyticall!
 ! R6    R(2,6)                  1.5678         calculate D2E/DX2
analyticall!
 ! R7    R(2,17)                 1.0776         calculate D2E/DX2
analyticall!
 ! R8    R(3,5)                  1.5149         calculate D2E/DX2
analyticall!
 ! R9    R(3,10)                 1.6024         calculate D2E/DX2
analyticall!
 ! R10   R(3,18)                 1.0758         calculate D2E/DX2
analyticall!
 ! R11   R(4,5)                  1.5206         calculate D2E/DX2
analyticall!
 ! R12   R(4,19)                 1.0773         calculate D2E/DX2
analyticall!
 ! R13   R(5,12)                 1.2137         calculate D2E/DX2
analyticall!
 ! R14   R(6,7)                  1.5586         calculate D2E/DX2
analyticall!
 ! R15   R(6,10)                 1.5597         calculate D2E/DX2
analyticall!
 ! R16   R(6,20)                 1.0762         calculate D2E/DX2
analyticall!
 ! R17   R(7,8)                  1.5497         calculate D2E/DX2
analyticall!
 ! R18   R(7,11)                 1.5344         calculate D2E/DX2
analyticall!
 ! R19   R(7,21)                 1.0747         calculate D2E/DX2
analyticall!
 ! R20   R(8,9)                  1.492          calculate D2E/DX2
analyticall!
```

```
 ! R21   R(8,22)                 1.0761         calculate D2E/DX2
analyticall!
 ! R22   R(9,10)                 1.4935         calculate D2E/DX2
analyticall!
 ! R23   R(9,13)                 2.4718         calculate D2E/DX2
analyticall!
 ! R24   R(9,15)                 1.2737         calculate D2E/DX2
analyticall!
 ! R25   R(10,23)                1.0732         calculate D2E/DX2
analyticall!
 ! R26   R(11,24)                1.0838         calculate D2E/DX2
analyticall!
 ! R27   R(11,25)                1.0841         calculate D2E/DX2
analyticall!
 ! R28   R(13,14)                1.1642         calculate D2E/DX2
analyticall!
 ! R29   R(13,21)                2.8173         calculate D2E/DX2
analyticall!
 ! R30   R(15,28)                1.0571         calculate D2E/DX2
analyticall!
 ! R31   R(26,27)                0.9613         calculate D2E/DX2
analyticall!
 ! R32   R(26,28)                1.4222         calculate D2E/DX2
analyticall!
 ! R33   R(26,29)                0.9978         calculate D2E/DX2
analyticall!
 ! A1    A(2,1,4)               101.6417         calculate D2E/DX2
analyticall!
 ! A2    A(2,1,11)              103.0171         calculate D2E/DX2
analyticall!
 ! A3    A(2,1,16)              115.0691         calculate D2E/DX2
analyticall!
 ! A4    A(4,1,11)              104.0689         calculate D2E/DX2
analyticall!
 ! A5    A(4,1,16)              113.6257         calculate D2E/DX2
analyticall!
 ! A6    A(11,1,16)             117.5096         calculate D2E/DX2
analyticall!
 ! A7    A(1,2,3)               107.2029         calculate D2E/DX2
analyticall!
 ! A8    A(1,2,6)               102.9992         calculate D2E/DX2
analyticall!
 ! A9    A(1,2,17)              115.3406         calculate D2E/DX2
analyticall!
 ! A10   A(3,2,6)                90.7922         calculate D2E/DX2
analyticall!
 ! A11   A(3,2,17)              117.9741         calculate D2E/DX2
analyticall!
 ! A12   A(6,2,17)              119.1009         calculate D2E/DX2
analyticall!
 ! A13   A(2,3,5)               103.3942         calculate D2E/DX2
analyticall!
 ! A14   A(2,3,10)               88.9362         calculate D2E/DX2
analyticall!
```

```
 ! A15   A(2,3,18)            120.312         calculate D2E/DX2
analyticall!
 ! A16   A(5,3,10)            110.4949        calculate D2E/DX2
analyticall!
 ! A17   A(5,3,18)            114.9771        calculate D2E/DX2
analyticall!
 ! A18   A(10,3,18)           115.522         calculate D2E/DX2
analyticall!
 ! A19   A(1,4,5)             101.8445        calculate D2E/DX2
analyticall!
 ! A20   A(1,4,19)            115.8888        calculate D2E/DX2
analyticall!
 ! A21   A(5,4,19)            113.5212        calculate D2E/DX2
analyticall!
 ! A22   A(3,5,4)             104.6487        calculate D2E/DX2
analyticall!
 ! A23   A(3,5,12)            127.6202        calculate D2E/DX2
analyticall!
 ! A24   A(4,5,12)            127.5364        calculate D2E/DX2
analyticall!
 ! A25   A(2,6,7)             103.1622        calculate D2E/DX2
analyticall!
 ! A26   A(2,6,10)             90.4724        calculate D2E/DX2
analyticall!
 ! A27   A(2,6,20)            119.4599        calculate D2E/DX2
analyticall!
 ! A28   A(7,6,10)            107.729         calculate D2E/DX2
analyticall!
 ! A29   A(7,6,20)            115.2636        calculate D2E/DX2
analyticall!
 ! A30   A(10,6,20)           117.384         calculate D2E/DX2
analyticall!
 ! A31   A(6,7,8)             101.4249        calculate D2E/DX2
analyticall!
 ! A32   A(6,7,11)            103.117         calculate D2E/DX2
analyticall!
 ! A33   A(6,7,21)            114.7752        calculate D2E/DX2
analyticall!
 ! A34   A(8,7,11)            103.9769        calculate D2E/DX2
analyticall!
 ! A35   A(8,7,21)            113.6261        calculate D2E/DX2
analyticall!
 ! A36   A(11,7,21)           117.9465        calculate D2E/DX2
analyticall!
 ! A37   A(7,8,9)             104.1249        calculate D2E/DX2
analyticall!
 ! A38   A(7,8,22)            116.7852        calculate D2E/DX2
analyticall!
 ! A39   A(9,8,22)            113.6391        calculate D2E/DX2
analyticall!
 ! A40   A(8,9,10)            107.0767        calculate D2E/DX2
analyticall!
 ! A41   A(8,9,13)            105.4513        calculate D2E/DX2
analyticall!
```

```
 ! A42   A(8,9,15)             122.0561         calculate D2E/DX2
analyticall!
 ! A43   A(10,9,13)             89.7048         calculate D2E/DX2
analyticall!
 ! A44   A(10,9,15)            127.3632         calculate D2E/DX2
analyticall!
 ! A45   A(13,9,15)             94.1383         calculate D2E/DX2
analyticall!
 ! A46   A(3,10,6)              89.7978         calculate D2E/DX2
analyticall!
 ! A47   A(3,10,9)             105.6727         calculate D2E/DX2
analyticall!
 ! A48   A(3,10,23)            116.437          calculate D2E/DX2
analyticall!
 ! A49   A(6,10,9)             104.1001         calculate D2E/DX2
analyticall!
 ! A50   A(6,10,23)            120.5764         calculate D2E/DX2
analyticall!
 ! A51   A(9,10,23)            116.3769         calculate D2E/DX2
analyticall!
 ! A52   A(1,11,7)              95.7001         calculate D2E/DX2
analyticall!
 ! A53   A(1,11,24)            113.1236         calculate D2E/DX2
analyticall!
 ! A54   A(1,11,25)            112.6234         calculate D2E/DX2
analyticall!
 ! A55   A(7,11,24)            113.2273         calculate D2E/DX2
analyticall!
 ! A56   A(7,11,25)            112.4152         calculate D2E/DX2
analyticall!
 ! A57   A(24,11,25)           109.2945         calculate D2E/DX2
analyticall!
 ! A58   A(9,13,21)             66.2527         calculate D2E/DX2
analyticall!
 ! A59   A(14,13,21)           168.7186         calculate D2E/DX2
analyticall!
 ! A60   A(9,15,28)            120.5498         calculate D2E/DX2
analyticall!
 ! A61   A(7,21,13)            100.2643         calculate D2E/DX2
analyticall!
 ! A62   A(27,26,28)           133.0626         calculate D2E/DX2
analyticall!
 ! A63   A(27,26,29)           115.4647         calculate D2E/DX2
analyticall!
 ! A64   A(28,26,29)           106.2603         calculate D2E/DX2
analyticall!
 ! A65   L(15,28,26,29,-1)     163.5774         calculate D2E/DX2
analyticall!
 ! A66   L(9,13,14,21,-2)      228.2174         calculate D2E/DX2
analyticall!
 ! A67   L(15,28,26,29,-2)     180.8017         calculate D2E/DX2
analyticall!
 ! D1    D(4,1,2,3)             20.8726         calculate D2E/DX2
analyticall!
```

```
 ! D2    D(4,1,2,6)            -74.0798         calculate D2E/DX2
analyticall!
 ! D3    D(4,1,2,17)           154.4977         calculate D2E/DX2
analyticall!
 ! D4    D(11,1,2,3)           128.4726         calculate D2E/DX2
analyticall!
 ! D5    D(11,1,2,6)            33.5202         calculate D2E/DX2
analyticall!
 ! D6    D(11,1,2,17)          -97.9022         calculate D2E/DX2
analyticall!
 ! D7    D(16,1,2,3)          -102.3647         calculate D2E/DX2
analyticall!
 ! D8    D(16,1,2,6)           162.6829         calculate D2E/DX2
analyticall!
 ! D9    D(16,1,2,17)           31.2605         calculate D2E/DX2
analyticall!
 ! D10   D(2,1,4,5)            -40.5293         calculate D2E/DX2
analyticall!
 ! D11   D(2,1,4,19)          -164.2429         calculate D2E/DX2
analyticall!
 ! D12   D(11,1,4,5)          -147.3104         calculate D2E/DX2
analyticall!
 ! D13   D(11,1,4,19)           88.976          calculate D2E/DX2
analyticall!
 ! D14   D(16,1,4,5)            83.6864         calculate D2E/DX2
analyticall!
 ! D15   D(16,1,4,19)          -40.0273         calculate D2E/DX2
analyticall!
 ! D16   D(2,1,11,7)           -52.9784         calculate D2E/DX2
analyticall!
 ! D17   D(2,1,11,24)         -171.2457         calculate D2E/DX2
analyticall!
 ! D18   D(2,1,11,25)           64.1993         calculate D2E/DX2
analyticall!
 ! D19   D(4,1,11,7)            52.7724         calculate D2E/DX2
analyticall!
 ! D20   D(4,1,11,24)          -65.495          calculate D2E/DX2
analyticall!
 ! D21   D(4,1,11,25)          169.9501         calculate D2E/DX2
analyticall!
 ! D22   D(16,1,11,7)          179.38           calculate D2E/DX2
analyticall!
 ! D23   D(16,1,11,24)          61.1127         calculate D2E/DX2
analyticall!
 ! D24   D(16,1,11,25)         -63.4423         calculate D2E/DX2
analyticall!
 ! D25   D(1,2,3,5)              6.6709         calculate D2E/DX2
analyticall!
 ! D26   D(1,2,3,10)          -104.1566         calculate D2E/DX2
analyticall!
 ! D27   D(1,2,3,18)           136.6133         calculate D2E/DX2
analyticall!
 ! D28   D(6,2,3,5)            110.5442         calculate D2E/DX2
analyticall!
```

```
 ! D29   D(6,2,3,10)            -0.2833         calculate D2E/DX2
analyticall!
 ! D30   D(6,2,3,18)          -119.5134         calculate D2E/DX2
analyticall!
 ! D31   D(17,2,3,5)          -125.5321         calculate D2E/DX2
analyticall!
 ! D32   D(17,2,3,10)          123.6404         calculate D2E/DX2
analyticall!
 ! D33   D(17,2,3,18)            4.4103         calculate D2E/DX2
analyticall!
 ! D34   D(1,2,6,7)              -0.1861         calculate D2E/DX2
analyticall!
 ! D35   D(1,2,6,10)            108.1548         calculate D2E/DX2
analyticall!
 ! D36   D(1,2,6,20)          -129.6415         calculate D2E/DX2
analyticall!
 ! D37   D(3,2,6,7)           -108.0499         calculate D2E/DX2
analyticall!
 ! D38   D(3,2,6,10)              0.291         calculate D2E/DX2
analyticall!
 ! D39   D(3,2,6,20)            122.4947         calculate D2E/DX2
analyticall!
 ! D40   D(17,2,6,7)            128.9535         calculate D2E/DX2
analyticall!
 ! D41   D(17,2,6,10)          -122.7056         calculate D2E/DX2
analyticall!
 ! D42   D(17,2,6,20)            -0.5019         calculate D2E/DX2
analyticall!
 ! D43   D(2,3,5,4)             -32.7348         calculate D2E/DX2
analyticall!
 ! D44   D(2,3,5,12)            142.4619         calculate D2E/DX2
analyticall!
 ! D45   D(10,3,5,4)             61.2007         calculate D2E/DX2
analyticall!
 ! D46   D(10,3,5,12)          -123.6026         calculate D2E/DX2
analyticall!
 ! D47   D(18,3,5,4)           -165.8348         calculate D2E/DX2
analyticall!
 ! D48   D(18,3,5,12)             9.3619         calculate D2E/DX2
analyticall!
 ! D49   D(2,3,10,6)              0.2847         calculate D2E/DX2
analyticall!
 ! D50   D(2,3,10,9)            104.8827         calculate D2E/DX2
analyticall!
 ! D51   D(2,3,10,23)          -124.211          calculate D2E/DX2
analyticall!
 ! D52   D(5,3,10,6)           -103.6257         calculate D2E/DX2
analyticall!
 ! D53   D(5,3,10,9)              0.9723         calculate D2E/DX2
analyticall!
 ! D54   D(5,3,10,23)           131.8786         calculate D2E/DX2
analyticall!
 ! D55   D(18,3,10,6)           123.687          calculate D2E/DX2
analyticall!
```

```
 ! D56   D(18,3,10,9)         -131.715         calculate D2E/DX2
analyticall!
 ! D57   D(18,3,10,23)          -0.8087         calculate D2E/DX2
analyticall!
 ! D58   D(1,4,5,3)             46.7392         calculate D2E/DX2
analyticall!
 ! D59   D(1,4,5,12)          -128.4629         calculate D2E/DX2
analyticall!
 ! D60   D(19,4,5,3)           172.0374         calculate D2E/DX2
analyticall!
 ! D61   D(19,4,5,12)           -3.1647         calculate D2E/DX2
analyticall!
 ! D62   D(2,6,7,8)             74.2795         calculate D2E/DX2
analyticall!
 ! D63   D(2,6,7,11)           -33.1844         calculate D2E/DX2
analyticall!
 ! D64   D(2,6,7,21)          -162.7923         calculate D2E/DX2
analyticall!
 ! D65   D(10,6,7,8)            -20.519         calculate D2E/DX2
analyticall!
 ! D66   D(10,6,7,11)          -127.9829         calculate D2E/DX2
analyticall!
 ! D67   D(10,6,7,21)           102.4092         calculate D2E/DX2
analyticall!
 ! D68   D(20,6,7,8)           -153.7411         calculate D2E/DX2
analyticall!
 ! D69   D(20,6,7,11)            98.795          calculate D2E/DX2
analyticall!
 ! D70   D(20,6,7,21)           -30.8129         calculate D2E/DX2
analyticall!
 ! D71   D(2,6,10,3)             -0.2846         calculate D2E/DX2
analyticall!
 ! D72   D(2,6,10,9)           -106.4045         calculate D2E/DX2
analyticall!
 ! D73   D(2,6,10,23)           120.7153         calculate D2E/DX2
analyticall!
 ! D74   D(7,6,10,3)            103.7027         calculate D2E/DX2
analyticall!
 ! D75   D(7,6,10,9)             -2.4172         calculate D2E/DX2
analyticall!
 ! D76   D(7,6,10,23)          -135.2974         calculate D2E/DX2
analyticall!
 ! D77   D(20,6,10,3)          -124.214          calculate D2E/DX2
analyticall!
 ! D78   D(20,6,10,9)           129.6661         calculate D2E/DX2
analyticall!
 ! D79   D(20,6,10,23)           -3.2141         calculate D2E/DX2
analyticall!
 ! D80   D(6,7,8,9)              36.1679         calculate D2E/DX2
analyticall!
 ! D81   D(6,7,8,22)            162.3395         calculate D2E/DX2
analyticall!
 ! D82   D(11,7,8,9)            142.9595         calculate D2E/DX2
analyticall!
```

```
 ! D83   D(11,7,8,22)          -90.8688         calculate D2E/DX2
analyticall!
 ! D84   D(21,7,8,9)           -87.5459         calculate D2E/DX2
analyticall!
 ! D85   D(21,7,8,22)           38.6258         calculate D2E/DX2
analyticall!
 ! D86   D(6,7,11,1)            52.9021         calculate D2E/DX2
analyticall!
 ! D87   D(6,7,11,24)          171.0867         calculate D2E/DX2
analyticall!
 ! D88   D(6,7,11,25)          -64.4432         calculate D2E/DX2
analyticall!
 ! D89   D(8,7,11,1)           -52.6191         calculate D2E/DX2
analyticall!
 ! D90   D(8,7,11,24)           65.5656         calculate D2E/DX2
analyticall!
 ! D91   D(8,7,11,25)         -169.9643         calculate D2E/DX2
analyticall!
 ! D92   D(21,7,11,1)         -179.4573         calculate D2E/DX2
analyticall!
 ! D93   D(21,7,11,24)         -61.2726         calculate D2E/DX2
analyticall!
 ! D94   D(21,7,11,25)          63.1975         calculate D2E/DX2
analyticall!
 ! D95   D(6,7,21,13)          -58.6109         calculate D2E/DX2
analyticall!
 ! D96   D(8,7,21,13)           57.494          calculate D2E/DX2
analyticall!
 ! D97   D(11,7,21,13)         179.5326         calculate D2E/DX2
analyticall!
 ! D98   D(7,8,9,10)           -40.0471         calculate D2E/DX2
analyticall!
 ! D99   D(7,8,9,13)            54.5024         calculate D2E/DX2
analyticall!
 ! D100  D(7,8,9,15)           159.6577         calculate D2E/DX2
analyticall!
 ! D101  D(22,8,9,10)         -168.1741         calculate D2E/DX2
analyticall!
 ! D102  D(22,8,9,13)          -73.6246         calculate D2E/DX2
analyticall!
 ! D103  D(22,8,9,15)           31.5306         calculate D2E/DX2
analyticall!
 ! D104  D(8,9,10,3)           -67.8264         calculate D2E/DX2
analyticall!
 ! D105  D(8,9,10,6)            25.9979         calculate D2E/DX2
analyticall!
 ! D106  D(8,9,10,23)          161.2329         calculate D2E/DX2
analyticall!
 ! D107  D(13,9,10,3)         -173.9153         calculate D2E/DX2
analyticall!
 ! D108  D(13,9,10,6)          -80.091          calculate D2E/DX2
analyticall!
 ! D109  D(13,9,10,23)          55.144          calculate D2E/DX2
analyticall!
```

```
 ! D110  D(15,9,10,3)           91.1016         calculate D2E/DX2
analyticall!
 ! D111  D(15,9,10,6)         -175.0741         calculate D2E/DX2
analyticall!
 ! D112  D(15,9,10,23)         -39.8391         calculate D2E/DX2
analyticall!
 ! D113  D(8,9,13,21)          -22.8352         calculate D2E/DX2
analyticall!
 ! D114  D(10,9,13,21)          84.8174         calculate D2E/DX2
analyticall!
 ! D115  D(15,9,13,21)        -147.7313         calculate D2E/DX2
analyticall!
 ! D116  D(8,9,15,28)         -170.3523         calculate D2E/DX2
analyticall!
 ! D117  D(10,9,15,28)          33.5714         calculate D2E/DX2
analyticall!
 ! D118  D(13,9,15,28)         -59.2226         calculate D2E/DX2
analyticall!
 ! D119  D(9,13,21,7)          -18.6312         calculate D2E/DX2
analyticall!
 ! D120  D(14,13,21,7)         113.1514         calculate D2E/DX2
analyticall!
 ! D121  D(9,15,26,27)        -157.6647         calculate D2E/DX2
analyticall!
 ! D122  D(9,15,26,29)          53.3054         calculate D2E/DX2
analyticall!
 ---------------------------------------------------------------------
-----
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
 Number of steps in this run= 174 maximum allowed number of steps= 174.
 Search for a saddle point of order  1.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.914380   -0.271354    1.721772
    2          6             0       -1.496997    1.143876    1.208317
    3          6             0       -1.411895    1.063439   -0.354696
    4          6             0       -1.512635   -1.171656    0.520841
    5          6             0       -1.942520   -0.321340   -0.664238
    6          6             0        0.066720    1.111387    1.316867
    7          6             0        0.353727   -0.312416    1.882192
    8          6             0        0.090102   -1.196113    0.636711
    9          6             0        0.588343   -0.374517   -0.504746
   10          6             0        0.185936    1.038536   -0.236583
   11          6             0       -0.856107   -0.577902    2.787759
   12          8             0       -2.638455   -0.655875   -1.600689
   13          6             0        2.924836    0.196179    0.065110
   14          7             0        3.644592    0.641005   -0.734613
   15          8             0        0.891532   -0.891880   -1.628410
   16          1             0       -2.951941   -0.367252    2.006674
```

17	1	0	-2.035529	1.969712	1.643409
18	1	0	-1.819555	1.852364	-0.961991
19	1	0	-1.934464	-2.162926	0.514274
20	1	0	0.579502	1.915537	1.815517
21	1	0	1.334775	-0.441076	2.301756
22	1	0	0.490849	-2.194653	0.656947
23	1	0	0.717053	1.796763	-0.779509
24	1	0	-0.901795	-1.597687	3.151992
25	1	0	-0.900982	0.105101	3.628473
26	8	0	2.308818	0.508124	-3.062110
27	1	0	2.531734	0.607679	-3.991932
28	1	0	1.382662	-0.318967	-2.368720
29	1	0	3.049607	0.696705	-2.420757

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.562280	0.000000			
3	C	2.519104	1.567394	0.000000		
4	C	1.553763	2.415483	2.402575	0.000000	
5	C	2.386699	2.419052	1.514923	1.520608	0.000000
6	C	2.449628	1.567816	2.232201	2.887959	3.164573
7	C	2.274145	2.449504	3.164501	2.464728	3.428868
8	C	2.459774	2.884643	2.888678	1.607107	2.566953
9	C	3.351365	3.096570	2.468033	2.470095	2.536440
10	C	3.156311	2.220607	1.602384	2.888561	2.561733
11	C	1.533050	2.422787	3.588583	2.433617	3.628002
12	O	3.422117	3.525982	2.452140	2.456499	1.213746
13	C	5.136256	4.664510	4.442478	4.665813	4.948830
14	N	6.145600	5.519402	5.088305	5.608824	5.669822
15	O	4.413832	4.230412	3.278932	3.236908	3.047457
16	H	1.080231	2.244492	3.161438	2.219542	2.855662
17	H	2.245706	1.077649	2.280937	3.376651	3.253122
18	H	3.423704	2.305697	1.075823	3.381965	2.197445
19	H	2.244214	3.407053	3.381955	1.077311	2.186411
20	H	3.318242	2.296955	3.066196	3.947656	4.184901
21	H	3.304875	3.424415	4.106641	3.437027	4.421778
22	H	3.258537	3.924451	3.906280	2.253663	3.343069
23	H	4.178272	3.046265	2.291429	3.933692	3.401907
24	H	2.197730	3.412961	4.431553	2.734518	4.156414
25	H	2.191850	2.700267	4.128569	3.414910	4.437794
26	O	6.428726	5.755429	4.634886	5.501155	4.950927
27	H	7.292945	6.600058	5.384181	6.315700	5.652926
28	H	5.254034	4.819496	3.711723	4.178443	3.736589
29	H	6.537496	5.834531	4.930325	5.740891	5.389166

		6	7	8	9	10
6	C	0.000000				
7	C	1.558582	0.000000			
8	C	2.405767	1.549723	0.000000		
9	C	2.407961	2.399245	1.492041	0.000000	
10	C	1.559720	2.518419	2.401142	1.493507	0.000000
11	C	2.422567	1.534352	2.429919	3.601165	3.584045
12	O	4.353541	4.604517	3.569711	3.419426	3.564968
13	C	3.251665	3.189209	3.209504	2.471766	2.881346

14	N	4.151025	4.311203	4.229649	3.228743	3.516869
15	O	3.656234	3.598519	2.421904	1.273659	2.482247
16	H	3.431402	3.308466	3.437708	4.340610	4.105450
17	H	2.294080	3.312653	3.943881	4.122461	3.055547
18	H	3.049635	4.183157	3.936477	3.311502	2.282658
19	H	3.920461	3.245213	2.246906	3.255974	3.912703
20	H	1.076223	2.240356	3.363252	3.260068	2.266085
21	H	2.233409	1.074729	2.211711	2.904831	3.154719
22	H	3.397835	2.250077	1.076146	2.161465	3.368216
23	H	2.299449	3.415449	3.369874	2.192377	1.073201
24	H	3.412446	2.200148	2.733453	4.133811	4.428914
25	H	2.700477	2.190459	3.409699	4.419459	4.122057
26	O	4.956448	5.379757	4.637715	3.206119	3.573733
27	H	5.874807	6.332110	5.535301	4.111197	4.448713
28	H	4.166674	4.373671	3.387139	2.026925	2.796601
29	H	4.799939	5.177013	4.657203	3.297944	3.617745

		11	12	13	14	15
11	C	0.000000				
12	O	4.737227	0.000000			
13	C	4.723087	5.869505	0.000000		
14	N	5.843726	6.473690	1.164249	0.000000	
15	O	4.759766	3.537976	2.861154	3.275355	0.000000
16	H	2.246551	3.632443	6.214791	7.214256	5.316141
17	H	3.031652	4.216799	5.499242	6.299542	5.240343
18	H	4.571111	2.714736	5.129047	5.601428	3.914713
19	H	2.973868	2.690701	5.420325	6.367701	3.767347
20	H	3.037017	5.351436	3.394216	4.185973	4.454164
21	H	2.248307	5.573309	2.817263	3.965563	3.980690
22	H	2.994751	4.154190	3.462751	4.463574	2.660943
23	H	4.565005	4.236650	2.854743	3.147742	2.824867
24	H	1.083842	5.146938	5.233536	6.386477	5.154263
25	H	1.084116	5.562556	5.229027	6.323445	5.642862
26	O	6.739227	5.288304	3.202545	2.686856	2.454426
27	H	7.671198	5.834849	4.096761	3.442338	3.244253
28	H	5.627469	4.107646	2.926979	2.950963	1.057117
29	H	6.633843	5.903900	2.538825	1.788908	2.794406

		16	17	18	19	20
16	H	0.000000				
17	H	2.536370	0.000000			
18	H	3.875818	2.616969	0.000000		
19	H	2.546951	4.285307	4.279616	0.000000	
20	H	4.209366	2.621249	3.670697	4.964587	0.000000
21	H	4.297495	4.195745	5.085441	4.104605	2.522002
22	H	4.124798	4.969671	4.933282	2.429713	4.271277
23	H	5.089921	3.671124	2.543771	4.937971	2.601381
24	H	2.651193	4.035779	5.447017	2.888505	4.040192
25	H	2.657026	2.950331	4.996905	3.988768	2.959108
26	O	7.357611	6.568981	4.822960	6.158772	5.363077
27	H	8.185625	7.380521	5.446420	6.923082	6.264835
28	H	6.159154	5.746239	4.116765	4.766043	4.811020
29	H	7.533441	6.632994	5.212704	6.452353	5.053018

		21	22	23	24	25
21	H	0.000000				
22	H	2.548066	0.000000			

23	H	3.857940	4.248056	0.000000		
24	H	2.657611	2.919089	5.440557	0.000000	
25	H	2.656520	4.006998	4.990998	1.768197	0.000000
26	O	5.533607	4.943824	3.066689	7.304625	7.431631
27	H	6.491772	5.799168	3.876422	8.227297	8.372974
28	H	4.672317	3.669903	2.728542	6.110003	6.431266
29	H	5.151439	4.937556	3.056900	7.206480	7.249161

		26	27	28	29
26	O	0.000000			
27	H	0.961338	0.000000		
28	H	1.422194	2.194050	0.000000	
29	H	0.997830	1.656716	1.952692	0.000000

Stoichiometry C12H13NO3
Framework group C1[X(C12H13NO3)]
Deg. of freedom 81
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.572698	-0.288596	-0.030360
2	6	0	-1.790011	-0.245400	1.321030
3	6	0	-0.826952	0.989702	1.259683
4	6	0	-1.648230	0.550713	-0.955076
5	6	0	-1.222888	1.679740	-0.029532
6	6	0	-0.590003	-1.221326	1.064909
7	6	0	-0.833216	-1.707155	-0.395912
8	6	0	-0.420014	-0.454193	-1.208926
9	6	0	0.728605	0.113489	-0.444335
10	6	0	0.395950	-0.014197	1.006044
11	6	0	-2.363523	-1.731371	-0.504586
12	8	0	-1.280644	2.873044	-0.243705
13	6	0	2.351103	-1.737925	-0.222082
14	7	0	3.442273	-1.538521	0.131560
15	8	0	1.568768	0.908467	-0.977574
16	1	0	-3.587345	0.079102	0.016410
17	1	0	-2.390789	-0.374473	2.206318
18	1	0	-0.723694	1.640487	2.110101
19	1	0	-2.089815	0.893086	-1.876153
20	1	0	-0.378536	-1.998856	1.778340
21	1	0	-0.294650	-2.595719	-0.670581
22	1	0	-0.211822	-0.601423	-2.254426
23	1	0	1.218921	0.052436	1.691638
24	1	0	-2.717667	-1.903059	-1.514446
25	1	0	-2.813793	-2.458687	0.161429
26	8	0	3.690858	1.134821	0.234740
27	1	0	4.418710	1.757062	0.319688
28	1	0	2.453934	1.177070	-0.465881
29	1	0	3.940049	0.171080	0.303827

Rotational constants (GHZ): 0.9148638 0.4991978 0.3975386

```
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,O-16,C-
12,N-14,
 O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,O-16,H-1,H-1,H-1
 Standard basis: 3-21+G* (6D, 7F)
 There are   234 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    131072 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
   234 basis functions      343 primitive gaussians
    58 alpha electrons       58 beta electrons
       nuclear repulsion energy      1163.4005857738 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   234 RedAO= T  NBF=   234
 NBsUse=   234 1.00D-04 NBFU=   234
 Initial guess read from the checkpoint file:
 mech1s1tsF.chk
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -736.914161664     A.U. after    2 cycles
             Convg  =    0.3695D-08             -V/T =  2.0024
             S**2   =   0.0000
 Range of M.O.s used for correlation:     1   234
 NBasis=   234 NAE=    58 NBE=    58 NFC=     0 NFV=     0
 NROrb=    234 NOA=    58 NOB=    58 NVA=   176 NVB=   176

 **** Warning!!: The largest alpha MO coefficient is  0.10292376D+03

          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   3 vectors were produced by pass 12.
   3 vectors were produced by pass 13.
 Inv2:  IOpt= 1 Iter= 1 AM= 7.17D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  42 with in-core refinement.
 G2DrvN: will do   29 atoms at a time, making    1 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
```

```
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  90 IRICut=      82 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
          There are  90 degrees of freedom in the 1st order CPHF.
  87 vectors were produced by pass  0.
 AX will form  87 AO Fock derivatives at one time.
  87 vectors were produced by pass  1.
  87 vectors were produced by pass  2.
  87 vectors were produced by pass  3.
  87 vectors were produced by pass  4.
  87 vectors were produced by pass  5.
  87 vectors were produced by pass  6.
  39 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
 Inv2:  IOpt= 1 Iter= 1 AM= 5.01D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 651 with in-core refinement.

 ********************************************************************

            Population analysis using the SCF density.

 ********************************************************************

 Alpha  occ. eigenvalues --  -20.56489 -20.51970 -20.51294 -15.43460 -
11.38021
 Alpha  occ. eigenvalues --  -11.31963 -11.23733 -11.23532 -11.23247 -
11.23161
 Alpha  occ. eigenvalues --  -11.22032 -11.21972 -11.21642 -11.21032 -
11.19886
 Alpha  occ. eigenvalues --  -11.13718  -1.49705  -1.44227  -1.38935  -
1.28253
 Alpha  occ. eigenvalues --   -1.17615  -1.13551  -1.10848  -1.08434  -
0.95931
 Alpha  occ. eigenvalues --   -0.94570  -0.92920  -0.86073  -0.83022  -
0.79330
 Alpha  occ. eigenvalues --   -0.77394  -0.76869  -0.75561  -0.71012  -
0.70343
 Alpha  occ. eigenvalues --   -0.67849  -0.67196  -0.65735  -0.64902  -
0.62952
 Alpha  occ. eigenvalues --   -0.61016  -0.58607  -0.56668  -0.55996  -
0.55246
 Alpha  occ. eigenvalues --   -0.54240  -0.53004  -0.51816  -0.51556  -
0.50218
 Alpha  occ. eigenvalues --   -0.49396  -0.48940  -0.47483  -0.45884  -
0.41706
 Alpha  occ. eigenvalues --   -0.41441  -0.40877  -0.39564
 Alpha virt. eigenvalues --    0.04855   0.05578   0.06524   0.07180
0.07832
 Alpha virt. eigenvalues --    0.08741   0.08965   0.09443   0.09997
0.10362
```

```
 Alpha virt. eigenvalues --    0.10847   0.12181   0.12318   0.13428
0.13631
 Alpha virt. eigenvalues --    0.14357   0.14497   0.15292   0.16896
0.17417
 Alpha virt. eigenvalues --    0.17773   0.17989   0.18810   0.19179
0.19346
 Alpha virt. eigenvalues --    0.19748   0.19969   0.21189   0.22317
0.23134
 Alpha virt. eigenvalues --    0.23215   0.23805   0.24155   0.24201
0.24715
 Alpha virt. eigenvalues --    0.25159   0.25743   0.26276   0.26610
0.27006
 Alpha virt. eigenvalues --    0.27593   0.27704   0.28443   0.28680
0.28920
 Alpha virt. eigenvalues --    0.29493   0.29807   0.30508   0.31065
0.31609
 Alpha virt. eigenvalues --    0.32525   0.32828   0.33094   0.34409
0.35007
 Alpha virt. eigenvalues --    0.35702   0.37002   0.37059   0.37946
0.38387
 Alpha virt. eigenvalues --    0.39300   0.40199   0.40660   0.41266
0.41520
 Alpha virt. eigenvalues --    0.42483   0.43130   0.43506   0.44873
0.45637
 Alpha virt. eigenvalues --    0.45787   0.46156   0.47230   0.47412
0.48477
 Alpha virt. eigenvalues --    0.48689   0.49239   0.50009   0.51231
0.51696
 Alpha virt. eigenvalues --    0.52915   0.53520   0.54741   0.55638
0.57229
 Alpha virt. eigenvalues --    0.57928   0.58577   0.59165   0.59885
0.60586
 Alpha virt. eigenvalues --    0.61609   0.62868   0.63262   0.64552
0.65413
 Alpha virt. eigenvalues --    0.66748   0.70551   0.77542   0.83906
1.06713
 Alpha virt. eigenvalues --    1.08273   1.10122   1.10918   1.12073
1.12968
 Alpha virt. eigenvalues --    1.14019   1.14631   1.15713   1.16168
1.17070
 Alpha virt. eigenvalues --    1.17718   1.18689   1.19034   1.19309
1.20598
 Alpha virt. eigenvalues --    1.21398   1.22897   1.24011   1.25067
1.26551
 Alpha virt. eigenvalues --    1.27977   1.31593   1.32077   1.32777
1.35616
 Alpha virt. eigenvalues --    1.37417   1.39352   1.42393   1.45279
1.47452
 Alpha virt. eigenvalues --    1.48397   1.49563   1.50823   1.51765
1.51841
 Alpha virt. eigenvalues --    1.53009   1.55286   1.56395   1.57138
1.58360
 Alpha virt. eigenvalues --    1.61908   1.64176   1.69719   1.71297
1.72429
```

```
 Alpha virt. eigenvalues --    1.75367   1.77402   1.77778   1.84383
1.92483
 Alpha virt. eigenvalues --    1.95406   1.98889   2.00518   2.05804
2.09390
 Alpha virt. eigenvalues --    2.13408   2.13908   2.17701   2.20487
2.21237
 Alpha virt. eigenvalues --    2.25370   2.29055   2.31186   2.38595
2.46589
 Alpha virt. eigenvalues --    2.54689   2.57904   2.88068   2.95819
2.99499
 Alpha virt. eigenvalues --    3.16507   3.38141   3.48570   3.74649
3.90459
 Alpha virt. eigenvalues --    4.02984
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   14.965090  -8.912957   4.403164  -5.117663  -1.852259   6.174978
  2  C   -8.912957  23.369302 -12.349188   2.954390   5.255635 -14.335569
  3  C    4.403164 -12.349188  24.247595   2.515548 -13.120176   9.443171
  4  C   -5.117663   2.954390   2.515548  18.710939 -10.713172  -3.171265
  5  C   -1.852259   5.255635 -13.120176 -10.713172  28.589010  -2.786332
  6  C    6.174978 -14.335569   9.443171  -3.171265  -2.786332  25.388425
  7  C   -2.506977   4.470267  -1.532709   4.186291  -0.525115  -8.530773
  8  C    4.725233  -3.514302  -1.278110 -12.064912   8.231924   5.332835
  9  C   -0.718769  -1.310079   5.966203   9.256135 -11.804474   0.525525
 10  C   -2.346169   9.297718 -12.863353  -2.190549   6.057521 -11.924544
 11  C   -4.092801   2.031505  -0.669865   0.556576   0.536336  -1.152977
 12  O    0.042955  -0.228167   0.501776   0.365738  -0.678651   0.114093
 13  C    0.362083  -0.630389   0.360397  -0.321679  -0.129723   0.845283
 14  N   -0.036707   0.059713  -0.029466   0.058536  -0.020967  -0.105284
 15  O    0.036404  -0.062281  -0.037770  -0.151709   0.074540   0.113323
 16  H    0.476930  -0.066045  -0.000361  -0.130783   0.030937   0.014942
 17  H   -0.079923   0.551061  -0.130490   0.004339   0.025810  -0.109070
 18  H    0.029447  -0.094420   0.486725  -0.019188  -0.017030   0.058448
 19  H   -0.025509  -0.003511   0.012706   0.474739  -0.057753   0.012361
 20  H   -0.006225  -0.090499   0.070543   0.004235   0.003399   0.498336
 21  H   -0.054137   0.056374  -0.012892   0.057033   0.005386  -0.103085
 22  H   -0.000391   0.011413  -0.026360  -0.108786   0.062056   0.004010
 23  H    0.001035   0.012017  -0.043410  -0.008309   0.019968  -0.009792
 24  H   -0.051954   0.009199   0.006466   0.010564  -0.013756   0.047410
 25  H   -0.044076  -0.016018  -0.001366   0.018417   0.001296   0.033631
 26  O    0.006636  -0.017609  -0.012834  -0.016475   0.024890   0.030706
 27  H   -0.000158   0.000527   0.000075   0.000324  -0.000197  -0.002024
 28  H   -0.000141   0.007476   0.000881  -0.002205  -0.004253  -0.027779
 29  H   -0.000135   0.000773  -0.000132   0.000754  -0.001945  -0.000127
               7          8          9         10         11         12
  1  C   -2.506977   4.725233  -0.718769  -2.346169  -4.092801   0.042955
  2  C    4.470267  -3.514302  -1.310079   9.297718   2.031505  -0.228167
  3  C   -1.532709  -1.278110   5.966203 -12.863353  -0.669865   0.501776
  4  C    4.186291 -12.064912   9.256135  -2.190549   0.556576   0.365738
  5  C   -0.525115   8.231924 -11.804474   6.057521   0.536336  -0.678651
  6  C   -8.530773   5.332835   0.525525 -11.924544  -1.152977   0.114093
  7  C   17.927010 -11.769596   7.564569   0.898814  -4.254689  -0.045372
  8  C  -11.769596  51.753744 -46.839632  10.539329  -0.982652   0.105044
  9  C    7.564569 -46.839632  70.563654 -24.085314  -0.181556  -0.213027
```

10	C	0.898814	10.539329	-24.085314	30.545034	0.279139	-0.008520
11	C	-4.254689	-0.982652	-0.181556	0.279139	16.018645	0.000169
12	O	-0.045372	0.105044	-0.213027	-0.008520	0.000169	8.621365
13	C	-1.011515	2.225134	-3.471370	1.006893	-0.449301	0.010975
14	N	0.086535	-0.239777	0.312551	-0.019188	0.034389	-0.000119
15	O	-0.346001	1.607174	-2.063626	0.591144	-0.007779	0.019457
16	H	-0.019307	0.024100	0.015309	-0.010312	0.014842	0.000122
17	H	-0.005456	0.015096	-0.011162	0.078411	0.025901	0.000373
18	H	-0.009527	0.031655	-0.062419	-0.045305	0.000598	-0.004720
19	H	0.001298	-0.061990	-0.026527	0.003741	0.020443	-0.001263
20	H	-0.083412	0.054989	-0.035460	-0.079905	0.029198	-0.000044
21	H	0.474332	-0.064930	-0.047795	0.021865	0.016709	-0.000010
22	H	-0.061348	0.653659	-0.279698	0.071349	0.015248	0.000144
23	H	-0.013463	0.100047	-0.219591	0.501983	0.001360	0.000687
24	H	-0.070445	0.067132	-0.026085	0.002630	0.332399	0.000150
25	H	-0.086033	0.066696	-0.011475	-0.000173	0.353741	-0.000036
26	O	-0.034018	-0.070292	-0.000701	-0.000230	-0.004126	-0.001147
27	H	0.000639	0.009107	0.008753	-0.001035	0.000058	0.000016
28	H	0.010839	0.037393	-0.039156	0.032502	0.001006	0.000369
29	H	0.002042	-0.013004	0.043800	-0.019330	0.000156	-0.000005

		13	14	15	16	17	18
1	C	0.362083	-0.036707	0.036404	0.476930	-0.079923	0.029447
2	C	-0.630389	0.059713	-0.062281	-0.066045	0.551061	-0.094420
3	C	0.360397	-0.029466	-0.037770	-0.000361	-0.130490	0.486725
4	C	-0.321679	0.058536	-0.151709	-0.130783	0.004339	-0.019188
5	C	-0.129723	-0.020967	0.074540	0.030937	0.025810	-0.017030
6	C	0.845283	-0.105284	0.113323	0.014942	-0.109070	0.058448
7	C	-1.011515	0.086535	-0.346001	-0.019307	-0.005456	-0.009527
8	C	2.225134	-0.239777	1.607174	0.024100	0.015096	0.031655
9	C	-3.471370	0.312551	-2.063626	0.015309	-0.011162	-0.062419
10	C	1.006893	-0.019188	0.591144	-0.010312	0.078411	-0.045305
11	C	-0.449301	0.034389	-0.007779	0.014842	0.025901	0.000598
12	O	0.010975	-0.000119	0.019457	0.000122	0.000373	-0.004720
13	C	6.974704	0.142781	0.215990	-0.000755	0.000218	-0.000314
14	N	0.142781	7.512097	-0.010540	0.000002	0.000000	0.000018
15	O	0.215990	-0.010540	8.641611	-0.000072	-0.000001	0.002754
16	H	-0.000755	0.000002	-0.000072	0.366936	-0.000735	-0.000006
17	H	0.000218	0.000000	-0.000001	-0.000735	0.354712	-0.000204
18	H	-0.000314	0.000018	0.002754	-0.000006	-0.000204	0.335132
19	H	-0.000001	-0.000002	0.002139	-0.000278	-0.000009	-0.000007
20	H	-0.001056	0.000969	0.000381	-0.000008	-0.000495	-0.000067
21	H	0.000195	-0.001516	0.000368	-0.000017	-0.000008	0.000000
22	H	0.002167	0.000199	0.008095	-0.000002	0.000000	-0.000001
23	H	0.004317	-0.002101	0.003732	0.000000	-0.000026	-0.000938
24	H	0.001746	-0.000010	0.000078	-0.000258	-0.000023	0.000000
25	H	0.001978	-0.000008	0.000023	-0.000417	0.000218	0.000000
26	O	0.041353	-0.070006	-0.066403	0.000000	0.000000	-0.000064
27	H	-0.004164	0.002824	0.002604	0.000000	0.000000	0.000000
28	H	-0.017642	-0.003738	0.161248	0.000000	0.000000	-0.000003
29	H	-0.022324	0.065342	0.001107	0.000000	0.000000	0.000000

		19	20	21	22	23	24
1	C	-0.025509	-0.006225	-0.054137	-0.000391	0.001035	-0.051954
2	C	-0.003511	-0.090499	0.056374	0.011413	0.012017	0.009199
3	C	0.012706	0.070543	-0.012892	-0.026360	-0.043410	0.006466

4	C	0.474739	0.004235	0.057033	-0.108786	-0.008309	0.010564
5	C	-0.057753	0.003399	0.005386	0.062056	0.019968	-0.013756
6	C	0.012361	0.498336	-0.103085	0.004010	-0.009792	0.047410
7	C	0.001298	-0.083412	0.474332	-0.061348	-0.013463	-0.070445
8	C	-0.061990	0.054989	-0.064930	0.653659	0.100047	0.067132
9	C	-0.026527	-0.035460	-0.047795	-0.279698	-0.219591	-0.026085
10	C	0.003741	-0.079905	0.021865	0.071349	0.501983	0.002630
11	C	0.020443	0.029198	0.016709	0.015248	0.001360	0.332399
12	O	-0.001263	-0.000044	-0.000010	0.000144	0.000687	0.000150
13	C	-0.000001	-0.001056	0.000195	0.002167	0.004317	0.001746
14	N	-0.000002	0.000969	-0.001516	0.000199	-0.002101	-0.000010
15	O	0.002139	0.000381	0.000368	0.008095	0.003732	0.000078
16	H	-0.000278	-0.000008	-0.000017	-0.000002	0.000000	-0.000258
17	H	-0.000009	-0.000495	-0.000008	0.000000	-0.000026	-0.000023
18	H	-0.000007	-0.000067	0.000000	-0.000001	-0.000938	0.000000
19	H	0.339708	0.000000	-0.000011	-0.000672	-0.000001	0.000143
20	H	0.000000	0.346349	-0.000161	-0.000007	-0.000128	-0.000026
21	H	-0.000011	-0.000161	0.323516	0.000370	0.000006	-0.000183
22	H	-0.000672	-0.000007	0.000370	0.325360	-0.000005	-0.000007
23	H	-0.000001	-0.000128	0.000006	-0.000005	0.313429	0.000000
24	H	0.000143	-0.000026	-0.000183	-0.000007	0.000000	0.425760
25	H	-0.000038	0.000114	-0.000303	-0.000028	0.000000	-0.014741
26	O	0.000002	-0.000013	0.000020	-0.000014	0.002988	0.000000
27	H	0.000000	0.000000	0.000000	0.000000	0.000002	0.000000
28	H	0.000001	0.000002	0.000000	-0.000017	-0.000308	0.000000
29	H	0.000000	0.000000	0.000000	0.000000	-0.000242	0.000000

		25	26	27	28	29
1	C	-0.044076	0.006636	-0.000158	-0.000141	-0.000135
2	C	-0.016018	-0.017609	0.000527	0.007476	0.000773
3	C	-0.001366	-0.012834	0.000075	0.000881	-0.000132
4	C	0.018417	-0.016475	0.000324	-0.002205	0.000754
5	C	0.001296	0.024890	-0.000197	-0.004253	-0.001945
6	C	0.033631	0.030706	-0.002024	-0.027779	-0.000127
7	C	-0.086033	-0.034018	0.000639	0.010839	0.002042
8	C	0.066696	-0.070292	0.009107	0.037393	-0.013004
9	C	-0.011475	-0.000701	0.008753	-0.039156	0.043800
10	C	-0.000173	-0.000230	-0.001035	0.032502	-0.019330
11	C	0.353741	-0.004126	0.000058	0.001006	0.000156
12	O	-0.000036	-0.001147	0.000016	0.000369	-0.000005
13	C	0.001978	0.041353	-0.004164	-0.017642	-0.022324
14	N	-0.000008	-0.070006	0.002824	-0.003738	0.065342
15	O	0.000023	-0.066403	0.002604	0.161248	0.001107
16	H	-0.000417	0.000000	0.000000	0.000000	0.000000
17	H	0.000218	0.000000	0.000000	0.000000	0.000000
18	H	0.000000	-0.000064	0.000000	-0.000003	0.000000
19	H	-0.000038	0.000002	0.000000	0.000001	0.000000
20	H	0.000114	-0.000013	0.000000	0.000002	0.000000
21	H	-0.000303	0.000020	0.000000	0.000000	0.000000
22	H	-0.000028	-0.000014	0.000000	-0.000017	0.000000
23	H	0.000000	0.002988	0.000002	-0.000308	-0.000242
24	H	-0.014741	0.000000	0.000000	0.000000	0.000000
25	H	0.421467	0.000000	0.000000	0.000000	0.000000
26	O	0.000000	8.777176	0.208766	0.059346	0.180534
27	H	0.000000	0.208766	0.269415	-0.000796	-0.009367

```
28  H    0.000000   0.059346  -0.000796   0.157274  -0.003959
29  H    0.000000   0.180534  -0.009367  -0.003959   0.205159
Total atomic charges:
             1
 1  C    0.622996
 2  C   -0.456335
 3  C    0.093231
 4  C    0.842137
 5  C   -1.192906
 6  C   -0.378854
 7  C    1.283121
 8  C   -2.681092
 9  C    3.191418
10  C   -0.334145
11  C   -2.472673
12  O   -0.602352
13  C   -0.135979
14  N   -0.736528
15  O   -0.735991
16  H    0.285236
17  H    0.281463
18  H    0.309437
19  H    0.310292
20  H    0.288993
21  H    0.328875
22  H    0.323267
23  H    0.336739
24  H    0.273810
25  H    0.277130
26  O   -1.038484
27  H    0.514631
28  H    0.631659
29  H    0.570903
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  C    0.908232
 2  C   -0.174872
 3  C    0.402668
 4  C    1.152429
 5  C   -1.192906
 6  C   -0.089861
 7  C    1.611996
 8  C   -2.357825
 9  C    3.191418
10  C    0.002594
11  C   -1.921733
12  O   -0.602352
13  C   -0.135979
14  N   -0.736528
15  O   -0.104332
16  H    0.000000
17  H    0.000000
18  H    0.000000
```

```
 19  H    0.000000
 20  H    0.000000
 21  H    0.000000
 22  H    0.000000
 23  H    0.000000
 24  H    0.000000
 25  H    0.000000
 26  O    0.047050
 27  H    0.000000
 28  H    0.000000
 29  H    0.000000
 Sum of Mulliken charges=   0.00000
 Electronic spatial extent (au):  <R**2>=  3001.8780
 Charge=     0.0000 electrons
 Dipole moment (Debye):
    X=    -4.9089    Y=     0.9393    Z=     1.7710  Tot=     5.3025
 Quadrupole moment (Debye-Ang):
   XX=   -97.0265   YY=  -114.6810   ZZ=   -91.8287
   XY=    27.7690   XZ=     2.3305   YZ=     3.6698
 Octapole moment (Debye-Ang**2):
  XXX=    11.5678  YYY=   -10.5375  ZZZ=     1.0029  XYY=     6.4686
  XXY=    89.7237  XXZ=     6.3530  XZZ=    -9.2108  YZZ=     5.7673
  YYZ=     8.8422  XYZ=     2.5233
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -2123.5316 YYYY= -1319.2522 ZZZZ=  -480.6033 XXXY=   424.4636
 XXXZ=    29.0007 YYYX=   205.2701 YYYZ=    13.1691 ZZZX=    10.3740
 ZZZY=     3.7842 XXYY=  -622.7949 XXZZ=  -482.2685 YYZZ=  -274.6840
 XXYZ=    17.5542 YYXZ=    -5.2116 ZZXY=    14.4456
 N-N= 1.163400585774D+03 E-N=-4.049095830197D+03  KE= 7.351470463416D+02
  Exact polarizability: 144.106  -0.264 131.821   3.243  -0.410 104.754
 Approx polarizability: 121.255   2.828 121.361   3.642  -1.833 103.405
 Full mass-weighted force constant matrix:
 Low frequencies --- -247.9451   -0.1774   -0.0015   -0.0011   -0.0007
0.7086
 Low frequencies ---    1.0774   71.6232   90.0411
 ******    1 imaginary frequencies (negative Signs) ******
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                      1                      2                      3
                     ?A                     ?A                     ?A
 Frequencies --  -247.9451                71.6232                90.0411
 Red. masses --     9.1386                 5.3793                 6.7627
 Frc consts  --     0.3310                 0.0163                 0.0323
 IR Inten    --    61.1727                 4.4324                 4.1820
 Raman Activ --    32.3073                 0.9316                 0.8697
 Depolar     --     0.6171                 0.6271                 0.7493
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.03   0.01  -0.02    -0.03  -0.02  -0.08    -0.03   0.06  -
0.03
   2   6     0.00   0.02  -0.01    -0.10  -0.02  -0.03    -0.05  -0.03  -
0.02
```

3	6	0.04	-0.01	-0.02	-0.12	0.00	0.03	0.02	-0.09	0.04
4	6	0.09	-0.04	-0.02	0.01	0.01	-0.02	0.04	0.02	0.01
5	6	0.07	-0.03	-0.02	-0.08	0.01	0.02	0.13	-0.03	0.04
6	6	-0.02	-0.03	0.04	-0.06	0.01	0.02	-0.11	-0.10	-0.02
7	6	-0.02	-0.06	0.04	0.03	0.02	0.00	-0.12	-0.05	-0.03
8	6	0.06	-0.11	0.03	0.04	0.04	0.04	-0.02	-0.07	0.01
9	6	0.13	-0.22	0.03	0.00	0.05	0.11	-0.02	-0.12	0.03
10	6	0.00	-0.05	0.04	-0.08	0.03	0.09	-0.03	-0.15	0.03
11	6	-0.02	0.00	0.01	0.04	-0.01	-0.09	-0.12	0.05	-0.06
12	8	0.01	-0.03	-0.01	-0.12	0.01	0.04	0.32	-0.03	0.04
13	6	-0.27	0.63	-0.04	0.00	0.04	0.16	0.05	0.03	0.09
14	7	-0.10	-0.28	-0.08	0.09	-0.07	-0.02	0.00	0.24	0.13
15	8	-0.08	0.09	-0.03	0.03	0.03	0.13	-0.08	-0.06	0.03
16	1	0.04	0.06	-0.05	-0.04	-0.05	-0.13	-0.01	0.13	-0.04
17	1	-0.02	0.05	-0.02	-0.14	-0.05	-0.07	-0.08	-0.02	-0.03
18	1	0.03	0.00	-0.02	-0.19	-0.01	0.05	0.05	-0.12	0.06
19	1	0.13	-0.05	-0.04	0.05	0.01	-0.04	0.09	0.08	0.01
20	1	-0.07	-0.02	0.06	-0.08	0.00	0.02	-0.17	-0.13	-0.03
21	1	-0.07	-0.10	0.06	0.07	0.04	0.02	-0.17	-0.09	-0.04
22	1	0.05	-0.14	0.03	0.10	0.06	0.05	-0.02	-0.06	0.00
23	1	-0.03	-0.05	0.08	-0.12	0.04	0.14	-0.04	-0.23	0.04
24	1	0.00	-0.01	0.01	0.10	-0.01	-0.11	-0.11	0.10	-0.08
25	1	-0.06	0.03	0.02	0.02	-0.03	-0.12	-0.19	0.07	-0.09
26	8	0.09	0.08	0.06	0.26	-0.07	-0.29	0.00	0.22	-0.19
27	1	0.09	0.07	0.19	0.30	-0.10	-0.50	-0.03	0.28	-0.36
28	1	-0.25	0.11	-0.11	0.13	-0.04	0.05	-0.06	0.03	-0.03
29	1	0.17	0.17	0.02	0.21	-0.08	-0.25	0.04	0.24	-0.08

		4			5			6		
		?A			?A			?A		
Frequencies --		92.8893			147.2228			157.5628		
Red. masses --		8.5268			9.0039			7.9111		
Frc consts --		0.0433			0.1150			0.1157		
IR Inten --		14.5814			16.1959			16.8104		
Raman Activ --		1.1852			2.5328			0.6631		
Depolar --		0.7491			0.5778			0.7229		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	-0.03	0.05	-0.03	0.10	0.01	-0.07	-0.12	0.07
2	6	0.11	-0.07	0.01	0.00	0.05	-0.01	-0.02	-0.10	0.04
3	6	0.07	-0.04	0.01	0.07	0.00	-0.02	-0.15	-0.02	0.05
4	6	-0.04	0.04	0.04	-0.01	0.05	-0.01	-0.19	0.00	0.07
5	6	-0.03	0.01	0.07	-0.01	0.04	0.03	-0.06	-0.01	0.03
6	6	0.12	-0.02	-0.11	-0.05	-0.01	-0.05	0.06	0.02	-0.04
7	6	0.04	0.03	-0.12	-0.12	0.00	-0.04	0.06	0.05	-0.06
8	6	-0.03	0.07	-0.09	-0.07	-0.03	-0.05	-0.09	0.12	-0.02
9	6	0.02	0.03	-0.14	-0.02	-0.09	-0.08	-0.09	0.16	-0.03
10	6	0.08	0.01	-0.12	0.00	-0.05	-0.08	-0.05	0.10	-0.02
11	6	0.03	0.00	-0.02	-0.13	0.09	0.00	0.06	-0.09	0.00
12	8	-0.12	0.02	0.15	-0.19	0.04	0.12	0.42	-0.02	-0.14
13	6	-0.12	0.06	0.10	0.32	0.12	0.25	0.05	0.13	0.12
14	7	-0.23	-0.08	0.52	0.46	-0.22	0.02	0.15	-0.22	0.03
15	8	0.02	0.01	-0.18	-0.02	-0.13	-0.14	-0.07	0.12	-0.03
16	1	0.03	-0.05	0.13	-0.01	0.16	0.03	-0.10	-0.23	0.13
17	1	0.17	-0.13	0.04	0.01	0.07	0.01	0.02	-0.20	0.06
18	1	0.11	-0.08	0.03	0.12	-0.02	-0.01	-0.18	-0.03	0.06
19	1	-0.10	0.07	0.08	-0.01	0.08	0.01	-0.24	0.00	0.10
20	1	0.20	-0.05	-0.16	-0.06	-0.02	-0.05	0.16	0.00	-0.09
21	1	0.04	0.05	-0.19	-0.18	-0.04	-0.05	0.13	0.12	-0.11
22	1	-0.10	0.12	-0.11	-0.12	-0.03	-0.06	-0.12	0.19	-0.04

23	1	0.11	0.00	-0.16	0.02	-0.10	-0.10	-0.04	0.15	-0.04
24	1	-0.02	0.04	-0.01	-0.17	0.12	0.01	0.03	-0.08	0.01
25	1	0.09	-0.04	-0.03	-0.16	0.11	0.01	0.15	-0.16	-0.01
26	8	0.04	-0.01	-0.15	-0.10	0.04	0.04	-0.08	-0.07	-0.01
27	1	0.09	-0.06	-0.20	-0.22	0.16	0.15	-0.10	-0.06	0.08
28	1	0.02	-0.01	-0.21	-0.06	-0.10	-0.12	-0.05	0.05	-0.03
29	1	-0.05	-0.01	0.12	0.09	0.10	0.04	-0.05	-0.06	-0.03

	7	8	9
	?A	?A	?A
Frequencies --	210.5575	232.7665	276.7378
Red. masses --	10.2593	6.5762	7.0692
Frc consts --	0.2680	0.2099	0.3190
IR Inten --	2.4792	14.1829	48.9533
Raman Activ --	1.7245	0.7980	0.5919
Depolar --	0.7496	0.4544	0.2880

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	-0.04	0.02	0.10	0.03	-0.10	0.01	0.02	0.03
2	6	0.02	-0.06	0.01	0.02	0.02	-0.04	0.06	0.00	0.00
3	6	-0.05	-0.01	0.03	0.04	0.01	0.03	0.09	-0.02	-0.04
4	6	-0.03	0.02	0.04	0.17	0.01	-0.04	0.00	-0.02	-0.01
5	6	-0.04	0.00	0.06	0.09	0.02	0.02	0.04	-0.02	-0.04
6	6	0.06	0.01	-0.06	0.03	0.01	0.04	0.02	-0.04	-0.03
7	6	0.03	0.02	-0.06	0.09	-0.03	0.04	-0.04	-0.02	-0.03
8	6	-0.01	0.04	-0.04	0.13	-0.06	0.03	-0.02	-0.02	-0.03
9	6	0.03	-0.01	-0.07	0.01	0.03	0.04	0.00	-0.01	-0.03
10	6	-0.01	0.08	-0.05	0.03	0.02	0.05	0.03	-0.07	-0.04
11	6	0.03	-0.02	-0.03	0.10	0.01	-0.06	-0.05	0.02	0.03
12	8	0.04	0.01	0.06	-0.01	0.02	0.10	-0.03	-0.03	-0.04
13	6	-0.34	-0.02	0.55	-0.11	-0.15	0.21	0.02	0.26	0.16
14	7	-0.09	0.17	-0.34	-0.03	-0.13	-0.07	0.05	0.35	0.00
15	8	0.18	-0.24	-0.18	-0.17	0.16	-0.02	-0.06	0.12	0.07

```
  16   1    -0.01  -0.07   0.05     0.11   0.04  -0.16     0.02   0.06
0.07
  17   1     0.04  -0.13   0.01    -0.04   0.02  -0.09     0.08   0.03
0.03
  18   1    -0.05  -0.04   0.05    -0.01   0.00   0.04     0.12  -0.01  -
0.05
  19   1    -0.05   0.03   0.05     0.24   0.03  -0.07    -0.03  -0.02
0.00
  20   1     0.14   0.01  -0.08     0.00   0.04   0.07     0.00  -0.05  -
0.05
  21   1     0.04   0.04  -0.07     0.09  -0.04   0.09    -0.08  -0.04  -
0.06
  22   1    -0.07   0.07  -0.06     0.18  -0.08   0.05    -0.03  -0.01  -
0.04
  23   1     0.00   0.09  -0.06     0.04   0.02   0.04     0.04  -0.08  -
0.05
  24   1     0.02   0.00  -0.03     0.18   0.01  -0.09    -0.10   0.02
0.05
  25   1     0.07  -0.05  -0.04     0.02   0.04  -0.09    -0.03   0.03
0.06
  26   8     0.06   0.08   0.11    -0.34  -0.02  -0.16    -0.06  -0.41  -
0.02
  27   1     0.01   0.12   0.24    -0.36  -0.02  -0.01    -0.06  -0.43
0.07
  28   1     0.07  -0.12  -0.13    -0.12   0.20  -0.05     0.08  -0.08
0.10
  29   1     0.11   0.09  -0.03    -0.34  -0.03  -0.20    -0.13  -0.47  -
0.09
                     10                    11                    12
                     ?A                    ?A                    ?A
 Frequencies --   287.2625              328.3092              370.8175
 Red. masses --     6.3571                1.1478                4.2800
 Frc consts  --     0.3091                0.0729                0.3468
 IR Inten    --     4.1324              188.7219               47.5146
 Raman Activ --     0.7462                2.2046                1.0838
 Depolar     --     0.6571                0.7500                0.5935
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00  -0.03  -0.10     0.00   0.00   0.00    -0.01  -0.02  -
0.10
   2   6    -0.12   0.00  -0.02     0.00   0.00   0.00    -0.04   0.04  -
0.08
   3   6    -0.16   0.03   0.08     0.00   0.00   0.00    -0.04  -0.01  -
0.07
   4   6     0.07   0.02   0.00     0.00   0.00   0.00     0.01  -0.01  -
0.11
   5   6    -0.02   0.03   0.09     0.00   0.00   0.00     0.01   0.01  -
0.01
   6   6    -0.04   0.08   0.08    -0.01   0.00   0.00    -0.01   0.04
0.00
   7   6     0.06   0.00   0.10    -0.01   0.00   0.00    -0.01  -0.06
0.05
   8   6     0.04  -0.04   0.05     0.00   0.00   0.00    -0.02  -0.10  -
0.07
```

```
    9   6     0.02  -0.02  -0.01     0.00   0.00   0.00    -0.06   0.01  -
0.09
   10   6    -0.08   0.14   0.05     0.00  -0.01   0.00    -0.03   0.04  -
0.09
   11   6     0.09  -0.04  -0.05    -0.01   0.00   0.00    -0.01  -0.11
0.16
   12   8     0.07   0.05   0.16     0.00   0.00   0.00     0.09   0.05
0.23
   13   6     0.08   0.18  -0.21     0.01  -0.03   0.00     0.02  -0.07
0.04
   14   7     0.00   0.11   0.05    -0.01   0.01   0.01     0.01   0.02  -
0.01
   15   8     0.09  -0.24  -0.20    -0.02   0.02  -0.01    -0.10   0.13  -
0.04
   16   1    -0.01  -0.06  -0.19     0.00   0.00   0.00    -0.02  -0.03  -
0.14
   17   1    -0.20  -0.04  -0.09     0.00   0.00   0.00    -0.08   0.06  -
0.11
   18   1    -0.23  -0.01   0.11     0.00   0.00   0.00    -0.03   0.00  -
0.07
   19   1     0.15   0.05  -0.03     0.00   0.00   0.00     0.04   0.00  -
0.12
   20   1    -0.02   0.13   0.14    -0.01   0.00   0.00    -0.01   0.10
0.06
   21   1     0.12   0.01   0.17    -0.01   0.00   0.00     0.00  -0.07
0.11
   22   1     0.04  -0.11   0.06     0.00   0.00   0.00    -0.04  -0.18  -
0.06
   23   1    -0.09   0.19   0.07     0.00  -0.01   0.00     0.00   0.08  -
0.13
   24   1     0.21  -0.07  -0.09    -0.01   0.00   0.00    -0.13  -0.42
0.26
   25   1     0.01  -0.03  -0.08    -0.01   0.00   0.00     0.09   0.07
0.43
   26   8    -0.11  -0.14  -0.06     0.05   0.00  -0.07     0.15  -0.01
0.09
   27   1    -0.20  -0.08   0.19    -0.16   0.10   0.96     0.28  -0.13  -
0.07
   28   1     0.09  -0.17  -0.21    -0.03   0.05  -0.05    -0.14   0.08  -
0.03
   29   1    -0.09  -0.14   0.02     0.10   0.01  -0.12     0.05  -0.03
0.05
                      13                    14                    15
                      ?A                    ?A                    ?A
 Frequencies --    411.1742              451.6891              498.9235
 Red. masses --      3.3290                3.4794                3.1478
 Frc consts  --      0.3316                0.4182                0.4617
 IR Inten    --     56.8202               11.2142               23.9319
 Raman Activ --      0.4928                1.0882                1.7745
 Depolar     --      0.3170                0.5970                0.7455
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.02  -0.02  -0.03     0.05   0.08   0.00     0.01   0.01  -
0.08
```

2	6	0.02	0.03	-0.06	-0.04	-0.06	0.02	-0.02	-0.01	-0.07
3	6	0.04	-0.01	-0.09	-0.12	-0.01	0.15	0.03	-0.02	0.07
4	6	-0.07	0.03	-0.07	0.17	-0.03	0.02	0.02	0.08	0.02
5	6	0.00	0.02	-0.06	0.01	-0.06	0.09	0.03	0.06	0.04
6	6	0.00	-0.01	-0.04	0.02	0.02	-0.09	-0.03	-0.06	-0.03
7	6	0.02	0.04	-0.05	-0.04	-0.01	-0.08	0.04	0.05	-0.07
8	6	-0.02	0.08	-0.03	0.08	-0.04	-0.08	-0.01	0.12	0.07
9	6	0.03	-0.02	0.05	0.03	0.06	-0.04	-0.02	-0.02	0.10
10	6	0.01	-0.05	0.01	-0.07	0.09	-0.03	0.04	-0.10	0.13
11	6	0.02	-0.09	0.15	-0.11	0.06	0.15	0.06	-0.06	0.09
12	8	0.02	0.05	0.08	-0.03	-0.10	-0.08	-0.04	0.04	-0.12
13	6	-0.03	0.07	-0.01	0.00	0.00	-0.02	0.01	-0.02	0.01
14	7	-0.02	-0.04	0.00	0.00	-0.02	0.00	0.01	0.02	0.00
15	8	0.13	-0.09	0.17	0.09	0.04	0.01	-0.13	-0.05	-0.14
16	1	-0.04	-0.08	-0.02	0.10	0.24	-0.06	-0.01	-0.03	-0.09
17	1	0.03	0.07	-0.05	-0.08	-0.23	-0.03	-0.06	-0.04	-0.10
18	1	0.03	0.01	-0.11	-0.15	-0.05	0.18	-0.02	-0.10	0.13
19	1	-0.09	0.00	-0.07	0.19	0.08	0.05	0.09	0.15	0.01
20	1	-0.06	-0.05	-0.06	0.11	0.01	-0.13	-0.15	-0.13	-0.07
21	1	0.06	0.07	-0.09	-0.15	-0.08	-0.07	0.10	0.11	-0.14
22	1	0.04	0.11	-0.02	0.08	0.00	-0.09	0.08	0.23	0.07
23	1	-0.02	-0.06	0.04	-0.08	0.05	-0.02	0.02	-0.17	0.15
24	1	-0.18	-0.36	0.27	-0.35	-0.16	0.27	-0.13	-0.34	0.20
25	1	0.23	0.04	0.42	0.05	0.21	0.42	0.24	0.08	0.37
26	8	-0.13	0.02	-0.09	-0.03	0.01	-0.02	0.04	-0.01	0.03
27	1	-0.32	0.22	0.08	-0.04	0.02	0.01	0.17	-0.15	-0.01
28	1	0.19	-0.10	0.22	0.10	0.05	0.07	-0.17	0.01	-0.27

```
  29   1     0.03   0.06  -0.07    -0.04   0.00  -0.02    -0.07  -0.03
0.05
                     16                    17                    18
                     ?A                    ?A                    ?A
 Frequencies --    524.2050              557.6971              592.4383
 Red. masses --      7.1425                3.7128                6.0528
 Frc consts  --      1.1564                0.6804                1.2517
 IR Inten    --      0.7867               12.1646               39.1676
 Raman Activ --      4.5892                1.7275               20.4804
 Depolar     --      0.3943                0.1752                0.0744
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.13  -0.04   0.04    -0.03  -0.03  -0.06    -0.12  -0.10
0.03
   2   6     0.07  -0.10   0.01    -0.10   0.13   0.03    -0.10   0.00
0.01
   3   6    -0.08   0.08   0.08     0.13   0.04   0.11     0.00   0.00  -
0.01
   4   6     0.08   0.07   0.08     0.03   0.03   0.10    -0.04   0.00
0.13
   5   6    -0.02   0.32   0.07     0.11  -0.05   0.15    -0.07   0.15
0.05
   6   6     0.09  -0.06  -0.03    -0.13   0.10   0.01    -0.14  -0.04  -
0.01
   7   6     0.03  -0.16  -0.03     0.05   0.05   0.03    -0.06  -0.06
0.03
   8   6    -0.02  -0.15  -0.08    -0.07   0.01  -0.10     0.09  -0.04
0.07
   9   6    -0.13  -0.15  -0.07    -0.07  -0.01  -0.14     0.32  -0.03  -
0.07
  10   6    -0.10   0.01  -0.12    -0.04  -0.06  -0.10     0.02  -0.12  -
0.04
  11   6     0.05  -0.07  -0.01     0.13  -0.09  -0.03    -0.08  -0.13  -
0.01
  12   8    -0.02   0.32  -0.13    -0.03  -0.10  -0.06     0.00   0.16  -
0.05
  13   6     0.00   0.00  -0.01    -0.01   0.01   0.01     0.01  -0.06
0.02
  14   7    -0.01   0.01   0.01    -0.01  -0.01   0.00     0.01   0.01
0.00
  15   8    -0.10  -0.09   0.17     0.02   0.01   0.05     0.21   0.21  -
0.10
  16   1     0.13  -0.06   0.09    -0.08  -0.14  -0.21    -0.13  -0.13  -
0.03
  17   1     0.04  -0.20  -0.02    -0.12   0.17   0.02    -0.04   0.05
0.07
  18   1     0.00  -0.16   0.26     0.25  -0.02   0.14     0.10  -0.15
0.09
  19   1     0.04   0.01   0.08     0.07   0.27   0.17     0.01  -0.10
0.07
  20   1     0.22   0.00   0.00    -0.18   0.10   0.03    -0.21  -0.03
0.02
  21   1     0.01  -0.17  -0.04     0.19   0.10   0.15    -0.05  -0.08
0.10
```

22	1	-0.12	-0.12	-0.11	-0.23	-0.03	-0.12	-0.12	-0.04	0.03
23	1	-0.01	0.08	-0.23	0.07	-0.20	-0.22	-0.13	-0.22	0.16
24	1	0.03	-0.02	-0.02	0.17	-0.13	-0.04	-0.09	-0.14	0.00
25	1	-0.02	-0.04	-0.03	0.16	-0.12	-0.03	-0.03	-0.15	0.00
26	8	0.02	-0.01	0.00	0.01	0.00	0.00	-0.06	0.01	-0.03
27	1	-0.11	0.14	0.02	-0.13	0.15	-0.02	0.12	-0.20	0.00
28	1	-0.12	-0.12	0.23	0.04	-0.08	0.14	0.22	0.26	-0.08
29	1	0.17	0.03	-0.06	0.15	0.04	-0.01	-0.29	-0.06	0.01

	19	20	21
	?A	?A	?A
Frequencies --	619.9575	665.6761	678.8224
Red. masses --	3.5713	1.2757	5.2172
Frc consts --	0.8087	0.3331	1.4165
IR Inten --	24.7387	117.8007	11.4134
Raman Activ --	1.9138	4.9483	5.3173
Depolar --	0.7474	0.4414	0.5108

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	-0.06	0.17	0.01	0.00	0.03	0.11	0.10	0.06
2	6	-0.04	0.10	0.12	-0.02	0.00	0.03	-0.09	-0.08	0.14
3	6	-0.01	0.12	-0.03	-0.03	0.00	-0.01	-0.13	-0.16	-0.07
4	6	0.04	-0.11	0.04	0.02	-0.02	0.00	0.01	0.09	-0.08
5	6	0.02	-0.01	-0.06	-0.01	0.00	-0.02	-0.09	-0.01	-0.07
6	6	-0.11	0.07	-0.09	-0.03	-0.01	0.00	-0.05	-0.12	0.14
7	6	0.03	0.05	-0.19	0.01	0.02	-0.02	0.09	0.14	0.11
8	6	0.12	-0.02	-0.11	0.04	0.01	0.00	0.01	0.06	-0.08
9	6	0.02	-0.09	0.05	0.03	-0.01	0.00	0.02	-0.09	-0.12
10	6	-0.11	0.02	0.03	-0.01	-0.02	0.01	-0.11	-0.17	-0.10
11	6	0.06	-0.02	-0.01	0.01	0.02	0.01	0.21	0.19	0.09
12	8	0.02	0.02	0.07	0.00	0.01	0.01	0.00	0.01	-0.02
13	6	0.02	-0.02	-0.01	0.00	-0.03	0.00	0.00	0.00	0.01
14	7	0.01	0.01	0.00	-0.01	0.01	0.00	0.01	0.00	0.00

```
  15   8    -0.07  -0.04  -0.01    -0.03   0.05  -0.05     0.02   0.01
0.00
  16   1     0.02  -0.06   0.03     0.01   0.01   0.01     0.08   0.04
0.03
  17   1     0.07   0.11   0.20    -0.02   0.01   0.03    -0.23   0.04
0.06
  18   1     0.06   0.25  -0.14    -0.02   0.02  -0.03     0.04  -0.17  -
0.09
  19   1    -0.10  -0.26   0.05    -0.01  -0.07  -0.01    -0.12   0.00  -
0.05
  20   1    -0.12  -0.02  -0.20    -0.03  -0.04  -0.03     0.05  -0.20
0.02
  21   1     0.06   0.02  -0.05     0.01   0.01   0.00     0.08   0.14
0.08
  22   1     0.23   0.16  -0.11     0.05   0.02   0.00    -0.11  -0.13  -
0.08
  23   1    -0.17  -0.07   0.11    -0.04  -0.03   0.05    -0.15  -0.04  -
0.07
  24   1    -0.14   0.13   0.04    -0.02   0.03   0.02     0.22   0.14
0.10
  25   1     0.26  -0.18  -0.04     0.05   0.00   0.02     0.21   0.21
0.12
  26   8     0.00   0.01   0.00     0.02  -0.06   0.02    -0.01   0.02  -
0.01
  27   1     0.21  -0.24   0.07    -0.46   0.53  -0.21     0.19  -0.22
0.07
  28   1    -0.15   0.11  -0.07     0.08  -0.24  -0.04    -0.04   0.10
0.02
  29   1    -0.23  -0.05  -0.02     0.58   0.12   0.09    -0.25  -0.05  -
0.01
                     22                    23                    24
                     ?A                    ?A                    ?A
 Frequencies --    733.6307              806.2886              832.6478
 Red. masses --      7.1502                4.4050                5.2933
 Frc consts  --      2.2674                1.6872                2.1622
 IR Inten    --     32.9443               13.8089                2.7035
 Raman Activ --     21.1018                2.7528                6.2864
 Depolar     --      0.6133                0.2510                0.0237
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.11  -0.03   0.07    -0.06  -0.08   0.00    -0.19   0.06
0.14
   2   6    -0.04   0.00   0.09    -0.08  -0.11   0.15    -0.08  -0.09  -
0.20
   3   6     0.10  -0.04   0.04    -0.01  -0.03  -0.11    -0.01  -0.10  -
0.07
   4   6     0.09  -0.11  -0.08     0.18   0.08   0.01    -0.03  -0.02
0.12
   5   6     0.19   0.06  -0.13     0.24   0.00  -0.09     0.30   0.02  -
0.08
   6   6    -0.13  -0.18   0.05     0.09  -0.04   0.12     0.02   0.04  -
0.21
   7   6     0.00  -0.14   0.03    -0.09   0.11  -0.01     0.09   0.03
0.06
```

8	6	-0.02	0.03	0.01	-0.11	0.13	0.02	-0.05	-0.13	0.09
9	6	-0.25	0.45	0.01	0.05	-0.09	-0.02	0.00	0.02	0.00
10	6	-0.14	-0.10	0.03	-0.06	0.11	-0.01	-0.08	0.06	0.02
11	6	-0.03	-0.07	0.00	-0.10	-0.15	-0.06	0.13	0.13	0.09
12	8	-0.03	0.10	0.01	-0.04	0.01	0.00	-0.06	0.03	0.01
13	6	-0.04	0.09	0.00	0.01	-0.03	0.00	0.00	0.00	0.00
14	7	-0.01	-0.04	-0.01	0.01	0.01	0.00	0.00	0.00	0.00
15	8	0.12	-0.01	-0.09	-0.01	0.02	0.01	0.01	0.00	0.00
16	1	0.14	0.06	0.01	-0.02	0.05	-0.05	-0.25	-0.10	0.13
17	1	-0.11	0.13	0.06	-0.06	0.06	0.19	0.18	-0.28	-0.05
18	1	0.15	0.01	-0.01	0.05	0.03	-0.17	-0.24	-0.21	0.03
19	1	-0.08	-0.25	-0.05	0.23	0.19	0.03	0.03	-0.04	0.09
20	1	-0.11	-0.16	0.07	0.38	-0.10	-0.03	-0.08	0.07	-0.15
21	1	0.05	-0.10	0.01	0.06	0.23	-0.13	-0.02	-0.04	0.06
22	1	0.19	-0.01	0.05	-0.20	0.08	0.01	-0.19	-0.21	0.08
23	1	-0.05	-0.28	-0.06	-0.12	0.38	0.04	-0.15	-0.02	0.10
24	1	-0.07	0.07	-0.01	-0.08	-0.23	-0.06	0.24	0.18	0.04
25	1	-0.10	-0.08	-0.06	-0.01	-0.17	-0.02	0.14	0.00	-0.04
26	8	0.02	0.03	0.00	0.00	0.00	0.00	0.01	0.00	0.00
27	1	0.05	-0.02	0.07	0.00	-0.01	0.01	0.00	0.01	0.01
28	1	0.23	-0.08	-0.05	-0.01	0.00	-0.01	0.04	-0.01	0.01
29	1	-0.10	-0.01	0.14	-0.01	0.00	0.06	-0.02	0.00	0.11

	25	26	27
	?A	?A	?A
Frequencies --	838.3684	851.8703	857.1581
Red. masses --	3.7301	1.5414	1.8626
Frc consts --	1.5447	0.6590	0.8063
IR Inten --	11.5521	112.7691	59.2326
Raman Activ --	11.0008	4.2256	2.3009
Depolar --	0.0170	0.2294	0.2764

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z

1	6	-0.13	-0.03	0.01	0.06	0.00	0.02	0.10	0.00	0.04
2	6	-0.02	-0.07	0.10	0.04	0.00	-0.03	0.03	0.02	-0.07
3	6	-0.01	-0.03	0.19	-0.04	0.05	0.05	-0.05	0.03	0.00
4	6	-0.06	-0.01	-0.21	-0.04	0.04	-0.04	-0.04	0.05	0.01
5	6	0.08	0.04	-0.06	0.04	-0.01	-0.01	0.07	-0.02	-0.02
6	6	0.03	0.08	0.02	-0.01	0.00	0.03	-0.04	-0.04	0.05
7	6	-0.03	0.14	0.04	0.00	-0.03	-0.01	0.01	-0.08	-0.03
8	6	0.03	-0.08	-0.18	-0.06	-0.01	-0.08	-0.08	0.01	-0.06
9	6	0.00	0.00	-0.02	0.03	-0.04	-0.02	0.04	-0.03	-0.03
10	6	0.15	-0.04	0.12	-0.01	0.00	0.08	-0.02	0.02	0.10
11	6	-0.03	-0.03	0.00	0.01	-0.02	0.00	0.01	-0.01	0.00
12	8	-0.02	0.07	-0.01	-0.01	-0.01	0.01	-0.02	-0.03	0.01
13	6	0.00	0.01	0.00	0.00	-0.01	0.01	0.01	-0.01	0.00
14	7	0.00	0.00	0.01	0.01	0.00	-0.02	0.00	0.00	0.02
15	8	0.01	0.00	-0.01	0.01	0.04	0.01	0.04	0.03	-0.03
16	1	-0.14	-0.04	0.03	0.05	-0.03	0.12	0.09	-0.03	0.15
17	1	0.03	-0.26	0.11	0.00	-0.05	-0.06	-0.04	0.06	-0.11
18	1	-0.16	0.01	0.19	-0.17	0.10	0.02	-0.24	0.08	-0.01
19	1	-0.12	0.05	-0.17	-0.13	0.13	0.03	-0.15	0.12	0.09
20	1	-0.02	-0.07	-0.13	-0.10	0.00	0.05	-0.17	-0.02	0.12
21	1	-0.04	0.09	0.19	0.02	-0.02	-0.01	0.03	-0.05	-0.08
22	1	0.22	-0.30	-0.11	-0.09	-0.05	-0.08	-0.17	0.03	-0.08
23	1	0.29	-0.21	-0.02	-0.02	-0.03	0.11	-0.03	0.05	0.11
24	1	0.09	-0.02	-0.05	0.02	0.04	-0.01	-0.03	0.07	0.01
25	1	0.03	-0.15	-0.09	-0.05	-0.02	-0.03	-0.05	0.01	-0.02
26	8	0.00	0.00	0.02	0.00	0.00	-0.04	-0.01	0.00	0.04
27	1	0.01	0.00	-0.03	-0.01	0.00	0.07	0.00	0.00	-0.07

```
  28   1    -0.06   0.07   0.06     0.16  -0.12  -0.12    -0.09   0.14
0.11
  29   1     0.06  -0.02  -0.37    -0.16   0.03   0.85     0.14  -0.03  -
0.77
                     28                     29                     30
                     ?A                     ?A                     ?A
 Frequencies --   869.1199               892.9974               919.9530
 Red. masses --     3.4001                 2.4388                 2.9295
 Frc consts  --     1.5132                 1.1458                 1.4607
 IR Inten    --     0.2543                 8.0378                 5.8943
 Raman Activ --    12.5297                 2.6843                 3.8882
 Depolar     --     0.0259                 0.6793                 0.3773
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.13  -0.02   0.06    -0.01   0.04  -0.05     0.02  -0.04
0.09
   2   6     0.09  -0.05  -0.09     0.07  -0.06   0.10     0.12  -0.04  -
0.06
   3   6    -0.12   0.02   0.00     0.03   0.16   0.04     0.03  -0.09  -
0.08
   4   6     0.16  -0.11   0.01    -0.01   0.09  -0.07    -0.02   0.19  -
0.05
   5   6    -0.03   0.00  -0.04    -0.04  -0.03  -0.03     0.00  -0.01
0.06
   6   6    -0.10   0.14  -0.07     0.02  -0.02  -0.14    -0.09   0.06  -
0.01
   7   6    -0.04   0.13   0.09    -0.02  -0.02   0.06    -0.03   0.02
0.09
   8   6    -0.11   0.10   0.08    -0.07  -0.04   0.09     0.17   0.01  -
0.06
   9   6    -0.01  -0.01  -0.03     0.03   0.01   0.02    -0.01   0.03
0.05
  10   6     0.08  -0.10  -0.07    -0.13  -0.05   0.00    -0.11   0.02  -
0.04
  11   6    -0.05  -0.07   0.00     0.05  -0.03  -0.01    -0.06  -0.09
0.01
  12   8     0.01   0.01   0.02     0.01  -0.03   0.01    -0.01  -0.04  -
0.03
  13   6     0.00   0.01   0.01     0.00  -0.01   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.01     0.00   0.00
0.00
  15   8    -0.01  -0.01   0.02     0.02   0.02  -0.02    -0.02  -0.02  -
0.01
  16   1     0.23   0.24   0.13    -0.03  -0.02   0.00     0.04  -0.02
0.38
  17   1     0.14  -0.26  -0.10     0.12  -0.33   0.09     0.23  -0.02
0.02
  18   1    -0.23  -0.02   0.04     0.20   0.43  -0.19     0.08  -0.23
0.02
  19   1     0.08  -0.28  -0.01     0.11   0.17  -0.10     0.02   0.42
0.02
  20   1    -0.28   0.12  -0.05     0.20  -0.01  -0.19    -0.14   0.11
0.05
```

21	1	0.20	0.26	0.18	0.01	0.01	0.02	0.05	0.00	0.31
22	1	-0.22	0.00	0.08	-0.12	-0.18	0.10	0.40	0.00	-0.02
23	1	0.10	-0.26	-0.08	-0.26	-0.35	0.17	-0.21	0.06	0.06
24	1	0.04	0.03	-0.05	0.17	-0.13	-0.03	0.00	0.01	-0.03
25	1	-0.08	-0.13	-0.09	-0.02	0.04	0.01	-0.09	-0.16	-0.07
26	8	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00
27	1	0.03	-0.03	0.01	-0.01	0.01	-0.02	-0.02	0.02	-0.01
28	1	-0.02	-0.01	0.03	0.00	0.04	0.01	-0.03	0.00	-0.05
29	1	-0.03	-0.01	-0.04	0.04	0.00	-0.16	0.03	0.00	-0.02

	31			32			33		
	?A			?A			?A		
Frequencies --	939.5888			963.8531			989.4729		
Red. masses --	2.3094			2.7193			2.1454		
Frc consts --	1.2012			1.4884			1.2376		
IR Inten --	1.7871			2.7982			8.8845		
Raman Activ --	2.5953			13.9946			3.2117		
Depolar --	0.5513			0.2484			0.2966		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.11	0.01	0.05	0.09	0.01	-0.04	0.03	0.00	0.01
2 6	0.10	0.13	0.03	0.08	0.01	-0.02	-0.03	0.15	-0.01
3 6	-0.12	0.01	-0.02	0.13	-0.07	0.03	-0.01	-0.10	0.04
4 6	0.10	0.06	-0.04	-0.05	-0.09	-0.02	0.02	-0.04	-0.09
5 6	-0.04	-0.01	0.03	-0.05	0.02	0.05	-0.02	0.02	0.03
6 6	-0.03	-0.12	-0.02	-0.06	-0.06	-0.01	0.11	0.02	-0.10
7 6	-0.03	0.02	-0.05	-0.04	0.18	-0.02	-0.02	-0.03	0.03
8 6	-0.02	-0.07	0.05	-0.06	-0.11	0.04	-0.07	0.06	-0.02
9 6	-0.04	0.04	-0.02	0.02	-0.01	-0.01	0.05	-0.03	0.04
10 6	0.07	-0.01	-0.01	-0.10	0.13	0.07	-0.07	-0.01	0.01
11 6	0.06	-0.03	0.00	0.00	-0.01	-0.06	0.00	-0.05	0.10
12 8	0.01	-0.02	0.00	0.01	0.02	-0.01	0.00	0.01	-0.01
13 6	0.00	0.01	0.00	0.00	-0.01	0.00	0.01	-0.01	0.00

14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.02	0.00	0.01	0.02	0.02	0.00	0.00	0.01	-0.01
16	1	-0.13	-0.06	0.05	0.15	0.13	0.07	0.02	-0.01	-0.09
17	1	0.30	0.37	0.20	-0.03	0.12	-0.09	-0.09	0.35	-0.02
18	1	-0.33	-0.05	0.05	0.18	-0.22	0.13	0.00	-0.30	0.19
19	1	0.34	0.21	-0.11	-0.13	-0.20	-0.02	-0.01	-0.03	-0.07
20	1	-0.18	-0.24	-0.10	-0.11	-0.27	-0.23	0.37	0.05	-0.14
21	1	-0.07	0.02	-0.15	0.04	0.24	-0.01	-0.02	0.00	-0.05
22	1	-0.07	-0.21	0.07	-0.15	-0.44	0.07	0.01	0.08	-0.01
23	1	0.11	0.14	-0.08	-0.16	0.31	0.12	-0.20	-0.16	0.18
24	1	0.05	0.00	0.00	-0.07	-0.14	-0.01	0.27	0.31	-0.07
25	1	0.21	-0.17	-0.06	0.19	-0.01	0.07	-0.26	-0.21	-0.26
26	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	1	0.01	0.00	0.01	-0.01	0.01	0.00	-0.01	0.00	-0.01
28	1	0.03	-0.01	0.04	0.02	0.03	0.02	0.00	0.02	-0.04
29	1	-0.02	0.00	0.03	0.01	0.00	0.00	0.02	0.00	-0.04

	34			35			36		
	?A			?A			?A		
Frequencies --	1005.3919			1018.2610			1032.0275		
Red. masses --	5.9328			2.6628			2.2411		
Frc consts --	3.5333			1.6267			1.4063		
IR Inten --	0.2156			3.4559			3.3800		
Raman Activ --	0.2394			6.4816			13.4703		
Depolar --	0.6535			0.1079			0.7320		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.14	-0.13	-0.09	-0.10	0.22	0.03	0.10	0.00	-0.03
2	6	0.12	-0.01	-0.18	0.00	0.03	0.01	-0.02	0.07	0.03
3	6	0.00	0.24	-0.06	-0.01	-0.01	0.01	-0.10	-0.02	-0.04
4	6	0.04	-0.16	0.12	-0.03	-0.02	0.02	-0.09	0.05	0.11
5	6	0.01	0.01	0.10	-0.03	0.00	-0.01	0.07	-0.01	-0.02
6	6	0.15	-0.16	0.10	0.04	-0.04	0.00	0.08	0.05	-0.03

7	6	0.02	0.19	0.13	0.23	-0.03	0.01	-0.04	0.06	0.01
8	6	0.11	0.06	-0.17	0.02	-0.01	-0.03	0.05	-0.10	0.03
9	6	-0.05	0.01	-0.07	0.00	-0.02	-0.03	-0.02	0.05	0.02
10	6	-0.16	-0.15	0.07	-0.03	-0.02	0.02	0.03	-0.09	-0.02
11	6	-0.10	0.09	0.07	-0.10	-0.12	-0.06	-0.03	-0.03	-0.10
12	8	0.01	0.00	0.01	0.00	0.00	0.00	-0.02	-0.01	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	-0.01	-0.02	-0.01	0.00	0.00	0.00	-0.01	0.00
16	1	-0.10	-0.03	-0.04	0.05	0.64	0.13	0.11	0.02	0.01
17	1	0.17	0.23	-0.12	0.06	0.03	0.05	-0.13	0.37	0.00
18	1	-0.21	0.23	-0.02	-0.02	0.01	0.00	-0.30	-0.02	-0.02
19	1	0.10	-0.02	0.15	-0.03	-0.07	0.00	-0.25	0.06	0.19
20	1	0.13	-0.30	-0.04	0.01	-0.03	0.03	0.42	-0.01	-0.20
21	1	-0.17	0.11	0.02	0.55	0.14	0.06	-0.01	0.04	0.16
22	1	0.07	0.02	-0.17	-0.06	0.02	-0.05	0.07	-0.17	0.04
23	1	-0.18	-0.15	0.09	-0.03	0.00	0.02	0.00	-0.31	0.03
24	1	0.19	0.07	-0.03	-0.07	-0.19	-0.06	-0.15	-0.27	-0.01
25	1	-0.16	0.00	-0.07	-0.11	-0.10	-0.03	0.08	0.14	0.16
26	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	1	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	-0.01	-0.02	0.01	-0.03	0.01	0.02	0.01	0.00	-0.01
29	1	-0.01	0.00	-0.03	0.00	0.00	0.01	0.00	0.00	0.00

	37	38	39
	?A	?A	?A
Frequencies --	1037.0250	1052.2436	1072.5461
Red. masses --	1.9029	2.0779	1.8122
Frc consts --	1.2057	1.3555	1.2282
IR Inten --	0.6011	2.2892	0.9721
Raman Activ --	2.6365	10.7943	5.5696
Depolar --	0.5354	0.5112	0.6759

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	-0.04	0.09	-0.07	-0.01	-0.05	0.03	-0.11	-0.02
2	6	-0.06	0.01	-0.09	0.15	0.02	0.03	-0.02	0.00	0.05
3	6	0.01	0.07	0.06	-0.02	-0.07	0.05	0.01	-0.03	-0.05
4	6	-0.02	0.03	-0.09	-0.01	-0.07	-0.03	0.04	0.04	-0.01
5	6	0.01	-0.01	0.01	0.04	0.01	-0.02	-0.03	0.01	0.02
6	6	0.05	0.00	0.08	0.00	0.10	0.09	-0.01	0.04	-0.03
7	6	0.04	0.05	-0.08	0.01	-0.04	-0.04	0.14	0.00	-0.02
8	6	0.02	-0.03	0.11	-0.03	0.04	0.02	-0.05	-0.05	0.00
9	6	0.00	-0.01	-0.01	0.01	-0.02	-0.01	-0.01	0.02	-0.01
10	6	-0.04	-0.05	-0.07	-0.12	-0.03	-0.01	0.02	-0.01	0.06
11	6	-0.04	0.00	-0.01	0.02	0.07	-0.09	-0.10	0.08	0.02
12	8	0.00	-0.02	0.00	-0.01	0.01	0.00	0.00	0.01	-0.01
13	6	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.01	0.01	-0.01	0.00	0.00	0.00
16	1	-0.01	-0.10	0.34	-0.09	-0.09	0.00	-0.08	-0.38	-0.19
17	1	-0.33	0.00	-0.28	0.38	0.07	0.19	0.11	0.06	0.14
18	1	0.09	0.04	0.07	-0.12	-0.25	0.19	0.00	-0.02	-0.06
19	1	0.16	0.06	-0.16	0.07	-0.14	-0.10	0.13	0.14	-0.02
20	1	0.18	0.16	0.21	0.08	0.35	0.33	-0.06	-0.05	-0.12
21	1	0.09	0.14	-0.28	-0.03	-0.05	-0.07	0.45	0.15	0.11
22	1	0.05	-0.26	0.15	-0.08	0.11	0.00	-0.15	-0.17	0.00
23	1	0.02	-0.16	-0.12	-0.18	-0.24	0.07	-0.03	-0.02	0.12
24	1	-0.30	0.20	0.05	-0.19	-0.20	0.04	-0.34	0.28	0.07
25	1	0.19	-0.17	-0.04	0.19	0.20	0.18	-0.29	0.22	0.05
26	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.01	0.02	0.00	0.01	0.00	0.00	0.00	0.02
29	1	0.00	0.00	0.00	0.00	0.00	-0.02	0.00	0.00	0.00

		40			41			42		
		?A			?A			?A		
Frequencies --		1092.2622			1155.7059			1180.1798		
Red. masses --		3.4342			1.8748			1.8557		
Frc consts --		2.4140			1.4754			1.5229		
IR Inten --		0.2115			18.5397			17.2584		
Raman Activ --		9.3342			4.7806			1.7560		
Depolar --		0.5229			0.5390			0.4989		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	-0.04	-0.05	-0.01	-0.03	0.06	0.04	0.01	-0.07
2	6	0.06	0.06	0.04	-0.02	0.01	-0.03	0.03	0.01	0.02
3	6	-0.07	0.05	0.15	0.10	-0.04	0.05	0.03	-0.06	0.01
4	6	-0.14	-0.02	-0.05	0.04	0.06	0.02	-0.04	0.07	0.08
5	6	0.16	0.00	-0.05	-0.09	-0.02	-0.10	-0.02	-0.01	-0.08
6	6	-0.08	-0.15	-0.07	0.01	-0.02	-0.03	0.01	0.01	0.04
7	6	0.05	0.00	0.08	-0.01	-0.02	0.06	-0.01	0.06	-0.07
8	6	0.09	0.12	0.10	0.05	0.03	0.01	0.09	-0.04	0.05
9	6	0.05	-0.09	-0.02	-0.02	-0.03	-0.09	-0.03	-0.01	-0.06
10	6	-0.02	0.09	-0.16	-0.03	0.08	0.08	-0.06	0.02	0.03
11	6	-0.06	0.02	0.01	0.00	0.01	-0.05	-0.03	-0.06	0.10
12	8	-0.03	-0.02	0.01	0.01	0.00	0.01	0.00	0.00	0.01
13	6	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	-0.02	0.00	0.02	0.00	0.00	0.01	0.01	0.00	0.00
16	1	-0.06	-0.29	-0.06	-0.03	-0.14	0.25	0.04	0.07	-0.43
17	1	0.04	0.07	0.03	-0.17	0.16	-0.11	0.17	-0.16	0.09
18	1	-0.13	0.01	0.19	-0.31	0.06	0.02	-0.27	0.08	-0.06
19	1	-0.15	-0.14	-0.09	0.31	-0.14	-0.17	-0.03	-0.05	0.03

20	1	-0.10	-0.25	-0.18	0.13	-0.11	-0.16	-0.14	0.13	0.20
21	1	0.25	0.12	0.09	-0.06	-0.10	0.23	-0.05	0.13	-0.39
22	1	0.22	0.09	0.14	-0.27	0.31	-0.09	-0.05	-0.07	0.03
23	1	0.13	0.18	-0.35	0.15	-0.33	-0.10	0.12	-0.26	-0.16
24	1	-0.06	0.05	0.01	-0.08	-0.13	0.00	0.15	0.24	-0.02
25	1	-0.29	0.20	0.05	0.07	0.08	0.09	-0.17	-0.22	-0.18
26	8	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00
27	1	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	-0.08	0.02	0.03	-0.10	0.03	0.14	-0.06	0.03	0.13
29	1	0.01	0.01	0.03	-0.01	0.00	0.06	-0.01	0.00	0.04

	43			44			45		
	?A			?A			?A		
Frequencies --	1225.8878			1245.7253			1267.6566		
Red. masses --	1.6611			2.0070			1.4469		
Frc consts --	1.4708			1.8350			1.3700		
IR Inten --	1.5162			11.1272			9.3079		
Raman Activ --	1.9240			1.7524			6.3153		
Depolar --	0.6572			0.5617			0.7009		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.03	-0.08	0.00	-0.02	0.03	0.03	0.01	0.00
2	6	0.08	-0.03	0.04	0.01	0.14	-0.03	-0.02	0.02	0.00
3	6	-0.04	-0.01	0.00	-0.06	-0.05	0.09	-0.01	0.00	-0.02
4	6	-0.07	-0.03	0.03	0.03	0.05	0.07	-0.05	0.02	-0.05
5	6	0.04	0.00	-0.02	-0.02	-0.02	-0.14	0.04	0.01	0.08
6	6	-0.04	0.07	0.06	0.11	-0.01	-0.02	0.05	0.02	-0.01
7	6	0.00	0.02	-0.08	-0.01	0.04	0.04	-0.01	-0.02	0.03
8	6	0.01	-0.08	0.02	0.03	-0.02	-0.03	0.02	0.03	0.06
9	6	-0.02	0.01	0.00	-0.01	0.02	0.01	-0.03	-0.02	-0.09
10	6	0.00	-0.04	-0.01	-0.02	-0.07	0.01	-0.01	-0.05	0.04
11	6	0.01	-0.01	0.07	-0.03	-0.02	-0.05	-0.01	-0.01	-0.02
12	8	-0.01	0.01	0.00	0.00	0.00	0.02	-0.01	-0.01	-0.01

13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.01	0.01	-0.01	0.00	0.00	0.00	0.01	0.00	0.00
16	1	-0.01	-0.03	0.27	-0.08	-0.24	-0.03	0.05	0.11	-0.33
17	1	-0.28	0.06	-0.19	0.00	-0.38	-0.12	0.13	-0.18	0.07
18	1	0.14	-0.02	-0.02	0.55	-0.04	0.01	-0.05	0.07	-0.07
19	1	0.44	0.03	-0.19	0.03	-0.03	0.04	-0.01	-0.14	-0.13
20	1	0.08	-0.18	-0.26	-0.30	0.01	0.11	-0.05	-0.10	-0.10
21	1	0.06	-0.03	0.19	-0.09	0.01	-0.02	-0.12	-0.18	0.34
22	1	-0.16	0.46	-0.08	-0.19	0.03	-0.07	-0.03	0.17	0.04
23	1	-0.05	0.15	0.03	-0.10	0.42	0.05	-0.10	0.23	0.13
24	1	0.13	0.15	-0.01	-0.07	-0.11	-0.02	-0.36	0.23	0.07
25	1	-0.12	-0.09	-0.11	-0.03	0.06	0.04	0.37	-0.29	-0.07
26	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	1	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.01
28	1	0.06	-0.03	-0.02	0.07	-0.06	-0.07	-0.06	-0.03	0.15
29	1	-0.01	-0.01	-0.02	0.00	-0.01	-0.04	-0.02	0.00	0.02

	46			47			48		
	?A			?A			?A		
Frequencies --	1274.7402			1298.0588			1306.3836		
Red. masses --	1.5052			1.5350			1.2610		
Frc consts --	1.4411			1.5239			1.2679		
IR Inten --	18.5230			59.7769			241.2967		
Raman Activ --	7.1121			2.5145			0.4798		
Depolar --	0.7158			0.7283			0.7462		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	-0.02	0.02	-0.01	-0.07	-0.06	0.02	-0.07	-0.02
2 6	-0.05	0.01	0.03	0.04	0.04	0.05	-0.02	0.00	0.03
3 6	-0.01	-0.01	-0.03	-0.05	-0.06	0.01	0.01	-0.01	0.00
4 6	-0.03	0.00	-0.04	-0.02	-0.04	0.02	-0.02	0.01	-0.02
5 6	0.04	0.02	0.09	0.02	0.00	-0.01	0.01	0.00	0.01

```
   6   6     0.04   0.06  -0.03    -0.04  -0.03  -0.05     0.01   0.01  -
0.03
   7   6     0.02   0.00  -0.01     0.07   0.00   0.04     0.08   0.01
0.02
   8   6     0.03   0.02   0.05     0.00   0.03  -0.01     0.00   0.00
0.01
   9   6    -0.04  -0.01  -0.10     0.02   0.02  -0.01     0.01  -0.02
0.01
  10   6     0.00  -0.04   0.05     0.05   0.05   0.00    -0.03   0.01
0.00
  11   6    -0.02   0.00  -0.01    -0.04   0.04   0.01    -0.05   0.03
0.00
  12   8    -0.01  -0.01  -0.01    -0.01   0.03   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.01   0.00   0.00    -0.01  -0.03   0.00    -0.02   0.01
0.03
  16   1     0.05  -0.03   0.35     0.12   0.25   0.14     0.14   0.23
0.07
  17   1     0.03   0.05   0.10    -0.19   0.02  -0.12     0.02   0.08
0.07
  18   1     0.02   0.06  -0.09     0.22   0.14  -0.18    -0.07   0.04  -
0.03
  19   1     0.10  -0.22  -0.18     0.07   0.31   0.10     0.05   0.06  -
0.04
  20   1    -0.28   0.00  -0.01    -0.03   0.13   0.13    -0.15  -0.01
0.00
  21   1    -0.15  -0.01  -0.34    -0.23  -0.14  -0.09    -0.27  -0.18  -
0.06
  22   1     0.10  -0.02   0.07    -0.12  -0.14  -0.01    -0.17   0.01  -
0.02
  23   1    -0.06   0.13   0.12    -0.10  -0.20   0.19     0.12  -0.05  -
0.17
  24   1     0.35  -0.33  -0.08    -0.03   0.03   0.01     0.06  -0.07  -
0.02
  25   1    -0.29   0.24   0.07     0.25  -0.19  -0.05     0.13  -0.10  -
0.02
  26   8     0.00   0.00  -0.01     0.01  -0.01  -0.01    -0.01   0.02
0.02
  27   1    -0.01   0.01   0.01    -0.05   0.05  -0.02     0.08  -0.08
0.03
  28   1    -0.12   0.02   0.22    -0.32   0.22   0.29     0.46  -0.36  -
0.48
  29   1    -0.02   0.00   0.05     0.02   0.01   0.13    -0.02  -0.01  -
0.20
                      49                     50                     51
                      ?A                     ?A                     ?A
 Frequencies --   1323.8346              1343.5885              1352.8591
 Red. masses --      1.5504                 1.4129                 1.4652
 Frc consts  --      1.6009                 1.5028                 1.5799
 IR Inten    --     56.8883                 8.5323                21.7351
```

Raman Activ --		1.5140			1.9501			3.2101		
Depolar --		0.3102			0.6278			0.2927		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	-0.07	0.00	0.00	-0.01	0.00	-0.03	-0.01	0.00
2	6	-0.03	-0.05	-0.02	0.00	0.04	0.05	0.03	0.00	-0.02
3	6	0.01	0.09	0.02	0.07	0.02	-0.02	-0.04	-0.06	0.02
4	6	0.02	0.06	-0.02	-0.02	-0.06	0.04	0.03	-0.03	0.02
5	6	-0.02	-0.02	-0.09	-0.03	-0.01	-0.07	-0.01	0.00	-0.01
6	6	0.01	0.05	0.03	-0.01	0.04	-0.01	0.07	0.05	0.03
7	6	0.06	-0.01	-0.03	-0.01	-0.04	0.00	-0.03	-0.04	-0.02
8	6	-0.03	-0.03	0.04	0.00	0.05	0.02	-0.05	0.01	0.04
9	6	0.00	0.01	0.02	-0.02	-0.02	-0.05	-0.02	-0.05	-0.04
10	6	-0.02	-0.03	-0.01	-0.01	-0.05	0.01	-0.06	0.04	0.03
11	6	-0.03	0.03	0.02	0.01	0.01	-0.01	0.02	0.01	-0.01
12	8	0.01	-0.03	0.02	0.01	0.02	0.01	0.00	0.02	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.02	0.00	-0.02	0.00	0.01	0.00	0.03	0.03	-0.01
16	1	0.12	0.29	-0.10	0.05	0.13	0.02	0.00	0.08	0.00
17	1	0.15	0.23	0.14	-0.15	-0.29	-0.10	-0.07	0.14	-0.07
18	1	0.16	-0.39	0.38	-0.39	-0.21	0.22	0.26	0.19	-0.21
19	1	-0.22	0.07	0.09	0.21	0.46	0.12	-0.12	0.21	0.18
20	1	-0.11	-0.19	-0.20	0.10	-0.04	-0.13	-0.31	-0.25	-0.18
21	1	-0.17	-0.17	0.04	0.01	-0.01	-0.09	0.12	0.01	0.13
22	1	-0.07	0.14	0.01	0.28	-0.24	0.11	0.54	0.01	0.16
23	1	0.04	0.07	-0.10	-0.08	0.32	0.06	0.16	-0.26	-0.20
24	1	0.14	-0.09	-0.02	0.00	-0.01	0.00	-0.04	0.04	0.01
25	1	0.03	-0.03	-0.01	0.00	0.05	0.02	0.02	0.03	0.01

26	8	0.00	-0.01	-0.01	0.00	0.01	0.00	0.00	0.00
0.00									
27	1	-0.04	0.04	-0.02	0.02	-0.02	0.01	0.02	-0.02
0.01									
28	1	-0.21	0.20	0.21	0.04	-0.08	0.02	0.06	-0.07
0.03									
29	1	0.01	0.01	0.10	-0.02	0.00	-0.03	-0.02	0.00 -
0.02									

	52	53	54
	?A	?A	?A
Frequencies --	1359.5111	1370.6057	1380.5081
Red. masses --	1.7001	1.5112	1.4417
Frc consts --	1.8514	1.6726	1.6189
IR Inten --	17.9860	5.7164	18.1413
Raman Activ --	2.4744	1.3543	2.9968
Depolar --	0.7495	0.4587	0.7403

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.07	0.03	0.02	-0.02	-0.06	-0.02	-0.02	-0.02	0.02
2	6	-0.07	0.05	0.02	0.01	0.09	-0.02	0.02	0.07	0.01
3	6	0.00	0.01	-0.07	0.03	-0.07	0.02	-0.01	0.02	- 0.04
4	6	-0.06	-0.08	-0.03	0.05	0.03	-0.02	0.04	0.03	- 0.02
5	6	0.01	0.01	0.04	0.00	0.01	0.04	0.00	0.01	0.01
6	6	0.07	-0.04	0.02	-0.06	0.01	0.03	-0.03	-0.04	0.06
7	6	0.00	0.05	0.02	0.04	0.00	-0.03	0.03	0.02	0.01
8	6	-0.04	-0.05	-0.02	-0.04	-0.03	0.02	-0.02	-0.07	0.02
9	6	0.03	0.00	0.09	0.01	-0.01	0.05	-0.02	0.00	- 0.06
10	6	-0.04	0.03	-0.02	-0.05	-0.06	0.00	0.06	0.07	- 0.03
11	6	0.00	-0.02	-0.03	-0.02	0.03	0.01	-0.03	0.02	0.00
12	8	0.00	0.01	0.00	0.00	0.01	-0.01	0.00	-0.02	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.02	0.00	-0.02	0.03	0.01	-0.02	-0.01	0.00	0.01
16	1	0.04	-0.06	0.03	0.03	0.06	0.18	-0.03	-0.04	- 0.05
17	1	0.18	-0.37	0.13	0.10	-0.33	-0.03	-0.07	-0.43	- 0.12
18	1	-0.10	-0.13	0.04	-0.23	0.32	-0.24	0.01	-0.20	0.11

```
  19   1     0.34   0.35  -0.06    -0.29  -0.10   0.10    -0.23  -0.06
0.07
  20   1    -0.26  -0.07   0.08     0.39  -0.01  -0.13     0.10  -0.15  -
0.10
  21   1    -0.07   0.01   0.05    -0.02  -0.06   0.06     0.00   0.05  -
0.15
  22   1    -0.03   0.31  -0.07     0.01   0.11   0.01     0.21   0.37
0.00
  23   1     0.21  -0.26  -0.29     0.19   0.29  -0.31    -0.23  -0.37
0.35
  24   1    -0.05  -0.02  -0.01     0.15  -0.10  -0.03     0.10  -0.12  -
0.03
  25   1    -0.03   0.07   0.04     0.02  -0.01  -0.01     0.03  -0.02
0.00
  26   8     0.00  -0.01   0.00     0.00  -0.01   0.00     0.00   0.01
0.00
  27   1    -0.04   0.04  -0.03    -0.03   0.03  -0.02     0.03  -0.03
0.02
  28   1    -0.14   0.23   0.04    -0.10   0.17   0.04     0.12  -0.18
0.00
  29   1     0.03   0.01   0.08     0.02   0.01   0.06    -0.03  -0.01  -
0.06
                     55                     56                     57
                     ?A                     ?A                     ?A
 Frequencies --  1385.6161              1401.5704              1416.1365
 Red. masses --     1.3839                 1.4271                 1.5774
 Frc consts  --     1.5655                 1.6518                 1.8638
 IR Inten    --     5.1933                 3.2903                 3.3941
 Raman Activ --     1.0298                 4.9024                 5.3237
 Depolar     --     0.6303                 0.7497                 0.7266
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01   0.01  -0.02     0.03  -0.06   0.01    -0.02  -0.07  -
0.01
   2   6    -0.02   0.04  -0.05    -0.06  -0.01  -0.06     0.03   0.03
0.06
   3   6    -0.06   0.01  -0.03    -0.01  -0.01   0.06    -0.03   0.04  -
0.07
   4   6    -0.03  -0.01   0.02    -0.04  -0.02  -0.01    -0.02   0.07
0.04
   5   6     0.01   0.01   0.00    -0.01  -0.01  -0.03     0.02   0.01
0.02
   6   6    -0.07   0.02   0.05    -0.03  -0.05  -0.03     0.02  -0.04  -
0.06
   7   6     0.00  -0.03   0.01    -0.06   0.02   0.02    -0.05  -0.03  -
0.02
   8   6     0.04   0.06  -0.01     0.00  -0.06   0.01    -0.02   0.01  -
0.04
   9   6    -0.02  -0.01  -0.02    -0.03  -0.03  -0.04    -0.02  -0.02
0.03
  10   6     0.01   0.03   0.07     0.03   0.00   0.02    -0.02   0.00
0.07
  11   6     0.04  -0.03   0.00     0.02   0.03   0.00    -0.02   0.07
0.02
```

12	8	0.00	-0.01	0.00	0.00	0.02	0.00	0.00	-0.03	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.01	0.02	0.00	0.03	0.02	-0.01
16	1	0.04	0.07	0.12	0.16	0.30	0.02	0.09	0.24	-0.05
17	1	0.32	-0.21	0.14	0.33	0.15	0.23	-0.23	-0.16	-0.14
18	1	0.42	-0.16	0.03	0.15	0.14	-0.06	0.11	-0.27	0.14
19	1	0.14	-0.03	-0.06	0.15	0.24	-0.01	0.17	-0.38	-0.22
20	1	0.42	-0.15	-0.28	0.25	0.24	0.20	-0.01	0.18	0.20
21	1	-0.10	-0.05	-0.14	0.28	0.24	-0.03	0.34	0.14	0.18
22	1	-0.11	-0.30	0.01	0.15	0.37	-0.02	0.15	-0.13	0.01
23	1	0.20	-0.19	-0.13	-0.06	0.14	0.12	0.22	-0.05	-0.21
24	1	-0.13	0.11	0.03	0.08	0.02	-0.01	0.17	-0.09	-0.02
25	1	-0.11	0.07	0.01	0.05	0.07	0.06	0.19	-0.09	-0.02
26	8	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
27	1	0.01	-0.02	0.01	0.02	-0.02	0.01	0.00	0.00	0.00
28	1	0.02	-0.06	-0.02	0.06	-0.12	0.04	-0.01	0.03	0.00
29	1	0.00	0.00	-0.01	-0.02	0.00	-0.03	0.01	0.01	0.02

	58	59	60
	?A	?A	?A
Frequencies --	1421.1368	1426.2773	1434.3799
Red. masses --	1.6201	1.6120	1.4931
Frc consts --	1.9278	1.9320	1.8099
IR Inten --	6.0481	4.7261	1.7530
Raman Activ --	1.9971	3.4508	1.0241
Depolar --	0.6109	0.7486	0.7402

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.05	0.05	0.03	-0.03	-0.09	-0.01	-0.01	-0.04	0.15
2	6	0.01	-0.03	-0.02	-0.03	0.04	-0.02	0.06	0.00	-0.03
3	6	0.00	0.00	0.02	0.03	-0.03	0.05	-0.02	-0.02	0.00
4	6	-0.02	0.03	0.06	-0.02	0.06	0.05	-0.04	-0.02	-0.05

```
    5   6    -0.01   0.00  -0.03     0.01   0.00  -0.01     0.01   0.00
0.03
    6   6    -0.06  -0.02  -0.01     0.04   0.00   0.06    -0.02  -0.01
0.02
    7   6     0.11   0.07   0.01    -0.01  -0.01  -0.03     0.01   0.02  -
0.07
    8   6    -0.12  -0.01  -0.04    -0.04   0.01  -0.05     0.03   0.02
0.03
    9   6    -0.02  -0.04   0.01     0.03   0.03   0.04     0.01   0.01  -
0.01
   10   6     0.01   0.00   0.00     0.02   0.02  -0.11     0.00   0.00
0.01
   11   6    -0.05  -0.03  -0.01     0.07  -0.01   0.00     0.00   0.00  -
0.02
   12   8     0.00  -0.01   0.01     0.00   0.00   0.00     0.00   0.01  -
0.01
   13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   15   8     0.03   0.02  -0.01    -0.02  -0.02   0.01    -0.01  -0.01
0.01
   16   1    -0.06  -0.24  -0.19     0.16   0.43   0.08     0.03   0.18  -
0.63
   17   1     0.07   0.11   0.03     0.12  -0.11   0.06    -0.16  -0.02  -
0.19
   18   1     0.05   0.05  -0.02    -0.19   0.16  -0.06     0.08   0.09  -
0.09
   19   1     0.34  -0.18  -0.17     0.24  -0.30  -0.21     0.13   0.19  -
0.05
   20   1     0.21   0.13   0.08    -0.19  -0.22  -0.10     0.12   0.02
0.01
   21   1    -0.39  -0.24   0.05     0.00  -0.04   0.12    -0.05  -0.11
0.23
   22   1     0.59  -0.03   0.10     0.12  -0.21   0.01    -0.21  -0.08
0.00
   23   1     0.00   0.07   0.01    -0.27  -0.09   0.25     0.01  -0.04  -
0.01
   24   1     0.02  -0.06  -0.03    -0.13   0.14   0.05     0.23  -0.24  -
0.05
   25   1     0.01  -0.07  -0.01    -0.19   0.19   0.04    -0.26   0.25
0.08
   26   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   27   1     0.00   0.00   0.00    -0.02   0.02  -0.01     0.00   0.00
0.00
   28   1    -0.01   0.00   0.06    -0.02   0.08  -0.05     0.01  -0.01  -
0.01
   29   1    -0.01   0.00   0.01     0.01   0.00   0.00     0.00   0.00
0.00
                      61                    62                    63
                      ?A                    ?A                    ?A
 Frequencies --   1450.9207             1460.0256             1614.1734
 Red. masses --      1.4820                1.5189                1.6548
```

Frc consts	--	1.8382			1.9077			2.5404		
IR Inten	--	12.4321			7.7136			352.0923		
Raman Activ	--	1.6498			1.9502			12.3000		
Depolar	--	0.6228			0.7234			0.3579		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	-0.02	0.05	0.06	0.03	0.02	0.00	0.00	0.00
2	6	0.05	-0.02	0.00	-0.03	0.00	-0.05	0.00	0.00	0.00
3	6	0.00	-0.01	0.00	0.00	-0.02	0.03	0.01	-0.01	0.01
4	6	-0.02	0.02	0.00	-0.03	-0.01	0.02	0.00	-0.01	-0.01
5	6	0.01	0.00	0.02	0.00	0.00	-0.01	0.00	0.01	0.00
6	6	-0.02	0.07	-0.01	0.01	0.03	0.06	0.01	0.00	0.00
7	6	0.00	-0.04	0.14	-0.03	-0.08	-0.01	0.01	0.00	0.00
8	6	0.00	-0.04	-0.05	0.01	0.03	-0.03	0.03	0.02	-0.02
9	6	0.00	-0.01	0.05	0.02	0.02	0.02	-0.09	-0.08	0.13
10	6	-0.01	-0.02	0.00	0.01	0.01	-0.05	0.02	0.01	-0.05
11	6	0.02	0.00	-0.04	-0.10	0.08	0.02	0.00	0.01	0.00
12	8	0.00	0.00	-0.01	0.00	0.01	0.00	0.00	-0.01	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.02	0.01	-0.01	-0.01	-0.01	0.01	0.06	0.07	-0.08
16	1	0.02	0.14	-0.31	-0.04	-0.24	-0.11	0.00	0.00	0.00
17	1	-0.17	0.09	-0.13	0.20	-0.01	0.10	-0.01	0.00	0.00
18	1	-0.01	0.06	-0.05	-0.01	0.11	-0.06	-0.07	0.04	-0.02
19	1	0.11	-0.08	-0.11	0.20	0.03	-0.07	-0.02	0.01	0.01
20	1	0.00	-0.13	-0.24	-0.02	-0.23	-0.21	-0.04	-0.03	-0.02
21	1	0.01	0.22	-0.70	0.27	0.11	-0.04	0.00	-0.01	0.00
22	1	0.02	0.20	-0.08	-0.05	-0.19	-0.01	-0.21	-0.10	-0.04
23	1	0.05	0.09	-0.09	-0.10	-0.06	0.09	-0.06	-0.03	0.04
24	1	-0.21	0.04	0.04	0.38	-0.32	-0.08	-0.04	-0.07	0.03

```
  25   1     0.09   0.02   0.04     0.40  -0.32  -0.08    -0.04  -0.03  -
0.07
  26   8     0.00  -0.01   0.00     0.00   0.00   0.00    -0.02   0.02  -
0.02
  27   1    -0.02   0.02  -0.01    -0.01   0.01  -0.01     0.16  -0.20
0.08
  28   1    -0.04   0.10  -0.05    -0.02   0.05  -0.05    -0.10  -0.68
0.56
  29   1     0.02   0.01   0.02     0.01   0.00   0.00     0.05   0.06  -
0.01
                     64                     65                     66
                     ?A                     ?A                     ?A
 Frequencies --  1637.8182              1696.8365              1710.4913
 Red. masses --     1.1016                 1.8702                 1.2783
 Frc consts  --     1.7410                 3.1725                 2.2035
 IR Inten    --     6.5777               299.3373                 9.0937
 Raman Activ --    10.4227                 6.1394                19.2829
 Depolar     --     0.6706                 0.1948                 0.5941
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   2   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   3   6     0.00   0.00   0.00    -0.01   0.00   0.00     0.00   0.00
0.00
   4   6     0.00   0.00   0.00    -0.01   0.01   0.01     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00  -0.01   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00    -0.01   0.00   0.00     0.00   0.00
0.00
   7   6     0.00   0.01   0.00    -0.01   0.00   0.01     0.00   0.00
0.01
   8   6     0.00   0.00   0.00    -0.04  -0.03  -0.01    -0.02  -0.01  -
0.01
   9   6     0.00   0.00  -0.01     0.19   0.13  -0.05     0.10   0.05
0.00
  10   6     0.00   0.00   0.00    -0.04  -0.02   0.03    -0.02  -0.01
0.01
  11   6     0.06   0.06   0.02     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.00   0.01   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.01
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.01
0.00
  15   8     0.00   0.00   0.01    -0.08  -0.05   0.02    -0.06  -0.02  -
0.02
  16   1     0.02   0.01   0.00     0.01   0.01  -0.02     0.00   0.01  -
0.01
  17   1     0.02   0.01   0.01     0.00   0.00   0.00     0.00   0.00
0.00
```

```
  18   1     0.01   0.00   0.00     0.03  -0.01   0.00     0.00   0.00
0.00
  19   1     0.02   0.02   0.00     0.04  -0.04  -0.03     0.02  -0.02  -
0.02
  20   1     0.02   0.02   0.01     0.01   0.00   0.00     0.01   0.00  -
0.01
  21   1     0.01   0.02   0.01     0.01   0.02  -0.03     0.02   0.01  -
0.02
  22   1     0.03   0.03   0.01     0.13   0.07   0.00     0.04   0.01  -
0.01
  23   1     0.00   0.00   0.00     0.12   0.05  -0.16     0.08   0.02  -
0.11
  24   1    -0.37  -0.53   0.26    -0.02  -0.01   0.01    -0.01   0.00
0.00
  25   1    -0.33  -0.26  -0.56     0.01  -0.01  -0.02     0.01  -0.01
0.00
  26   8     0.00   0.00   0.00    -0.05   0.02  -0.02     0.06   0.01
0.01
  27   1    -0.02   0.02  -0.01     0.33  -0.40   0.10    -0.25   0.35  -
0.04
  28   1     0.01   0.06  -0.05    -0.17  -0.42   0.28     0.10  -0.32
0.37
  29   1    -0.01  -0.01   0.00     0.50   0.20   0.07    -0.66  -0.26  -
0.13
                     67                     68                     69
                     ?A                     ?A                     ?A
 Frequencies --  1884.7355              2243.8669              2296.7996
 Red. masses --    10.8185                 1.1666                 7.3624
 Frc consts  --    22.6421                 3.4609                22.8831
 IR Inten    --   334.2445              2320.7429               412.4237
 Raman Activ --    46.8286                84.2781                49.0623
 Depolar     --     0.3608                 0.3642                 0.1769
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.01  -0.02   0.01     0.00   0.00   0.00     0.00   0.00
0.00
   2   6     0.00  -0.02   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   3   6     0.01  -0.07   0.03     0.00   0.00   0.00     0.00   0.00
0.00
   4   6     0.00  -0.07   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   5   6    -0.04   0.75  -0.13     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   7   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   8   6     0.00  -0.01   0.00     0.00  -0.01   0.00     0.00   0.00
0.00
   9   6     0.04   0.02  -0.02     0.01   0.02  -0.02    -0.01  -0.01
0.01
  10   6     0.00  -0.01   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

```
  11   6     0.00   0.01   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.02  -0.46   0.08     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.06   0.01   0.02     0.52   0.09
0.17
  14   7     0.00   0.00   0.00    -0.05   0.00  -0.01    -0.45  -0.09  -
0.14
  15   8    -0.01  -0.02   0.01     0.05   0.02   0.04    -0.04  -0.01  -
0.03
  16   1     0.00   0.03  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
  17   1    -0.01   0.02   0.02     0.00   0.00   0.00     0.00   0.00
0.00
  18   1    -0.05   0.24  -0.16    -0.01   0.00   0.00     0.01   0.00
0.00
  19   1     0.05   0.29   0.06     0.00   0.00   0.00     0.00   0.00
0.00
  20   1     0.00   0.00   0.00    -0.01   0.00   0.00     0.00   0.00
0.00
  21   1     0.01   0.01  -0.01     0.00   0.00   0.00    -0.01  -0.01  -
0.01
  22   1     0.01   0.04  -0.01     0.01   0.01   0.00     0.00   0.00
0.00
  23   1     0.01   0.04   0.00    -0.01   0.00   0.00     0.00   0.00
0.00
  24   1    -0.01  -0.01   0.01     0.00   0.00   0.00     0.00   0.00
0.00
  25   1    -0.02   0.01  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
  26   8     0.00   0.00   0.00     0.01  -0.01   0.00     0.00   0.01
0.00
  27   1    -0.01   0.01   0.00    -0.09   0.08  -0.03     0.05  -0.04
0.02
  28   1    -0.05  -0.01  -0.02    -0.75  -0.39  -0.46     0.53   0.26
0.32
  29   1     0.01   0.00   0.00    -0.19   0.03  -0.04     0.10   0.00
0.02
                      70                     71                     72
                      ?A                     ?A                     ?A
 Frequencies --   3218.4099              3264.0924              3281.0389
 Red. masses --      1.0586                 1.1068                 1.0881
 Frc consts  --      6.4605                 6.9478                 6.9018
 IR Inten    --     31.5168                18.2550                15.5123
 Raman Activ --    136.1503                89.7620               108.2681
 Depolar     --      0.1713                 0.7495                 0.3928
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01   0.00   0.00     0.00   0.00   0.00    -0.08   0.03
0.00
   2   6     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.00  -
0.02
   3   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	-0.04	-0.05	-0.02	0.00	-0.03	0.09	0.00	-0.01	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	-0.10	0.03	0.00	0.02	-0.01	0.00	0.89	-0.32	-0.04
17	1	0.00	0.00	0.01	-0.01	0.00	0.01	-0.15	-0.03	0.21
18	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	-0.02
19	1	0.00	0.00	-0.01	0.00	0.00	0.01	-0.05	0.04	-0.11
20	1	0.00	-0.01	0.01	0.00	0.00	0.00	0.00	0.01	-0.01
21	1	0.02	-0.04	-0.01	0.00	0.00	0.00	0.02	-0.03	-0.01
22	1	0.00	0.00	-0.01	0.00	0.00	0.01	0.00	0.00	0.01
23	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	1	0.22	0.10	0.65	-0.24	-0.12	-0.66	0.02	0.01	0.08
25	1	0.29	0.47	-0.45	0.29	0.47	-0.42	0.02	0.04	-0.04
26	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.00
			73			74			75	
			?A			?A			?A	

Frequencies --		3300.7826			3306.0598			3322.3999		
Red. masses --		1.0649			1.0892			1.0889		
Frc consts --		6.8361			7.0143			7.0819		
IR Inten --		792.0891			18.5560			8.4001		
Raman Activ --		46.7528			108.0266			63.4193		
Depolar --		0.5144			0.4044			0.3684		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.02	-0.01	0.00	-0.01	0.00	0.00
2	6	0.00	0.00	0.00	0.04	0.01	-0.06	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00
4	6	0.00	0.00	0.00	0.00	0.00	-0.01	-0.03	0.02	-0.07
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	-0.02	0.02	0.00	0.01	-0.01
7	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	0.00	0.00	0.00	-0.23	0.08	0.01	0.12	-0.04	-0.01
17	1	0.02	0.01	-0.04	-0.50	-0.11	0.74	0.01	0.00	-0.02
18	1	0.00	0.00	-0.01	-0.01	-0.10	-0.14	0.01	0.03	0.05
19	1	0.00	0.00	0.01	0.04	-0.03	0.09	0.37	-0.28	0.78
20	1	0.01	-0.02	0.02	-0.05	0.20	-0.18	0.02	-0.08	0.08
21	1	0.01	-0.01	0.00	0.00	0.00	0.00	-0.02	0.03	0.01
22	1	0.00	0.00	-0.01	0.00	0.00	-0.01	0.06	-0.05	-0.35
23	1	0.00	0.00	0.00	0.02	0.00	0.02	-0.01	0.00	-0.01

```
  24   1     0.00   0.00   0.00    -0.01   0.00  -0.02     0.01   0.00
0.02
  25   1     0.00   0.00   0.00    -0.01  -0.02   0.01     0.00   0.01
0.00
  26   8    -0.02   0.06  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
  27   1     0.08   0.07   0.01     0.00   0.00   0.00     0.00   0.00
0.00
  28   1    -0.08  -0.02  -0.04     0.00   0.00   0.00     0.00   0.00
0.00
  29   1     0.30  -0.94   0.09     0.01  -0.04   0.00     0.00   0.01
0.00
                     76                    77                    78
                     ?A                    ?A                    ?A
 Frequencies --  3328.0074             3338.2978             3340.5134
 Red. masses --     1.0897                1.0896                1.0886
 Frc consts  --     7.1110                7.1542                7.1572
 IR Inten    --    12.6033                9.7313                1.6849
 Raman Activ --   103.8411               76.4184              135.3838
 Depolar     --     0.3620                0.2151                0.2306
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   2   6    -0.01   0.00   0.02     0.01   0.00  -0.01     0.00   0.00
0.00
   3   6     0.00  -0.01  -0.01    -0.01  -0.05  -0.06     0.00   0.01
0.02
   4   6     0.00   0.00  -0.01     0.00   0.00   0.00    -0.01   0.01  -
0.03
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.02  -0.06   0.05     0.00   0.01  -0.01     0.00   0.00
0.00
   7   6    -0.01   0.01   0.00     0.00   0.00   0.00    -0.01   0.02
0.01
   8   6     0.00   0.00   0.00     0.00   0.00  -0.02     0.01  -0.01  -
0.07
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6    -0.01   0.00  -0.01     0.01   0.00   0.01     0.00   0.00
0.00
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.05  -0.02   0.00    -0.03   0.01   0.00     0.04  -0.01
0.00
```

17	1	0.13	0.02	-0.20	-0.11	-0.03	0.17	0.03	0.01	-0.05
18	1	0.02	0.11	0.15	0.09	0.55	0.72	-0.03	-0.15	-0.20
19	1	0.04	-0.03	0.08	0.02	-0.01	0.04	0.14	-0.11	0.30
20	1	-0.18	0.66	-0.61	0.02	-0.08	0.08	0.01	-0.02	0.02
21	1	0.09	-0.15	-0.04	0.01	-0.02	-0.01	0.13	-0.22	-0.07
22	1	0.01	0.00	-0.03	-0.05	0.04	0.27	-0.15	0.12	0.83
23	1	0.07	0.00	0.06	-0.13	-0.01	-0.11	0.05	0.00	0.04
24	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
25	1	0.01	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
26	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	1	0.00	-0.01	0.00	0.00	-0.02	0.00	0.00	0.00	0.00

	79			80			81		
	?A			?A			?A		
Frequencies --	3358.2122			3372.3730			3980.2824		
Red. masses --	1.0902			1.0905			1.0695		
Frc consts --	7.2437			7.3072			9.9831		
IR Inten --	5.2571			0.2831			191.6184		
Raman Activ --	130.7438			110.7335			142.3657		
Depolar --	0.1280			0.1006			0.2631		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3 6	0.00	0.00	0.00	0.00	-0.01	-0.01	0.00	0.00	0.00
4 6	0.00	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
5 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6 6	0.00	-0.01	0.01	0.00	0.01	-0.01	0.00	0.00	0.00
7 6	0.04	-0.07	-0.02	0.00	0.01	0.00	0.00	0.00	0.00
8 6	0.00	0.00	-0.02	0.00	0.00	0.00	0.00	0.00	0.00
9 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  10   6    -0.01   0.00  -0.01    -0.06  -0.01  -0.06     0.00   0.00
0.00
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.04  -0.01   0.00    -0.01   0.00   0.00     0.00   0.00
0.00
  17   1     0.02   0.00  -0.03    -0.02  -0.01   0.03     0.00   0.00
0.00
  18   1     0.00   0.00   0.00     0.01   0.10   0.13     0.00   0.00
0.00
  19   1     0.03  -0.02   0.06    -0.01   0.01  -0.02     0.00   0.00
0.00
  20   1    -0.03   0.12  -0.11     0.02  -0.10   0.09     0.00   0.00
0.00
  21   1    -0.47   0.78   0.24     0.04  -0.07  -0.02     0.00   0.00
0.00
  22   1    -0.05   0.03   0.25     0.01  -0.01  -0.04     0.00   0.00
0.00
  23   1     0.09   0.01   0.08     0.74   0.06   0.62     0.00   0.00
0.00
  24   1     0.02   0.01   0.03     0.00   0.00   0.00     0.00   0.00
0.00
  25   1     0.02   0.02  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
  26   8     0.00   0.00   0.00     0.00   0.00   0.00    -0.04  -0.05  -
0.01
  27   1     0.00   0.00   0.00     0.00   0.00   0.00     0.74   0.66
0.09
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  29   1     0.00  -0.01   0.00     0.00   0.01   0.00    -0.05   0.07  -
0.01

 -------------------
 - Thermochemistry -
 -------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Atom  1 has atomic number  6 and mass  12.00000
 Atom  2 has atomic number  6 and mass  12.00000
 Atom  3 has atomic number  6 and mass  12.00000
 Atom  4 has atomic number  6 and mass  12.00000
 Atom  5 has atomic number  6 and mass  12.00000
 Atom  6 has atomic number  6 and mass  12.00000
 Atom  7 has atomic number  6 and mass  12.00000
 Atom  8 has atomic number  6 and mass  12.00000
 Atom  9 has atomic number  6 and mass  12.00000
```

```
Atom 10 has atomic number  6 and mass  12.00000
Atom 11 has atomic number  6 and mass  12.00000
Atom 12 has atomic number  8 and mass  15.99491
Atom 13 has atomic number  6 and mass  12.00000
Atom 14 has atomic number  7 and mass  14.00307
Atom 15 has atomic number  8 and mass  15.99491
Atom 16 has atomic number  1 and mass   1.00783
Atom 17 has atomic number  1 and mass   1.00783
Atom 18 has atomic number  1 and mass   1.00783
Atom 19 has atomic number  1 and mass   1.00783
Atom 20 has atomic number  1 and mass   1.00783
Atom 21 has atomic number  1 and mass   1.00783
Atom 22 has atomic number  1 and mass   1.00783
Atom 23 has atomic number  1 and mass   1.00783
Atom 24 has atomic number  1 and mass   1.00783
Atom 25 has atomic number  1 and mass   1.00783
Atom 26 has atomic number  8 and mass  15.99491
Atom 27 has atomic number  1 and mass   1.00783
Atom 28 has atomic number  1 and mass   1.00783
Atom 29 has atomic number  1 and mass   1.00783
Molecular mass:   219.08954 amu.
Principal axes and moments of inertia in atomic units:
                          1         2         3
    EIGENVALUES --  1972.68829 3615.28256 4539.78810
          X            0.99878   0.04906   0.00623
          Y           -0.04914   0.99872   0.01238
          Z           -0.00561  -0.01267   0.99990
THIS MOLECULE IS AN ASYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER  1.
WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
          MAY CAUSE SIGNIFICANT ERROR
ROTATIONAL TEMPERATURES (KELVIN)      0.04391     0.02396     0.01908
ROTATIONAL CONSTANTS (GHZ)            0.91486     0.49920     0.39754
   1 IMAGINARY FREQUENCIES IGNORED.
Zero-point vibrational energy     646268.1 (Joules/Mol)
                                 154.46179 (Kcal/Mol)
WARNING-- EXPLICIT CONSIDERATION OF  18 DEGREES OF FREEDOM AS
          VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
VIBRATIONAL TEMPERATURES:    103.05   129.55   133.65   211.82   226.70
         (KELVIN)            302.94   334.90   398.16   413.30   472.36
                             533.52   591.58   649.88   717.84   754.21
                             802.40   852.38   891.98   957.75   976.67
                            1055.52  1160.06  1197.99  1206.22  1225.64
                            1233.25  1250.46  1284.82  1323.60  1351.85
                            1386.76  1423.62  1446.53  1465.04  1484.85
                            1492.04  1513.94  1543.15  1571.51  1662.79
                            1698.01  1763.77  1792.31  1823.86  1834.06
                            1867.61  1879.58  1904.69  1933.11  1946.45
                            1956.02  1971.98  1986.23  1993.58  2016.54
                            2037.49  2044.69  2052.08  2063.74  2087.54
                            2100.64  2322.42  2356.44  2441.36  2461.00
                            2711.70  3228.41  3304.56  4630.55  4696.27
                            4720.66  4749.06  4756.66  4780.16  4788.23
                            4803.04  4806.23  4831.69  4852.06  5726.71
```

Zero-point correction=	0.246151
(Hartree/Particle)	
Thermal correction to Energy=	0.258148
Thermal correction to Enthalpy=	0.259092
Thermal correction to Gibbs Free Energy=	0.207803
Sum of electronic and zero-point Energies=	-736.668011
Sum of electronic and thermal Energies=	-736.656014
Sum of electronic and thermal Enthalpies=	-736.655069
Sum of electronic and thermal Free Energies=	-736.706359

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	161.990	47.987	107.948
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	42.056
ROTATIONAL	0.889	2.981	31.849
VIBRATIONAL	160.213	42.026	34.043
VIBRATION 1	0.598	1.968	4.108
VIBRATION 2	0.602	1.956	3.659
VIBRATION 3	0.602	1.954	3.598
VIBRATION 4	0.617	1.906	2.708
VIBRATION 5	0.621	1.894	2.579
VIBRATION 6	0.643	1.825	2.039
VIBRATION 7	0.654	1.791	1.858
VIBRATION 8	0.678	1.716	1.554
VIBRATION 9	0.684	1.697	1.490
VIBRATION 10	0.712	1.619	1.268
VIBRATION 11	0.743	1.532	1.076
VIBRATION 12	0.775	1.446	0.922
VIBRATION 13	0.810	1.357	0.791
VIBRATION 14	0.854	1.252	0.661
VIBRATION 15	0.879	1.196	0.600
VIBRATION 16	0.913	1.123	0.528
VIBRATION 17	0.950	1.048	0.463
VIBRATION 18	0.980	0.990	0.417

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.261834D-95	-95.581974	-220.085628
TOTAL V=0	0.435153D+18	17.638642	40.614475
VIB (BOT)	0.100848-109	-109.996334	-253.275919
VIB (BOT) 1	0.287893D+01	0.459231	1.057417
VIB (BOT) 2	0.228345D+01	0.358592	0.825689
VIB (BOT) 3	0.221232D+01	0.344848	0.794042
VIB (BOT) 4	0.137839D+01	0.139373	0.320919
VIB (BOT) 5	0.128404D+01	0.108579	0.250011
VIB (BOT) 6	0.943081D+00	-0.025451	-0.058603
VIB (BOT) 7	0.845138D+00	-0.073072	-0.168255
VIB (BOT) 8	0.695937D+00	-0.157430	-0.362496
VIB (BOT) 9	0.666703D+00	-0.176068	-0.405411
VIB (BOT) 10	0.569711D+00	-0.244346	-0.562627
VIB (BOT) 11	0.490695D+00	-0.309188	-0.711932
VIB (BOT) 12	0.429910D+00	-0.366623	-0.844180
VIB (BOT) 13	0.379139D+00	-0.421201	-0.969852
VIB (BOT) 14	0.329732D+00	-0.481839	-1.109474

VIB (BOT) 15	0.306734D+00	-0.513238	-1.181773
VIB (BOT) 16	0.279313D+00	-0.553909	-1.275423
VIB (BOT) 17	0.254003D+00	-0.595162	-1.370410
VIB (BOT) 18	0.235901D+00	-0.627271	-1.444344
VIB (V=0)	0.167603D+04	3.224282	7.424184
VIB (V=0) 1	0.342202D+01	0.534283	1.230232
VIB (V=0) 2	0.283755D+01	0.452944	1.042942
VIB (V=0) 3	0.276812D+01	0.442185	1.018168
VIB (V=0) 4	0.196628D+01	0.293645	0.676142
VIB (V=0) 5	0.187795D+01	0.273685	0.630183
VIB (V=0) 6	0.156743D+01	0.195188	0.449436
VIB (V=0) 7	0.148197D+01	0.170838	0.393370
VIB (V=0) 8	0.135693D+01	0.132557	0.305225
VIB (V=0) 9	0.133336D+01	0.124948	0.287704
VIB (V=0) 10	0.125800D+01	0.099682	0.229526
VIB (V=0) 11	0.120056D+01	0.079383	0.182787
VIB (V=0) 12	0.115941D+01	0.064237	0.147912
VIB (V=0) 13	0.112749D+01	0.052114	0.119996
VIB (V=0) 14	0.109894D+01	0.040972	0.094342
VIB (V=0) 15	0.108659D+01	0.036065	0.083043
VIB (V=0) 16	0.107273D+01	0.030489	0.070204
VIB (V=0) 17	0.106082D+01	0.025641	0.059041
VIB (V=0) 18	0.105286D+01	0.022369	0.051506
ELECTRONIC	0.100000D+01	0.000000	0.000000
TRANSLATIONAL	0.127466D+09	8.105393	18.663357
ROTATIONAL	0.203689D+07	6.308968	14.526935

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000167	-0.000000089	0.000000056
2	6	-0.000000086	0.000000105	0.000000013
3	6	0.000000617	0.000000427	-0.000000657
4	6	-0.000000636	-0.000000200	-0.000000200
5	6	0.000000196	0.000000478	0.000000446
6	6	0.000000028	-0.000000346	-0.000000353
7	6	0.000000167	0.000000324	-0.000000336
8	6	-0.000000847	-0.000000001	-0.000001148
9	6	0.000012088	0.000004183	0.000007385
10	6	-0.000002533	-0.000001758	-0.000001113
11	6	-0.000000066	0.000000135	-0.000000057
12	8	-0.000000789	0.000000169	-0.000000134
13	6	-0.000002163	-0.000006308	-0.000002069
14	7	-0.000007909	0.000003734	-0.000011265
15	8	0.000001791	0.000001192	-0.000009108
16	1	0.000000009	0.000000008	0.000000021
17	1	0.000000092	0.000000047	-0.000000011
18	1	-0.000000563	-0.000000039	0.000000163
19	1	-0.000000086	0.000000007	-0.000000032
20	1	0.000000001	-0.000000072	0.000000064
21	1	-0.000001605	0.000000607	0.000000860
22	1	0.000000210	0.000000126	0.000000048
23	1	0.000000361	0.000000448	0.000000304

```
  24          1           0.000000001   -0.000000013   -0.000000051
  25          1          -0.000000047   -0.000000007   -0.000000008
  26          8           0.000009937    0.000002187    0.000014421
  27          1           0.000003347    0.000001471   -0.000000945
  28          1          -0.000007833   -0.000006092    0.000009419
  29          1          -0.000003518   -0.000000725   -0.000005713
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000014421 RMS     0.000003615

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000035576 RMS     0.000004448
Search for a saddle point.
Step number   1 out of a maximum of 174
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Swaping is turned off.
Second derivative matrix not updated -- analytic derivatives used.
    Eigenvalues ---   -0.00784   0.00062   0.00542   0.00668   0.01024
    Eigenvalues ---    0.01258   0.01328   0.01636   0.01826   0.01933
    Eigenvalues ---    0.02141   0.02225   0.02419   0.02529   0.02762
    Eigenvalues ---    0.02961   0.03005   0.03134   0.03244   0.03725
    Eigenvalues ---    0.04000   0.04140   0.04401   0.04521   0.04603
    Eigenvalues ---    0.04930   0.05083   0.05548   0.06032   0.06281
    Eigenvalues ---    0.06395   0.06426   0.07007   0.07544   0.07741
    Eigenvalues ---    0.08107   0.08416   0.08578   0.08892   0.09287
    Eigenvalues ---    0.09405   0.12164   0.13024   0.13186   0.14494
    Eigenvalues ---    0.15140   0.15526   0.17795   0.18277   0.18836
    Eigenvalues ---    0.19422   0.19844   0.21889   0.23652   0.23740
    Eigenvalues ---    0.23841   0.25867   0.27046   0.29018   0.29727
    Eigenvalues ---    0.30417   0.34005   0.36730   0.36955   0.37134
    Eigenvalues ---    0.37627   0.37727   0.38139   0.38606   0.39082
    Eigenvalues ---    0.39315   0.39410   0.40098   0.40366   0.46277
    Eigenvalues ---    0.56802   0.59676   0.88172   0.91478   0.95629
    Eigenvalues ---    1.300321000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
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    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
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    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.00000
Eigenvectors required to have negative eigenvalues:
                      R1        R2        R3        R4        R5
        1           0.00090  -0.00308   0.00170   0.00005   0.00179
                      R6        R7        R8        R9        R10
        1          -0.00319  -0.00018   0.00199   0.00764  -0.00030
                      R11       R12       R13       R14       R15
        1           0.00137  -0.00010  -0.00015  -0.00351  -0.00164
                      R16       R17       R18       R19       R20
        1          -0.00095   0.00912   0.00019   0.00554  -0.00265
                      R21       R22       R23       R24       R25
        1           0.00033  -0.01068   0.64443  -0.05419   0.00136
                      R26       R27       R28       R29       R30
        1          -0.00021   0.00006   0.00610   0.05391   0.11746
                      R31       R32       R33       A1        A2
        1          -0.00180  -0.27818   0.04218   0.00082   0.00054
                      A3        A4        A5        A6        A7
        1           0.00112  -0.00094  -0.00148   0.00004   0.00161
                      A8        A9        A10       A11       A12
        1          -0.00103  -0.00004  -0.00119  -0.00086   0.00137
                      A13       A14       A15       A16       A17
        1          -0.00047   0.00001   0.00215  -0.00110   0.00124
                      A18       A19       A20       A21       A22
        1          -0.00210   0.00387   0.00202   0.00108   0.00117
                      A23       A24       A25       A26       A27
        1          -0.00007  -0.00036   0.00383   0.00485   0.00401
                      A28       A29       A30       A31       A32
        1          -0.00198  -0.00366  -0.00480  -0.00006  -0.00102
                      A33       A34       A35       A36       A37
        1          -0.01185  -0.00479   0.01065   0.00594  -0.00315
                      A38       A39       A40       A41       A42
        1          -0.00426   0.00014   0.00628  -0.01587   0.03031
                      A43       A44       A45       A46       A47
        1          -0.08326   0.03052  -0.07495  -0.00368  -0.01170
                      A48       A49       A50       A51       A52
        1           0.01139   0.00425  -0.00540   0.00256   0.00146
                      A53       A54       A55       A56       A57
        1           0.00038  -0.00111   0.00205  -0.00246  -0.00021
                      A58       A59       A60       A61       A62
        1          -0.07758   0.38095   0.06817   0.10167  -0.04700
                      A63       A64       A65       A66       A67
        1           0.03370  -0.00365   0.02851   0.13357  -0.05577
                      D1        D2        D3        D4        D5
        1          -0.00414  -0.00294  -0.00387  -0.00474  -0.00354
                      D6        D7        D8        D9        D10
        1          -0.00447  -0.00350  -0.00230  -0.00323   0.00642
                      D11       D12       D13       D14       D15
```

```
         1              0.00110   0.00585   0.00053   0.00753   0.00221
                          D16       D17       D18       D19       D20
         1              0.00327   0.00001   0.00088   0.00403   0.00078
                          D21       D22       D23       D24       D25
         1              0.00165   0.00131  -0.00195  -0.00108   0.00002
                          D26       D27       D28       D29       D30
         1              0.00119   0.00304  -0.00129  -0.00013   0.00173
                          D31       D32       D33       D34       D35
         1             -0.00074   0.00042   0.00227   0.00192   0.00142
                          D36       D37       D38       D39       D40
         1              0.00037   0.00064   0.00015  -0.00091   0.00196
                          D41       D42       D43       D44       D45
         1              0.00146   0.00041   0.00507   0.01411   0.00460
                          D46       D47       D48       D49       D50
         1              0.01365   0.00164   0.01069   0.00012   0.00267
                          D51       D52       D53       D54       D55
         1              0.00479   0.00070   0.00325   0.00537   0.00198
                          D56       D57       D58       D59       D60
         1              0.00453   0.00665  -0.00646  -0.01552  -0.00073
                          D61       D62       D63       D64       D65
         1             -0.00978  -0.00528   0.00013   0.00134  -0.01132
                          D66       D67       D68       D69       D70
         1             -0.00590  -0.00469   0.00058   0.00599   0.00721
                          D71       D72       D73       D74       D75
         1             -0.00013   0.01262   0.00927   0.00533   0.01809
                          D76       D77       D78       D79       D80
         1              0.01473  -0.00621   0.00655   0.00319  -0.00059
                          D81       D82       D83       D84       D85
         1             -0.00586  -0.00307  -0.00834   0.00815   0.00288
                          D86       D87       D88       D89       D90
         1             -0.00283  -0.00090  -0.00153  -0.00095   0.00098
                          D91       D92       D93       D94       D95
         1              0.00035  -0.01531  -0.01338  -0.01401   0.08828
                          D96       D97       D98       D99      D100
         1              0.08750   0.09534   0.01135  -0.08265  -0.17512
                         D101      D102      D103      D104      D105
         1              0.01908  -0.07492  -0.16739  -0.00985  -0.01569
                         D106      D107      D108      D109      D110
         1             -0.01703   0.03278   0.02694   0.02560   0.18910
                         D111      D112      D113      D114      D115
         1              0.18326   0.18192   0.04957   0.03077   0.05048
                         D116      D117      D118      D119      D120
         1              0.11823  -0.10328   0.05609  -0.05279  -0.18636
                         D121      D122
         1              0.00269   0.04863
 Angle between quadratic step and forces=  87.00 degrees.
 Linear search not attempted -- option 19 set.
 Iteration  1 RMS(Cart)=  0.00013523 RMS(Int)=  0.00000024
 Iteration  2 RMS(Cart)=  0.00000020 RMS(Int)=  0.00000000
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                  (Linear)    (Quad)   (Total)
    R1        2.95228   0.00000   0.00000   0.00000   0.00000   2.95228
    R2        2.93619   0.00000   0.00000   0.00000   0.00000   2.93619
    R3        2.89705   0.00000   0.00000   0.00000   0.00000   2.89704
```

R4	2.04134	0.00000	0.00000	0.00000	0.00000	2.04134
R5	2.96195	0.00000	0.00000	0.00000	0.00000	2.96195
R6	2.96274	0.00000	0.00000	0.00000	0.00000	2.96274
R7	2.03646	0.00000	0.00000	0.00000	0.00000	2.03646
R8	2.86279	0.00000	0.00000	0.00000	0.00000	2.86279
R9	3.02807	0.00000	0.00000	0.00000	0.00000	3.02806
R10	2.03301	0.00000	0.00000	0.00000	0.00000	2.03301
R11	2.87353	0.00000	0.00000	0.00000	0.00000	2.87354
R12	2.03582	0.00000	0.00000	0.00000	0.00000	2.03582
R13	2.29365	0.00000	0.00000	0.00000	0.00000	2.29365
R14	2.94529	0.00000	0.00000	0.00000	0.00000	2.94529
R15	2.94744	0.00000	0.00000	0.00000	0.00000	2.94744
R16	2.03377	0.00000	0.00000	0.00000	0.00000	2.03377
R17	2.92855	0.00000	0.00000	0.00000	0.00000	2.92855
R18	2.89950	0.00000	0.00000	0.00000	0.00000	2.89950
R19	2.03094	0.00000	0.00000	0.00000	0.00000	2.03094
R20	2.81955	0.00000	0.00000	-0.00001	-0.00001	2.81954
R21	2.03362	0.00000	0.00000	0.00000	0.00000	2.03362
R22	2.82232	0.00000	0.00000	0.00000	0.00000	2.82232
R23	4.67096	-0.00002	0.00000	-0.00010	-0.00010	4.67086
R24	2.40687	-0.00001	0.00000	0.00002	0.00002	2.40688
R25	2.02806	0.00000	0.00000	0.00000	0.00000	2.02805
R26	2.04816	0.00000	0.00000	0.00000	0.00000	2.04816
R27	2.04868	0.00000	0.00000	0.00000	0.00000	2.04868
R28	2.20011	0.00000	0.00000	0.00000	0.00000	2.20011
R29	5.32386	0.00000	0.00000	0.00018	0.00018	5.32404
R30	1.99766	-0.00001	0.00000	-0.00009	-0.00009	1.99757
R31	1.81667	0.00000	0.00000	0.00000	0.00000	1.81667
R32	2.68756	0.00000	0.00000	0.00022	0.00022	2.68778
R33	1.88563	-0.00001	0.00000	0.00001	0.00001	1.88564
A1	1.77398	0.00000	0.00000	0.00000	0.00000	1.77398
A2	1.79799	0.00000	0.00000	0.00000	0.00000	1.79799
A3	2.00833	0.00000	0.00000	0.00000	0.00000	2.00833
A4	1.81634	0.00000	0.00000	0.00000	0.00000	1.81635
A5	1.98314	0.00000	0.00000	0.00000	0.00000	1.98314
A6	2.05093	0.00000	0.00000	0.00000	0.00000	2.05093
A7	1.87104	0.00000	0.00000	0.00000	0.00000	1.87104
A8	1.79768	0.00000	0.00000	0.00000	0.00000	1.79768
A9	2.01307	0.00000	0.00000	0.00000	0.00000	2.01307
A10	1.58462	0.00000	0.00000	0.00000	0.00000	1.58462
A11	2.05904	0.00000	0.00000	0.00000	0.00000	2.05904
A12	2.07870	0.00000	0.00000	0.00000	0.00000	2.07870
A13	1.80457	0.00000	0.00000	-0.00001	-0.00001	1.80456
A14	1.55223	0.00000	0.00000	0.00000	0.00000	1.55223
A15	2.09984	0.00000	0.00000	0.00000	0.00000	2.09984
A16	1.92850	0.00000	0.00000	0.00001	0.00001	1.92851
A17	2.00673	0.00000	0.00000	0.00000	0.00000	2.00673
A18	2.01624	0.00000	0.00000	0.00000	0.00000	2.01624
A19	1.77752	0.00000	0.00000	-0.00001	-0.00001	1.77751
A20	2.02264	0.00000	0.00000	0.00000	0.00000	2.02264
A21	1.98132	0.00000	0.00000	0.00000	0.00000	1.98132
A22	1.82646	0.00000	0.00000	0.00000	0.00000	1.82646
A23	2.22739	0.00000	0.00000	0.00000	0.00000	2.22739
A24	2.22593	0.00000	0.00000	0.00000	0.00000	2.22593

A25	1.80052	0.00000	0.00000	0.00000	0.00000	1.80052
A26	1.57904	0.00000	0.00000	0.00000	0.00000	1.57904
A27	2.08497	0.00000	0.00000	0.00000	0.00000	2.08497
A28	1.88023	0.00000	0.00000	0.00000	0.00000	1.88023
A29	2.01173	0.00000	0.00000	0.00000	0.00000	2.01173
A30	2.04874	0.00000	0.00000	0.00000	0.00000	2.04874
A31	1.77020	0.00000	0.00000	0.00000	0.00000	1.77020
A32	1.79973	0.00000	0.00000	0.00000	0.00000	1.79973
A33	2.00320	0.00000	0.00000	0.00000	0.00000	2.00321
A34	1.81474	0.00000	0.00000	0.00000	0.00000	1.81474
A35	1.98315	0.00000	0.00000	0.00001	0.00001	1.98316
A36	2.05855	0.00000	0.00000	-0.00001	-0.00001	2.05854
A37	1.81732	0.00000	0.00000	0.00001	0.00001	1.81733
A38	2.03829	0.00000	0.00000	0.00000	0.00000	2.03829
A39	1.98338	0.00000	0.00000	0.00001	0.00001	1.98338
A40	1.86884	0.00000	0.00000	0.00000	0.00000	1.86884
A41	1.84047	0.00001	0.00000	0.00002	0.00002	1.84049
A42	2.13028	0.00000	0.00000	-0.00001	-0.00001	2.13027
A43	1.56564	0.00000	0.00000	0.00002	0.00002	1.56567
A44	2.22291	0.00000	0.00000	-0.00002	-0.00002	2.22288
A45	1.64302	-0.00001	0.00000	0.00003	0.00003	1.64306
A46	1.56727	0.00000	0.00000	0.00000	0.00000	1.56727
A47	1.84434	0.00000	0.00000	-0.00001	-0.00001	1.84433
A48	2.03221	0.00000	0.00000	0.00000	0.00000	2.03221
A49	1.81689	0.00000	0.00000	0.00000	0.00000	1.81689
A50	2.10446	0.00000	0.00000	0.00000	0.00000	2.10446
A51	2.03116	0.00000	0.00000	0.00000	0.00000	2.03116
A52	1.67028	0.00000	0.00000	0.00000	0.00000	1.67028
A53	1.97438	0.00000	0.00000	0.00000	0.00000	1.97438
A54	1.96565	0.00000	0.00000	0.00000	0.00000	1.96565
A55	1.97619	0.00000	0.00000	0.00000	0.00000	1.97619
A56	1.96201	0.00000	0.00000	0.00000	0.00000	1.96202
A57	1.90755	0.00000	0.00000	0.00000	0.00000	1.90755
A58	1.15633	0.00000	0.00000	-0.00001	-0.00001	1.15632
A59	2.94470	0.00001	0.00000	-0.00013	-0.00013	2.94457
A60	2.10399	-0.00004	0.00000	-0.00007	-0.00007	2.10392
A61	1.74994	0.00000	0.00000	-0.00004	-0.00004	1.74990
A62	2.32238	0.00000	0.00000	0.00009	0.00009	2.32247
A63	2.01524	0.00000	0.00000	-0.00002	-0.00002	2.01522
A64	1.85459	0.00000	0.00000	-0.00005	-0.00005	1.85454
A65	2.85496	-0.00003	0.00000	-0.00004	-0.00004	2.85493
A66	3.98315	0.00000	0.00000	0.00366	0.00366	3.98681
A67	3.15559	0.00000	0.00000	0.00010	0.00010	3.15569
D1	0.36429	0.00000	0.00000	0.00000	0.00000	0.36430
D2	-1.29294	0.00000	0.00000	0.00000	0.00000	-1.29294
D3	2.69649	0.00000	0.00000	0.00000	0.00000	2.69650
D4	2.24227	0.00000	0.00000	0.00000	0.00000	2.24227
D5	0.58504	0.00000	0.00000	0.00000	0.00000	0.58504
D6	-1.70872	0.00000	0.00000	0.00000	0.00000	-1.70871
D7	-1.78660	0.00000	0.00000	0.00000	0.00000	-1.78660
D8	2.83935	0.00000	0.00000	0.00000	0.00000	2.83935
D9	0.54560	0.00000	0.00000	0.00000	0.00000	0.54560
D10	-0.70737	0.00000	0.00000	-0.00001	-0.00001	-0.70738
D11	-2.86658	0.00000	0.00000	0.00000	0.00000	-2.86658

D12	-2.57105	0.00000	0.00000	-0.00001	-0.00001	-2.57106
D13	1.55292	0.00000	0.00000	0.00000	0.00000	1.55292
D14	1.46060	0.00000	0.00000	-0.00001	-0.00001	1.46059
D15	-0.69861	0.00000	0.00000	0.00000	0.00000	-0.69861
D16	-0.92465	0.00000	0.00000	0.00000	0.00000	-0.92465
D17	-2.98880	0.00000	0.00000	0.00000	0.00000	-2.98880
D18	1.12049	0.00000	0.00000	0.00000	0.00000	1.12049
D19	0.92105	0.00000	0.00000	0.00000	0.00000	0.92105
D20	-1.14310	0.00000	0.00000	0.00000	0.00000	-1.14310
D21	2.96619	0.00000	0.00000	0.00000	0.00000	2.96619
D22	3.13077	0.00000	0.00000	0.00000	0.00000	3.13077
D23	1.06662	0.00000	0.00000	0.00000	0.00000	1.06662
D24	-1.10728	0.00000	0.00000	0.00000	0.00000	-1.10728
D25	0.11643	0.00000	0.00000	0.00001	0.00001	0.11644
D26	-1.81788	0.00000	0.00000	0.00000	0.00000	-1.81787
D27	2.38435	0.00000	0.00000	0.00000	0.00000	2.38435
D28	1.92936	0.00000	0.00000	0.00001	0.00001	1.92937
D29	-0.00494	0.00000	0.00000	0.00000	0.00000	-0.00494
D30	-2.08590	0.00000	0.00000	0.00000	0.00000	-2.08590
D31	-2.19095	0.00000	0.00000	0.00001	0.00001	-2.19094
D32	2.15793	0.00000	0.00000	0.00000	0.00000	2.15793
D33	0.07698	0.00000	0.00000	0.00000	0.00000	0.07698
D34	-0.00325	0.00000	0.00000	0.00000	0.00000	-0.00325
D35	1.88766	0.00000	0.00000	0.00000	0.00000	1.88766
D36	-2.26267	0.00000	0.00000	0.00000	0.00000	-2.26267
D37	-1.88583	0.00000	0.00000	0.00000	0.00000	-1.88583
D38	0.00508	0.00000	0.00000	0.00000	0.00000	0.00508
D39	2.13794	0.00000	0.00000	0.00000	0.00000	2.13793
D40	2.25066	0.00000	0.00000	0.00000	0.00000	2.25066
D41	-2.14162	0.00000	0.00000	0.00000	0.00000	-2.14162
D42	-0.00876	0.00000	0.00000	0.00000	0.00000	-0.00876
D43	-0.57133	0.00000	0.00000	-0.00002	-0.00002	-0.57135
D44	2.48643	0.00000	0.00000	-0.00005	-0.00005	2.48638
D45	1.06815	0.00000	0.00000	-0.00002	-0.00002	1.06813
D46	-2.15727	0.00000	0.00000	-0.00005	-0.00005	-2.15733
D47	-2.89436	0.00000	0.00000	-0.00001	-0.00001	-2.89437
D48	0.16340	0.00000	0.00000	-0.00004	-0.00004	0.16335
D49	0.00497	0.00000	0.00000	0.00000	0.00000	0.00497
D50	1.83055	0.00000	0.00000	0.00000	0.00000	1.83055
D51	-2.16789	0.00000	0.00000	0.00000	0.00000	-2.16789
D52	-1.80861	0.00000	0.00000	0.00000	0.00000	-1.80860
D53	0.01697	0.00000	0.00000	0.00001	0.00001	0.01698
D54	2.30172	0.00000	0.00000	0.00001	0.00001	2.30172
D55	2.15875	0.00000	0.00000	0.00000	0.00000	2.15874
D56	-2.29886	0.00000	0.00000	0.00000	0.00000	-2.29886
D57	-0.01411	0.00000	0.00000	0.00000	0.00000	-0.01412
D58	0.81575	0.00000	0.00000	0.00002	0.00002	0.81577
D59	-2.24210	0.00000	0.00000	0.00005	0.00005	-2.24205
D60	3.00262	0.00000	0.00000	0.00001	0.00001	3.00263
D61	-0.05524	0.00000	0.00000	0.00004	0.00004	-0.05519
D62	1.29642	0.00000	0.00000	0.00000	0.00000	1.29643
D63	-0.57918	0.00000	0.00000	0.00000	0.00000	-0.57917
D64	-2.84126	0.00000	0.00000	0.00002	0.00002	-2.84125
D65	-0.35812	0.00000	0.00000	0.00001	0.00001	-0.35812

D66	-2.23372	0.00000	0.00000	0.00000	0.00000	-2.23372
D67	1.78738	0.00000	0.00000	0.00002	0.00002	1.78739
D68	-2.68329	0.00000	0.00000	0.00000	0.00000	-2.68329
D69	1.72430	0.00000	0.00000	0.00000	0.00000	1.72430
D70	-0.53779	0.00000	0.00000	0.00001	0.00001	-0.53777
D71	-0.00497	0.00000	0.00000	0.00000	0.00000	-0.00497
D72	-1.85711	0.00000	0.00000	0.00001	0.00001	-1.85710
D73	2.10688	0.00000	0.00000	0.00000	0.00000	2.10688
D74	1.80995	0.00000	0.00000	0.00000	0.00000	1.80996
D75	-0.04219	0.00000	0.00000	0.00001	0.00001	-0.04218
D76	-2.36139	0.00000	0.00000	0.00000	0.00000	-2.36139
D77	-2.16794	0.00000	0.00000	0.00001	0.00001	-2.16794
D78	2.26310	0.00000	0.00000	0.00001	0.00001	2.26311
D79	-0.05610	0.00000	0.00000	0.00000	0.00000	-0.05609
D80	0.63125	0.00000	0.00000	-0.00001	-0.00001	0.63124
D81	2.83336	0.00000	0.00000	0.00000	0.00000	2.83336
D82	2.49511	0.00000	0.00000	-0.00001	-0.00001	2.49510
D83	-1.58596	0.00000	0.00000	0.00000	0.00000	-1.58596
D84	-1.52796	0.00000	0.00000	-0.00002	-0.00002	-1.52798
D85	0.67415	0.00000	0.00000	0.00000	0.00000	0.67414
D86	0.92332	0.00000	0.00000	0.00000	0.00000	0.92331
D87	2.98603	0.00000	0.00000	0.00000	0.00000	2.98602
D88	-1.12475	0.00000	0.00000	0.00000	0.00000	-1.12475
D89	-0.91838	0.00000	0.00000	0.00000	0.00000	-0.91838
D90	1.14433	0.00000	0.00000	0.00000	0.00000	1.14433
D91	-2.96644	0.00000	0.00000	0.00000	0.00000	-2.96644
D92	-3.13212	0.00000	0.00000	-0.00001	-0.00001	-3.13213
D93	-1.06941	0.00000	0.00000	-0.00001	-0.00001	-1.06942
D94	1.10300	0.00000	0.00000	-0.00001	-0.00001	1.10300
D95	-1.02295	0.00000	0.00000	-0.00004	-0.00004	-1.02300
D96	1.00346	0.00000	0.00000	-0.00003	-0.00003	1.00342
D97	3.13344	0.00000	0.00000	-0.00004	-0.00004	3.13340
D98	-0.69895	0.00000	0.00000	0.00002	0.00002	-0.69893
D99	0.95125	0.00000	0.00000	0.00005	0.00005	0.95130
D100	2.78655	-0.00001	0.00000	0.00010	0.00010	2.78666
D101	-2.93519	0.00000	0.00000	0.00001	0.00001	-2.93518
D102	-1.28499	0.00000	0.00000	0.00004	0.00004	-1.28495
D103	0.55031	0.00000	0.00000	0.00009	0.00009	0.55041
D104	-1.18379	0.00000	0.00000	-0.00002	-0.00002	-1.18381
D105	0.45375	0.00000	0.00000	-0.00002	-0.00002	0.45373
D106	2.81405	0.00000	0.00000	-0.00001	-0.00001	2.81403
D107	-3.03539	0.00000	0.00000	-0.00005	-0.00005	-3.03544
D108	-1.39785	0.00000	0.00000	-0.00005	-0.00005	-1.39790
D109	0.96244	-0.00001	0.00000	-0.00004	-0.00004	0.96240
D110	1.59002	0.00001	0.00000	-0.00010	-0.00010	1.58992
D111	-3.05562	0.00001	0.00000	-0.00010	-0.00010	-3.05572
D112	-0.69532	0.00001	0.00000	-0.00010	-0.00010	-0.69542
D113	-0.39855	0.00000	0.00000	-0.00003	-0.00003	-0.39858
D114	1.48034	0.00000	0.00000	-0.00002	-0.00002	1.48033
D115	-2.57840	0.00000	0.00000	-0.00004	-0.00004	-2.57843
D116	-2.97321	0.00001	0.00000	-0.00019	-0.00019	-2.97340
D117	0.58593	0.00001	0.00000	-0.00010	-0.00010	0.58583
D118	-1.03363	0.00002	0.00000	-0.00015	-0.00015	-1.03378
D119	-0.32518	0.00000	0.00000	0.00003	0.00003	-0.32515

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   D120        1.97486   0.00000   0.00000  -0.00363  -0.00363   1.97123
   D121       -2.75177   0.00000   0.00000  -0.00002  -0.00002  -2.75178
   D122        0.93035   0.00000   0.00000  -0.00008  -0.00008   0.93027
         Item               Value     Threshold  Converged?
 Maximum Force            0.000036     0.000450     YES
 RMS     Force            0.000004     0.000300     YES
 Maximum Displacement     0.000915     0.001800     YES
 RMS     Displacement     0.000135     0.001200     YES
 Predicted change in Energy=-9.007330D-09
 Optimization completed.
    -- Stationary point found.
                          ----------------------------
                          !   Optimized Parameters   !
                          ! (Angstroms and Degrees)  !
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-----
 ! Name  Definition              Value          Derivative Info.
!
 --------------------------------------------------------------------------
-----
 ! R1    R(1,2)                  1.5623         -DE/DX =    0.
!
 ! R2    R(1,4)                  1.5538         -DE/DX =    0.
!
 ! R3    R(1,11)                 1.5331         -DE/DX =    0.
!
 ! R4    R(1,16)                 1.0802         -DE/DX =    0.
!
 ! R5    R(2,3)                  1.5674         -DE/DX =    0.
!
 ! R6    R(2,6)                  1.5678         -DE/DX =    0.
!
 ! R7    R(2,17)                 1.0776         -DE/DX =    0.
!
 ! R8    R(3,5)                  1.5149         -DE/DX =    0.
!
 ! R9    R(3,10)                 1.6024         -DE/DX =    0.
!
 ! R10   R(3,18)                 1.0758         -DE/DX =    0.
!
 ! R11   R(4,5)                  1.5206         -DE/DX =    0.
!
 ! R12   R(4,19)                 1.0773         -DE/DX =    0.
!
 ! R13   R(5,12)                 1.2137         -DE/DX =    0.
!
 ! R14   R(6,7)                  1.5586         -DE/DX =    0.
!
 ! R15   R(6,10)                 1.5597         -DE/DX =    0.
!
 ! R16   R(6,20)                 1.0762         -DE/DX =    0.
!
 ! R17   R(7,8)                  1.5497         -DE/DX =    0.
!
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 ! R18   R(7,11)                1.5344         -DE/DX =    0.
!
 ! R19   R(7,21)                1.0747         -DE/DX =    0.
!
 ! R20   R(8,9)                 1.492          -DE/DX =    0.
!
 ! R21   R(8,22)                1.0761         -DE/DX =    0.
!
 ! R22   R(9,10)                1.4935         -DE/DX =    0.
!
 ! R23   R(9,13)                2.4718         -DE/DX =    0.
!
 ! R24   R(9,15)                1.2737         -DE/DX =    0.
!
 ! R25   R(10,23)               1.0732         -DE/DX =    0.
!
 ! R26   R(11,24)               1.0838         -DE/DX =    0.
!
 ! R27   R(11,25)               1.0841         -DE/DX =    0.
!
 ! R28   R(13,14)               1.1642         -DE/DX =    0.
!
 ! R29   R(13,21)               2.8173         -DE/DX =    0.
!
 ! R30   R(15,28)               1.0571         -DE/DX =    0.
!
 ! R31   R(26,27)               0.9613         -DE/DX =    0.
!
 ! R32   R(26,28)               1.4222         -DE/DX =    0.
!
 ! R33   R(26,29)               0.9978         -DE/DX =    0.
!
 ! A1    A(2,1,4)              101.6417        -DE/DX =    0.
!
 ! A2    A(2,1,11)             103.0171        -DE/DX =    0.
!
 ! A3    A(2,1,16)             115.0691        -DE/DX =    0.
!
 ! A4    A(4,1,11)             104.0689        -DE/DX =    0.
!
 ! A5    A(4,1,16)             113.6257        -DE/DX =    0.
!
 ! A6    A(11,1,16)            117.5096        -DE/DX =    0.
!
 ! A7    A(1,2,3)              107.2029        -DE/DX =    0.
!
 ! A8    A(1,2,6)              102.9992        -DE/DX =    0.
!
 ! A9    A(1,2,17)             115.3406        -DE/DX =    0.
!
 ! A10   A(3,2,6)               90.7922        -DE/DX =    0.
!
 ! A11   A(3,2,17)             117.9741        -DE/DX =    0.
!
```

```
 ! A12   A(6,2,17)             119.1009         -DE/DX =    0.
!
 ! A13   A(2,3,5)              103.3942         -DE/DX =    0.
!
 ! A14   A(2,3,10)              88.9362         -DE/DX =    0.
!
 ! A15   A(2,3,18)             120.312          -DE/DX =    0.
!
 ! A16   A(5,3,10)             110.4949         -DE/DX =    0.
!
 ! A17   A(5,3,18)             114.9771         -DE/DX =    0.
!
 ! A18   A(10,3,18)            115.522          -DE/DX =    0.
!
 ! A19   A(1,4,5)              101.8445         -DE/DX =    0.
!
 ! A20   A(1,4,19)             115.8888         -DE/DX =    0.
!
 ! A21   A(5,4,19)             113.5212         -DE/DX =    0.
!
 ! A22   A(3,5,4)              104.6487         -DE/DX =    0.
!
 ! A23   A(3,5,12)             127.6202         -DE/DX =    0.
!
 ! A24   A(4,5,12)             127.5364         -DE/DX =    0.
!
 ! A25   A(2,6,7)              103.1622         -DE/DX =    0.
!
 ! A26   A(2,6,10)              90.4724         -DE/DX =    0.
!
 ! A27   A(2,6,20)             119.4599         -DE/DX =    0.
!
 ! A28   A(7,6,10)             107.729          -DE/DX =    0.
!
 ! A29   A(7,6,20)             115.2636         -DE/DX =    0.
!
 ! A30   A(10,6,20)            117.384          -DE/DX =    0.
!
 ! A31   A(6,7,8)              101.4249         -DE/DX =    0.
!
 ! A32   A(6,7,11)             103.117          -DE/DX =    0.
!
 ! A33   A(6,7,21)             114.7752         -DE/DX =    0.
!
 ! A34   A(8,7,11)             103.9769         -DE/DX =    0.
!
 ! A35   A(8,7,21)             113.6261         -DE/DX =    0.
!
 ! A36   A(11,7,21)            117.9465         -DE/DX =    0.
!
 ! A37   A(7,8,9)              104.1249         -DE/DX =    0.
!
 ! A38   A(7,8,22)             116.7852         -DE/DX =    0.
!
```

```
 ! A39   A(9,8,22)             113.6391         -DE/DX =    0.
!
 ! A40   A(8,9,10)             107.0767         -DE/DX =    0.
!
 ! A41   A(8,9,13)             105.4513         -DE/DX =    0.
!
 ! A42   A(8,9,15)             122.0561         -DE/DX =    0.
!
 ! A43   A(10,9,13)             89.7048         -DE/DX =    0.
!
 ! A44   A(10,9,15)            127.3632         -DE/DX =    0.
!
 ! A45   A(13,9,15)             94.1383         -DE/DX =    0.
!
 ! A46   A(3,10,6)              89.7978         -DE/DX =    0.
!
 ! A47   A(3,10,9)             105.6727         -DE/DX =    0.
!
 ! A48   A(3,10,23)            116.437          -DE/DX =    0.
!
 ! A49   A(6,10,9)             104.1001         -DE/DX =    0.
!
 ! A50   A(6,10,23)            120.5764         -DE/DX =    0.
!
 ! A51   A(9,10,23)            116.3769         -DE/DX =    0.
!
 ! A52   A(1,11,7)              95.7001         -DE/DX =    0.
!
 ! A53   A(1,11,24)            113.1236         -DE/DX =    0.
!
 ! A54   A(1,11,25)            112.6234         -DE/DX =    0.
!
 ! A55   A(7,11,24)            113.2273         -DE/DX =    0.
!
 ! A56   A(7,11,25)            112.4152         -DE/DX =    0.
!
 ! A57   A(24,11,25)           109.2945         -DE/DX =    0.
!
 ! A58   A(9,13,21)             66.2527         -DE/DX =    0.
!
 ! A59   A(14,13,21)           168.7186         -DE/DX =    0.
!
 ! A60   A(9,15,28)            120.5498         -DE/DX =    0.
!
 ! A61   A(7,21,13)            100.2643         -DE/DX =    0.
!
 ! A62   A(27,26,28)           133.0626         -DE/DX =    0.
!
 ! A63   A(27,26,29)           115.4647         -DE/DX =    0.
!
 ! A64   A(28,26,29)           106.2603         -DE/DX =    0.
!
 ! A65   L(15,28,26,29,-1)     163.5774         -DE/DX =    0.
!
```

```
 ! A66   L(9,13,14,21,-2)      228.2174         -DE/DX =    0.
!
 ! A67   L(15,28,26,29,-2)     180.8017         -DE/DX =    0.
!
 ! D1    D(4,1,2,3)             20.8726         -DE/DX =    0.
!
 ! D2    D(4,1,2,6)            -74.0798         -DE/DX =    0.
!
 ! D3    D(4,1,2,17)           154.4977         -DE/DX =    0.
!
 ! D4    D(11,1,2,3)           128.4726         -DE/DX =    0.
!
 ! D5    D(11,1,2,6)            33.5202         -DE/DX =    0.
!
 ! D6    D(11,1,2,17)          -97.9022         -DE/DX =    0.
!
 ! D7    D(16,1,2,3)          -102.3647         -DE/DX =    0.
!
 ! D8    D(16,1,2,6)           162.6829         -DE/DX =    0.
!
 ! D9    D(16,1,2,17)           31.2605         -DE/DX =    0.
!
 ! D10   D(2,1,4,5)            -40.5293         -DE/DX =    0.
!
 ! D11   D(2,1,4,19)          -164.2429         -DE/DX =    0.
!
 ! D12   D(11,1,4,5)          -147.3104         -DE/DX =    0.
!
 ! D13   D(11,1,4,19)           88.976          -DE/DX =    0.
!
 ! D14   D(16,1,4,5)            83.6864         -DE/DX =    0.
!
 ! D15   D(16,1,4,19)          -40.0273         -DE/DX =    0.
!
 ! D16   D(2,1,11,7)           -52.9784         -DE/DX =    0.
!
 ! D17   D(2,1,11,24)         -171.2457         -DE/DX =    0.
!
 ! D18   D(2,1,11,25)           64.1993         -DE/DX =    0.
!
 ! D19   D(4,1,11,7)            52.7724         -DE/DX =    0.
!
 ! D20   D(4,1,11,24)          -65.495          -DE/DX =    0.
!
 ! D21   D(4,1,11,25)          169.9501         -DE/DX =    0.
!
 ! D22   D(16,1,11,7)          179.38           -DE/DX =    0.
!
 ! D23   D(16,1,11,24)          61.1127         -DE/DX =    0.
!
 ! D24   D(16,1,11,25)         -63.4423         -DE/DX =    0.
!
 ! D25   D(1,2,3,5)              6.6709         -DE/DX =    0.
!
```

```
 ! D26   D(1,2,3,10)          -104.1566         -DE/DX =    0.
!
 ! D27   D(1,2,3,18)           136.6133         -DE/DX =    0.
!
 ! D28   D(6,2,3,5)            110.5442         -DE/DX =    0.
!
 ! D29   D(6,2,3,10)            -0.2833         -DE/DX =    0.
!
 ! D30   D(6,2,3,18)          -119.5134         -DE/DX =    0.
!
 ! D31   D(17,2,3,5)          -125.5321         -DE/DX =    0.
!
 ! D32   D(17,2,3,10)          123.6404         -DE/DX =    0.
!
 ! D33   D(17,2,3,18)            4.4103         -DE/DX =    0.
!
 ! D34   D(1,2,6,7)             -0.1861         -DE/DX =    0.
!
 ! D35   D(1,2,6,10)           108.1548         -DE/DX =    0.
!
 ! D36   D(1,2,6,20)          -129.6415         -DE/DX =    0.
!
 ! D37   D(3,2,6,7)           -108.0499         -DE/DX =    0.
!
 ! D38   D(3,2,6,10)             0.291          -DE/DX =    0.
!
 ! D39   D(3,2,6,20)           122.4947         -DE/DX =    0.
!
 ! D40   D(17,2,6,7)           128.9535         -DE/DX =    0.
!
 ! D41   D(17,2,6,10)         -122.7056         -DE/DX =    0.
!
 ! D42   D(17,2,6,20)           -0.5019         -DE/DX =    0.
!
 ! D43   D(2,3,5,4)            -32.7348         -DE/DX =    0.
!
 ! D44   D(2,3,5,12)           142.4619         -DE/DX =    0.
!
 ! D45   D(10,3,5,4)            61.2007         -DE/DX =    0.
!
 ! D46   D(10,3,5,12)         -123.6026         -DE/DX =    0.
!
 ! D47   D(18,3,5,4)          -165.8348         -DE/DX =    0.
!
 ! D48   D(18,3,5,12)            9.3619         -DE/DX =    0.
!
 ! D49   D(2,3,10,6)             0.2847         -DE/DX =    0.
!
 ! D50   D(2,3,10,9)           104.8827         -DE/DX =    0.
!
 ! D51   D(2,3,10,23)         -124.211          -DE/DX =    0.
!
 ! D52   D(5,3,10,6)          -103.6257         -DE/DX =    0.
!
```

```
 ! D53   D(5,3,10,9)             0.9723         -DE/DX =    0.
!
 ! D54   D(5,3,10,23)          131.8786         -DE/DX =    0.
!
 ! D55   D(18,3,10,6)          123.687          -DE/DX =    0.
!
 ! D56   D(18,3,10,9)         -131.715          -DE/DX =    0.
!
 ! D57   D(18,3,10,23)          -0.8087         -DE/DX =    0.
!
 ! D58   D(1,4,5,3)             46.7392         -DE/DX =    0.
!
 ! D59   D(1,4,5,12)          -128.4629         -DE/DX =    0.
!
 ! D60   D(19,4,5,3)           172.0374         -DE/DX =    0.
!
 ! D61   D(19,4,5,12)           -3.1647         -DE/DX =    0.
!
 ! D62   D(2,6,7,8)             74.2795         -DE/DX =    0.
!
 ! D63   D(2,6,7,11)           -33.1844         -DE/DX =    0.
!
 ! D64   D(2,6,7,21)          -162.7923         -DE/DX =    0.
!
 ! D65   D(10,6,7,8)           -20.519          -DE/DX =    0.
!
 ! D66   D(10,6,7,11)         -127.9829         -DE/DX =    0.
!
 ! D67   D(10,6,7,21)          102.4092         -DE/DX =    0.
!
 ! D68   D(20,6,7,8)          -153.7411         -DE/DX =    0.
!
 ! D69   D(20,6,7,11)           98.795          -DE/DX =    0.
!
 ! D70   D(20,6,7,21)          -30.8129         -DE/DX =    0.
!
 ! D71   D(2,6,10,3)            -0.2846         -DE/DX =    0.
!
 ! D72   D(2,6,10,9)          -106.4045         -DE/DX =    0.
!
 ! D73   D(2,6,10,23)          120.7153         -DE/DX =    0.
!
 ! D74   D(7,6,10,3)           103.7027         -DE/DX =    0.
!
 ! D75   D(7,6,10,9)            -2.4172         -DE/DX =    0.
!
 ! D76   D(7,6,10,23)         -135.2974         -DE/DX =    0.
!
 ! D77   D(20,6,10,3)         -124.214          -DE/DX =    0.
!
 ! D78   D(20,6,10,9)          129.6661         -DE/DX =    0.
!
 ! D79   D(20,6,10,23)          -3.2141         -DE/DX =    0.
!
```

```
 ! D80   D(6,7,8,9)             36.1679         -DE/DX =    0.
!
 ! D81   D(6,7,8,22)           162.3395         -DE/DX =    0.
!
 ! D82   D(11,7,8,9)           142.9595         -DE/DX =    0.
!
 ! D83   D(11,7,8,22)          -90.8688         -DE/DX =    0.
!
 ! D84   D(21,7,8,9)           -87.5459         -DE/DX =    0.
!
 ! D85   D(21,7,8,22)           38.6258         -DE/DX =    0.
!
 ! D86   D(6,7,11,1)            52.9021         -DE/DX =    0.
!
 ! D87   D(6,7,11,24)          171.0867         -DE/DX =    0.
!
 ! D88   D(6,7,11,25)          -64.4432         -DE/DX =    0.
!
 ! D89   D(8,7,11,1)           -52.6191         -DE/DX =    0.
!
 ! D90   D(8,7,11,24)           65.5656         -DE/DX =    0.
!
 ! D91   D(8,7,11,25)         -169.9643         -DE/DX =    0.
!
 ! D92   D(21,7,11,1)         -179.4573         -DE/DX =    0.
!
 ! D93   D(21,7,11,24)         -61.2726         -DE/DX =    0.
!
 ! D94   D(21,7,11,25)          63.1975         -DE/DX =    0.
!
 ! D95   D(6,7,21,13)           -58.6109         -DE/DX =    0.
!
 ! D96   D(8,7,21,13)            57.494          -DE/DX =    0.
!
 ! D97   D(11,7,21,13)         179.5326         -DE/DX =    0.
!
 ! D98   D(7,8,9,10)            -40.0471         -DE/DX =    0.
!
 ! D99   D(7,8,9,13)             54.5024         -DE/DX =    0.
!
 ! D100  D(7,8,9,15)            159.6577         -DE/DX =    0.
!
 ! D101  D(22,8,9,10)         -168.1741         -DE/DX =    0.
!
 ! D102  D(22,8,9,13)           -73.6246         -DE/DX =    0.
!
 ! D103  D(22,8,9,15)            31.5306         -DE/DX =    0.
!
 ! D104  D(8,9,10,3)            -67.8264         -DE/DX =    0.
!
 ! D105  D(8,9,10,6)             25.9979         -DE/DX =    0.
!
 ! D106  D(8,9,10,23)           161.2329         -DE/DX =    0.
!
```

```
 ! D107  D(13,9,10,3)         -173.9153         -DE/DX =    0.
!
 ! D108  D(13,9,10,6)          -80.091          -DE/DX =    0.
!
 ! D109  D(13,9,10,23)          55.144          -DE/DX =    0.
!
 ! D110  D(15,9,10,3)           91.1016         -DE/DX =    0.
!
 ! D111  D(15,9,10,6)         -175.0741         -DE/DX =    0.
!
 ! D112  D(15,9,10,23)         -39.8391         -DE/DX =    0.
!
 ! D113  D(8,9,13,21)          -22.8352         -DE/DX =    0.
!
 ! D114  D(10,9,13,21)          84.8174         -DE/DX =    0.
!
 ! D115  D(15,9,13,21)        -147.7313         -DE/DX =    0.
!
 ! D116  D(8,9,15,28)         -170.3523         -DE/DX =    0.
!
 ! D117  D(10,9,15,28)          33.5714         -DE/DX =    0.
!
 ! D118  D(13,9,15,28)         -59.2226         -DE/DX =    0.
!
 ! D119  D(9,13,21,7)          -18.6312         -DE/DX =    0.
!
 ! D120  D(14,13,21,7)         113.1514         -DE/DX =    0.
!
 ! D121  D(9,15,26,27)        -157.6647         -DE/DX =    0.
!
 ! D122  D(9,15,26,29)          53.3054         -DE/DX =    0.
!
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 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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0437,-0.00021085,-0.00058949,-0.00022162,0.00011287,0.00002722,0.00018
904,-0.00041618,-0.00267487,-0.00228472,0.00305308,-0.00002314,0.00000
647,0.00001369,-0.00001763,0.00000885,0.00001670,-0.00001191,-0.000003
73,0.00000498,-0.00000517,-0.00002281,0.00000489,-0.00000612,-0.000000
57,0.00001617,0.00000280,0.00001286,-0.00002866,-0.00000757,0.00000217
,0.00001011,0.00007628,-0.00009711,-0.00004598,-0.00000561,-0.00001850
,0.00000477,-0.00001120,0.00001079,0.00001450,0.08689398,0.04572477,-0
.52249985,-0.10504805,-0.05109307,0.54000427,0.00011750,0.00019422,-0.
00001768,-0.00012444,0.00005502,-0.00006680,-0.00117202,0.00069150,0.0
0009796,-0.00038942,0.00028432,-0.00120047,-0.00130772,0.00031765,0.00
080329,-0.00007945,-0.00115915,0.00046365,0.00087170,0.00048123,0.0002
3564,0.00532199,-0.00245632,-0.00153774,0.00718686,0.01231619,0.016612
20,-0.00248809,-0.00055799,-0.00301619,-0.00002376,-0.00030089,-0.0004
7349,0.00089127,-0.00002543,-0.00026728,-0.00452809,-0.00032176,-0.005
13649,0.00070205,-0.00043955,0.00945610,-0.06533532,-0.04274868,0.0366
0021,0.00009619,-0.00010357,-0.00020503,0.00008231,-0.00009632,-0.0001
4455,0.00000665,0.00008094,0.00003484,0.00038702,-0.00007220,-0.000025
62,0.00026440,-0.00015567,-0.00063548,-0.00001107,-0.00003158,-0.00038
569,-0.00001296,-0.00026702,0.00046505,0.00077387,-0.00044269,-0.00022
134,0.00001219,0.00011447,0.00003202,0.00012117,-0.00010394,-0.0001926
9,-0.01307710,0.01395704,-0.02200938,0.00853763,0.00597795,0.00333561,
0.07384556,0.00017103,0.00022003,0.00016522,0.00000536,0.00000726,-0.0
0004000,-0.00097797,-0.00046553,-0.00008798,-0.00099925,-0.00046058,0.
00004097,-0.00148267,0.00106569,-0.00099988,-0.00047332,-0.00070335,-0
.00050359,0.00071489,0.00164319,-0.00018806,-0.00109983,-0.00483473,-0
.00425821,0.01617188,0.03266144,-0.00434781,0.00199761,0.00218708,-0.0
0126320,-0.00025676,-0.00080501,-0.00066909,0.00055992,-0.00043006,0.0
0079655,-0.00404550,-0.00094809,-0.00470815,0.00091941,-0.00197618,0.0
0795174,-0.04614245,-0.12380920,0.06384667,0.00007807,-0.00014827,-0.0
0012977,0.00003011,-0.00008178,-0.00006179,0.00050831,-0.00021309,-0.0
0014533,0.00027009,-0.00005825,0.00004366,0.00016666,-0.00014734,-0.00
032136,0.00003999,-0.00018888,-0.00028045,-0.00003936,-0.00005280,-0.0
0012808,0.00003805,-0.00180480,-0.00082633,-0.00006669,0.00003085,0.00
010151,0.00030575,0.00000572,-0.00023810,0.00631211,-0.01292034,-0.016
00337,0.00903377,0.00626671,0.00244737,0.02588317,0.10475990,-0.000216
81,-0.00012573,-0.00008950,-0.00024700,-0.00004481,0.00037034,0.001234
64,0.00073527,0.00022946,0.00154291,0.00068827,-0.00054686,0.00238262,
0.00067329,0.00233852,-0.00002886,0.00099843,-0.00019047,-0.00068264,-
0.00147796,-0.00011180,0.00340178,0.00006768,0.00684576,0.01140198,-0.
00425089,-0.05638418,-0.00371409,-0.00149364,0.00148336,0.00030308,0.0
0050752,0.00053116,-0.00125476,-0.00051875,-0.00232392,0.00495831,0.00

103466,0.00578115,0.00024371,0.00202123,-0.01122762,0.03511683,0.05817
713,-0.09742577,-0.00016499,0.00010970,0.00015637,-0.00017557,0.000081
50,0.00018925,-0.00086289,0.00014774,0.00028384,-0.00024444,-0.0000020
9,0.00000446,-0.00015529,0.00010187,0.00051712,-0.00003840,0.00015983,
0.00017482,-0.00020509,0.00006734,0.00034206,0.00019546,-0.00053596,0.
00027754,0.00002312,-0.00013193,-0.00002579,-0.00028977,0.00007529,0.0
0019855,-0.02630477,-0.02292301,-0.01781100,-0.00031899,0.00100908,-0.
00213476,-0.02626181,-0.03154791,0.14601928,-0.00014525,0.00000826,0.0
0003207,0.00001075,-0.00002407,-0.00005503,-0.00018181,0.00026778,-0.0
0002908,-0.00008622,0.00001164,-0.00002637,0.00000486,-0.00017955,0.00
035793,0.00023306,0.00007767,0.00012514,0.00030512,-0.00004101,0.00004
117,-0.00028476,-0.00002862,-0.00030868,0.00312666,0.00146853,0.006551
75,-0.00125131,-0.00049328,-0.00033193,-0.00005984,0.00007041,-0.00018
477,0.00001329,0.00004562,-0.00029954,-0.00406543,-0.00139530,-0.00166
737,-0.00158485,0.00132011,0.01355343,0.00159000,0.00054648,-0.0069013
5,-0.00001059,0.00001659,-0.00002317,0.00001197,-0.00000168,-0.0000269
1,-0.00012993,0.00004992,0.00004000,-0.00002856,0.00001844,-0.00000143
,0.00007326,-0.00008695,-0.00013350,0.00001915,0.00004075,-0.00023275,
0.00010808,0.00012188,-0.00006078,-0.00036581,0.00049427,0.00065535,0.
00001850,0.00002430,-0.00000880,0.00001187,-0.00001057,-0.00001154,-0.
26377528,-0.06709588,-0.17498647,0.01991170,0.00545670,0.01740647,-0.0
1066890,-0.00762239,0.00036173,0.25720027,0.00006873,0.00004204,0.0000
3471,0.00001043,-0.00000568,0.00000356,-0.00021180,-0.00023278,0.00001
385,-0.00007606,-0.00007004,-0.00007877,-0.00006760,0.00040010,0.00004
187,-0.00004500,-0.00018229,-0.00015879,-0.00002640,0.00013774,0.00006
337,0.00023334,-0.00023370,-0.00006451,-0.00166074,0.00214950,0.003345
50,0.00021244,0.00039332,-0.00021466,0.00000130,-0.00008960,-0.0000139
1,0.00000132,-0.00019593,-0.00007418,-0.00154521,0.00064607,0.00101576
,0.00251736,-0.01049381,0.00125197,0.00324288,-0.00103152,-0.00186396,
0.00000496,-0.00003199,-0.00002010,0.00000301,-0.00001252,-0.00000807,
0.00009071,-0.00001553,-0.00001115,0.00002968,-0.00002628,0.00002161,0
.00001752,-0.00000444,-0.00008389,0.00000443,-0.00002291,0.00003329,-0
.00005861,-0.00008798,0.00007424,0.00052398,-0.00016468,-0.00033069,-0
.00001941,-0.00001149,0.00002617,0.00002415,-0.00000004,-0.00002936,-0
.06517609,-0.04331439,-0.04188943,0.00603168,0.00283023,0.00527193,-0.
01107093,0.00120041,-0.00360316,0.06693996,0.04842820,-0.00031600,0.00
004278,0.00013177,-0.00011812,-0.00004127,-0.00000805,-0.00010462,0.00
002439,0.00005176,0.00013979,-0.00006237,-0.00000725,0.00044401,0.0006
7090,0.00138291,0.00017394,-0.00006247,-0.00023763,0.00041257,0.000021
70,0.00011797,-0.00067189,-0.00042850,-0.00043611,0.01048695,0.0060650
8,0.00799043,-0.00191070,-0.00033043,-0.00058949,-0.00008855,0.0000191
2,-0.00035296,-0.00051024,-0.00038952,-0.00124016,-0.00571390,0.000574
03,-0.00878204,0.00908262,-0.00108209,0.01432276,0.00156025,0.00126045
,-0.01748912,-0.00010236,0.00002090,-0.00000983,-0.00009056,0.00001528
,0.00003003,-0.00039390,0.00004631,0.00010524,-0.00014354,0.00001192,0
.00001472,0.00015492,-0.00017350,-0.00017483,0.00001596,0.00010297,-0.
00055020,0.00012500,0.00015859,0.00005686,0.00059594,-0.00063007,0.000
47453,-0.00000492,-0.00004506,0.00002271,-0.00000131,0.00003417,0.0000
1400,-0.12453461,-0.02717892,-0.18754936,-0.02831228,-0.00724600,-0.01
700693,-0.00633886,-0.00864521,0.02252863,0.14616443,0.03724683,0.1871
8963\\0.00000017,0.00000009,-0.00000006,0.00000009,-0.00000010,-0.0000
0001,-0.00000062,-0.00000043,0.00000066,0.00000064,0.00000020,0.000000
20,-0.00000020,-0.00000048,-0.00000045,-0.00000003,0.00000035,0.000000
35,-0.00000017,-0.00000032,0.00000034,0.00000085,0.,0.00000115,-0.0000

1209,-0.00000418,-0.00000739,0.00000253,0.00000176,0.00000111,0.000000
07,-0.00000013,0.00000006,0.00000079,-0.00000017,0.00000013,0.00000216
,0.00000631,0.00000207,0.00000791,-0.00000373,0.00001127,-0.00000179,-
0.00000119,0.00000911,0.,0.,-0.00000002,-0.00000009,-0.00000005,0.0000
0001,0.00000056,0.00000004,-0.00000016,0.00000009,0.,0.00000003,0.,0.0
0000007,-0.00000006,0.00000160,-0.00000061,-0.00000086,-0.00000021,-0.
00000013,-0.00000005,-0.00000036,-0.00000045,-0.00000030,0.,0.00000001
,0.00000005,0.00000005,0.,0.,-0.00000994,-0.00000219,-0.00001442,-0.00
000335,-0.00000147,0.00000094,0.00000783,0.00000609,-0.00000942,0.0000
0352,0.00000072,0.00000571\\\@

IF GOD HAD MEANT MAN TO SEE THE SUN RISE, HE
WOULD HAVE SCHEDULED IT FOR A LATER HOUR.
Job cpu time: 0 days 2 hours 44 minutes 40.7 seconds.
File lengths (MBytes): RWF= 216 Int=   0 D2E=   0 Chk=   8 Scr=
1
Normal termination of Gaussian 98.

```
%nproc=2
# opt=(gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity optcyc=100

H2O added

0  1
 C                  0.000000    0.000000    0.000000
 C                  0.000000    0.000000    1.556380
 C                  1.489384    0.000000    2.014803
 C                  1.418734   -0.528801   -0.302284
 C                  2.336350    0.128287    0.740227
 C                 -0.110252   -1.530481    1.905828
 C                 -0.168488   -2.212207    0.506975
 C                  1.309182   -2.067739    0.039740
 C                  2.111469   -2.330363    1.312158
 C                  1.393415   -1.523964    2.380585
 C                 -0.921081   -1.179140   -0.351294
 O                  2.452226    1.536560    0.407462
 C                  3.555654   -2.481829    1.284405
 N                  4.551336   -3.059438    1.360585
 O                  3.558595   -0.485673    0.852884
 H                 -0.215326    0.954528   -0.452623
 H                 -0.696282    0.679154    2.022865
 H                  1.808370    0.654398    2.807429
 H                  1.769523   -0.361544   -1.308344
 H                 -0.870504   -1.829219    2.614193
 H                 -0.550416   -3.222800    0.487212
 H                  1.597019   -2.715082   -0.774306
 H                  1.642370   -1.811327    3.389568
 H                 -0.912783   -1.424181   -1.407760
 H                 -1.945923   -1.035727   -0.024212
 H                  3.395939    1.744789    0.349881
 O                  1.750798   -3.897882    1.692806
 H                  2.525018   -4.484793    1.703902
 O                 -0.280424   -4.736121    3.046761
 H                 -0.423914   -5.642525    3.346857
 H                  0.939756   -4.204555    2.202603
 H                 -0.987920   -4.145745    3.338683

 1  2 1.0  4 1.0  11 1.0  16 1.0
 2  3 1.0  6 1.0  17 1.0
 3  5 1.0  10 1.0  18 1.0
 4  5 1.0  8 1.0  19 1.0
 5  12 1.0  15 1.0
 6  7 1.0  10 1.0  20 1.0
 7  8 1.0  11 1.0  21 1.0
 8  9 1.0  22 1.0
 9  10 1.0  13 1.0
 10  23 1.0
 11  24 1.0  25 1.0
 12  26 1.0
 13  14 3.0
 14
 15
```

```
16
17
18
19
20
21
22
23
24
25
26
27  28 1.0  31 1.0
28
29  30 1.0  32 1.0
30
31
32
```

```
 Entering Gaussian System, Link 0=g98
 Input=m1s8H2Onew3F.gjf
 Output=m1s8H2Onew3F.out
 Initial command:
 /usr/g98/l1.exe /usr/scratch/Singh/Gau-11025.inp -
scrdir=/usr/scratch/Singh/
 Default is to use a total of   2 processors:
                                2 via shared-memory
                                1 via Linda
 Entering Link 1 = /usr/g98/l1.exe PID=     11024.
```

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

Cite this work as:
Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

```
**********************************************
Gaussian 98:  DEC-AXP-OSF/1-G98RevA.7 11-Apr-1999
                  25-Feb-2003
**********************************************
%nproc=2
Will use up to    2 processors via shared memory.
%chk=m1s8H2Onew3F
%nosave
-------------------
#N RHF/3-21+G* FREQ
-------------------
1/10=4,30=1,38=1/1,3;
2/17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
```

```
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;
-------------------------------------
H2O added-freq calc of m1s8H2Onew3.out
-------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                    -0.27803  -0.40215  -2.28757
C                    -0.51518   1.03644  -1.74303
C                     0.69836   1.38701  -0.83043
C                     0.73459  -0.95138  -1.25958
C                     1.68448   0.21583  -0.94983
C                    -1.4042    0.78567  -0.46891
C                    -1.57121  -0.76245  -0.44987
C                    -0.1568   -1.21225   0.01897
C                     0.21354  -0.17492   1.07656
C                    -0.17769   1.15309   0.45148
C                    -1.58892  -1.12784  -1.94534
O                     2.51666   0.4355   -2.11885
C                     1.38889  -0.32884   1.91574
N                     1.95568  -0.52593   2.90099
O                     2.42335   0.02757   0.19129
H                     0.0674   -0.44871  -3.3078
H                    -0.85752   1.75885  -2.46733
H                     1.16919   2.35163  -0.90832
H                     1.27111  -1.83523  -1.56638
H                    -2.31183   1.36472  -0.36933
H                    -2.38645  -1.1444    0.14768
H                    -0.09806  -2.22381   0.39028
H                    -0.256     1.96474   1.15696
H                    -1.5394   -2.1975   -2.11744
H                    -2.45244  -0.7209   -2.46165
H                     3.43941   0.41472  -1.82667
O                    -0.91396  -0.39857   2.26435
H                    -0.53258  -0.64846   3.12232
O                    -3.27627   0.63548   2.37356
H                    -3.88435   0.5769    3.12124
H                    -1.83894  -0.00357   2.27506
H                    -3.64464   1.16349   1.65257

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 106 maximum allowed number of steps= 192.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

---------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
---------------------------------------------------------------------
```

1	1	C	0	-0.278033	-0.402152	-2.287571
2	2	C	0	-0.515179	1.036444	-1.743033
3	3	C	0	0.698361	1.387007	-0.830430
4	4	C	0	0.734588	-0.951375	-1.259581
5	5	C	0	1.684483	0.215829	-0.949831
6	6	C	0	-1.404204	0.785670	-0.468910
7	7	C	0	-1.571209	-0.762451	-0.449868
8	8	C	0	-0.156797	-1.212247	0.018970
9	9	C	0	0.213535	-0.174923	1.076559
10	10	C	0	-0.177693	1.153095	0.451479
11	11	C	0	-1.588917	-1.127843	-1.945336
12	12	O	0	2.516663	0.435500	-2.118854
13	13	C	0	1.388893	-0.328844	1.915739
14	14	N	0	1.955684	-0.525933	2.900992
15	15	O	0	2.423349	0.027570	0.191290
16	16	H	0	0.067395	-0.448713	-3.307801
17	17	H	0	-0.857516	1.758850	-2.467327
18	18	H	0	1.169195	2.351628	-0.908323
19	19	H	0	1.271108	-1.835235	-1.566376
20	20	H	0	-2.311834	1.364722	-0.369333
21	21	H	0	-2.386445	-1.144403	0.147677
22	22	H	0	-0.098059	-2.223807	0.390277
23	23	H	0	-0.255997	1.964741	1.156959
24	24	H	0	-1.539397	-2.197498	-2.117441
25	25	H	0	-2.452437	-0.720895	-2.461646
26	26	H	0	3.439412	0.414717	-1.826671
27	27	O	0	-0.913956	-0.398574	2.264347
28	28	H	0	-0.532582	-0.648462	3.122318
29	29	O	0	-3.276266	0.635481	2.373562
30	30	H	0	-3.884349	0.576897	3.121237
31	31	H	0	-1.838936	-0.003571	2.275060
32	32	H	0	-3.644638	1.163489	1.652574

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.278033	-0.402152	-2.287571
2	6	0	-0.515179	1.036444	-1.743033
3	6	0	0.698361	1.387007	-0.830430
4	6	0	0.734588	-0.951375	-1.259581
5	6	0	1.684483	0.215829	-0.949831
6	6	0	-1.404204	0.785670	-0.468910
7	6	0	-1.571209	-0.762451	-0.449868
8	6	0	-0.156797	-1.212247	0.018970
9	6	0	0.213535	-0.174923	1.076559
10	6	0	-0.177693	1.153095	0.451479
11	6	0	-1.588917	-1.127843	-1.945336
12	8	0	2.516663	0.435500	-2.118854
13	6	0	1.388893	-0.328844	1.915739
14	7	0	1.955684	-0.525933	2.900992
15	8	0	2.423349	0.027570	0.191290
16	1	0	0.067395	-0.448713	-3.307801

17	1	0	-0.857516	1.758850	-2.467327
18	1	0	1.169195	2.351628	-0.908323
19	1	0	1.271108	-1.835235	-1.566376
20	1	0	-2.311834	1.364722	-0.369333
21	1	0	-2.386445	-1.144403	0.147677
22	1	0	-0.098059	-2.223807	0.390277
23	1	0	-0.255997	1.964741	1.156959
24	1	0	-1.539397	-2.197498	-2.117441
25	1	0	-2.452437	-0.720895	-2.461646
26	1	0	3.439412	0.414717	-1.826671
27	8	0	-0.913956	-0.398574	2.264347
28	1	0	-0.532582	-0.648462	3.122318
29	8	0	-3.276266	0.635481	2.373562
30	1	0	-3.884349	0.576897	3.121237
31	1	0	-1.838936	-0.003571	2.275060
32	1	0	-3.644638	1.163489	1.652574

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.556380	0.000000			
3	C	2.505533	1.558338	0.000000		
4	C	1.543959	2.397304	2.377712	0.000000	
5	C	2.454163	2.478123	1.535692	1.536428	0.000000
6	C	2.446775	1.573735	2.216547	2.866517	3.177419
7	C	2.275801	2.454282	3.148959	2.451128	3.436062
8	C	2.447669	2.879185	2.865117	1.580289	2.523547
9	C	3.407439	3.154130	2.512228	2.516331	2.534291
10	C	3.151390	2.223373	1.570183	2.861604	2.511939
11	C	1.536935	2.424454	3.577587	2.429007	3.675817
12	O	2.922405	3.113590	2.423143	2.416105	1.451686
13	C	4.522370	4.344665	3.310955	3.301260	2.931814
14	N	5.650310	5.487545	4.377638	4.356885	3.930979
15	O	3.691460	3.659833	2.422306	2.432134	1.372414
16	H	1.078127	2.234633	3.147277	2.212017	2.935407
17	H	2.244558	1.078734	2.288767	3.367308	3.338483
18	H	3.402954	2.294246	1.076218	3.349939	2.197472
19	H	2.230176	3.386528	3.354474	1.078511	2.181254
20	H	3.307239	2.285342	3.045387	3.929063	4.198510
21	H	3.305567	3.439842	4.108620	3.429064	4.430261
22	H	3.243715	3.918448	3.893891	2.243750	3.305324
23	H	4.179408	3.055956	2.279099	3.914672	3.355998
24	H	2.200739	3.412856	4.417311	2.731255	4.192954
25	H	2.204525	2.712492	4.126941	3.413973	4.503015
26	H	3.833941	4.004039	3.074281	3.082835	1.971847
27	O	4.596125	4.275207	3.919887	3.929549	4.178554
28	H	5.421472	5.148869	4.613304	4.571489	4.716437
29	O	5.638461	4.973000	5.160234	5.639574	5.985823
30	H	6.574135	5.934948	6.105177	6.546889	6.907666
31	H	4.838686	4.356493	4.244485	4.473818	4.781479
32	H	5.413871	4.619502	5.007685	5.668414	6.005839

		6	7	8	9	10
6	C	0.000000				
7	C	1.557219	0.000000			

8	C	2.405353	1.556498	0.000000		
9	C	2.434809	2.420843	1.526984	0.000000	
10	C	1.576847	2.534488	2.404650	1.519018	0.000000
11	C	2.423940	1.539561	2.432404	3.645372	3.597076
12	O	4.268270	4.575074	3.799046	3.985935	3.792243
13	C	3.837979	3.813963	2.601402	1.452371	2.606606
14	N	4.936131	4.870644	3.638633	2.546929	3.656576
15	O	3.957365	4.122100	2.867751	2.389138	2.846037
16	H	3.427624	3.309265	3.420622	4.395331	4.093659
17	H	2.289021	3.307031	3.937016	4.176812	3.057536
18	H	3.044288	4.173426	3.913992	3.352089	2.258240
19	H	3.902675	3.236699	2.222690	3.295482	3.885985
20	H	1.081207	2.253858	3.381676	3.292203	2.296318
21	H	2.251701	1.080536	2.234390	2.926194	3.201465
22	H	3.391337	2.238655	1.079154	2.183117	3.378395
23	H	2.313447	3.427718	3.376109	2.192051	1.078241
24	H	3.411044	2.200266	2.728838	4.167159	4.436222
25	H	2.709156	2.196711	3.415384	4.463674	4.143983
26	H	5.043980	5.328005	4.357307	4.379806	4.338043
27	O	3.018853	2.816265	2.505408	1.652905	2.497249
28	H	3.964010	3.721861	3.176450	2.228466	3.241132
29	O	3.406878	3.582344	4.323111	3.810208	3.682863
30	H	4.368508	4.460635	5.169114	4.640969	4.604227
31	H	2.888125	2.841269	3.062749	2.382940	2.724528
32	H	3.108534	3.525424	4.525242	4.124153	3.669120

		11	12	13	14	15
11	C	0.000000				
12	O	4.396582	0.000000			
13	C	4.941017	4.258407	0.000000		
14	N	6.034351	5.141780	1.153612	0.000000	
15	O	4.690248	2.347739	2.042267	2.804917	0.000000
16	H	2.249644	2.862576	5.389443	6.490047	4.245115
17	H	3.023313	3.641122	5.349401	6.477127	4.563951
18	H	4.559528	2.636779	3.899811	4.838368	2.860646
19	H	2.970481	2.648184	3.795815	4.705347	2.808397
20	H	3.036326	5.219067	4.667451	5.699238	4.952195
21	H	2.239872	5.627941	4.247865	5.178545	4.950711
22	H	2.979745	4.494933	2.851131	3.661192	3.386118
23	H	4.578754	4.556004	2.922660	3.759872	3.444422
24	H	1.084543	4.835732	5.322902	6.339905	5.097502
25	H	1.085288	5.113385	5.837039	6.944597	5.601032
26	H	5.260957	0.968126	4.331644	5.043517	2.292255
27	O	4.325371	5.628257	2.330129	2.942171	3.951806
28	H	5.198727	6.159769	2.291300	2.501093	4.217283
29	O	4.960780	7.333473	4.785732	5.385199	6.133309
30	H	5.817672	8.273542	5.484585	5.947329	6.976633
31	H	4.374727	6.202460	3.264015	3.881210	4.744485
32	H	4.735097	7.260528	5.256686	5.981329	6.343984

		16	17	18	19	20
16	H	0.000000				
17	H	2.536768	0.000000			
18	H	3.848814	2.624774	0.000000		
19	H	2.530599	4.273196	4.239486	0.000000	
20	H	4.193313	2.583013	3.658149	4.950769	0.000000

21	H	4.294839	4.195801	5.097053	4.097917	2.562923
22	H	4.105376	4.960265	4.922083	2.419524	4.284314
23	H	5.085610	3.679628	2.538945	4.918173	2.629840
24	H	2.656499	4.029897	5.430744	2.886840	4.042518
25	H	2.672006	2.948379	4.996942	3.988490	2.957590
26	H	3.782824	4.547606	3.122318	3.135535	6.008592
27	O	5.658127	5.200616	4.687106	4.638204	3.464036
28	H	6.461138	6.094659	5.304965	5.161936	4.405709
29	O	6.680826	5.526890	5.786022	6.504319	2.997565
30	H	7.615818	6.464579	6.702636	7.373658	3.908651
31	H	5.916129	5.153596	4.972901	5.271053	3.014743
32	H	6.401852	5.009600	5.580578	6.596859	2.430014

		21	22	23	24	25
21	H	0.000000				
22	H	2.541786	0.000000			
23	H	3.901825	4.261066	0.000000		
24	H	2.637662	2.892542	5.449132	0.000000	
25	H	2.644292	3.991905	5.013112	1.769880	0.000000
26	H	6.345827	4.938661	4.996065	5.629987	6.033796
27	O	2.684171	2.740311	2.691556	4.777800	4.980545
28	H	3.539951	3.183484	3.281458	5.555921	5.905230
29	O	2.985688	4.712743	3.516970	5.586734	5.088977
30	H	3.748153	5.444086	4.353095	6.374936	5.907895
31	H	2.475282	3.393009	2.762263	4.919055	4.829837
32	H	3.028883	5.064128	3.517176	5.471863	4.679642

		26	27	28	29	30
26	H	0.000000				
27	O	6.029070	0.000000			
28	H	6.434250	0.971599	0.000000		
29	O	7.924079	2.581028	3.120408	0.000000	
30	H	8.839998	3.241765	3.568732	0.965513	0.000000
31	H	6.697770	1.005848	1.685316	1.576073	2.288378
32	H	7.927772	3.204829	3.889500	0.966599	1.599538

		31	32
31	H	0.000000	
32	H	2.238320	0.000000

Interatomic angles:

C1-C2-C3=107.108	C2-C1-C4=101.2906	C1-C4-C3= 76.1335
C2-C3-C4= 71.6348	C2-C1-C5= 72.445	C1-C5-C3= 73.795
C2-C3-C5=106.437	C1-C4-C5=105.6331	C2-C4-C5= 74.5165
C3-C5-C4=101.4225	C1-C2-C6=102.8295	C1-C6-C3= 64.778
C3-C2-C6= 90.0937	C4-C1-C6= 88.8351	C4-C2-C6= 89.9484
C4-C3-C6= 77.1196	C5-C1-C6= 80.8313	C5-C2-C6=100.925
C5-C3-C6=114.5128	C5-C4-C6= 86.8662	C2-C1-C7= 77.1284
C3-C1-C7= 82.234	C3-C2-C7=101.0343	C4-C1-C7= 77.2157
C2-C4-C7= 60.8102	C3-C4-C7= 81.3871	C5-C1-C7= 93.1013
C5-C2-C7= 88.3132	C5-C4-C7=117.1576	C1-C7-C6= 76.8085
C2-C6-C7=103.2325	C3-C6-C7=111.9276	C4-C7-C6= 88.3783
C2-C1-C8= 89.0697	C3-C1-C8= 70.6704	C2-C3-C8= 74.7577
C1-C4-C8=103.1476	C2-C4-C8= 90.3427	C3-C4-C8= 90.4427
C5-C1-C8= 61.9703	C2-C5-C8= 70.2829	C3-C5-C8= 86.1699
C5-C4-C8=108.1213	C1-C6-C8= 60.5829	C2-C6-C8= 90.2069
C3-C6-C8= 76.4964	C4-C8-C6= 89.5017	C5-C8-C6= 80.2399
C1-C7-C8= 76.8572	C2-C7-C8= 88.8264	C3-C8-C7= 85.3978

C4-C8-C7=102.7777 C5-C8-C7=112.5732 C6-C7-C8=101.1582
C1-C3-C9= 85.5428 C2-C3-C9= 98.8813 C1-C4-C9=111.8738
C2-C4-C9= 79.8291 C4-C3-C9= 61.8683 C1-C5-C9= 86.1514
C2-C5-C9= 77.9827 C5-C3-C9= 73.0694 C5-C4-C9= 72.9288
C1-C6-C9= 88.5362 C2-C6-C9=101.6201 C3-C6-C9= 65.1846
C4-C9-C6= 70.7331 C5-C9-C6= 79.4719 C1-C7-C9= 92.9699
C2-C7-C9= 80.6261 C3-C9-C7= 79.3121 C4-C7-C9= 62.1907
C5-C9-C7= 87.774 C6-C7-C9= 71.782 C1-C8-C9=116.0939
C2-C8-C9= 85.6113 C3-C9-C8= 86.7567 C4-C8-C9=108.1444
C5-C8-C9= 72.8127 C6-C8-C9= 72.6621 C7-C8-C9=103.4557
C1-C2-C10=111.7588 C1-C3-C10= 98.6847 C2-C3-C10= 90.5795
C1-C4-C10= 85.8379 C4-C2-C10= 76.4276 C4-C3-C10= 90.5355
C1-C5-C10= 78.7682 C5-C2-C10= 64.3237 C5-C3-C10=107.9467
C4-C5-C10= 86.4223 C1-C6-C10=100.8922 C2-C6-C10= 89.7726
C3-C10-C6= 89.5506 C4-C10-C6= 74.1929 C5-C10-C6= 99.443
C1-C7-C10= 81.6681 C7-C2-C10= 65.3991 C3-C10-C7= 97.4125
C4-C7-C10= 70.0325 C5-C10-C7= 85.8253 C7-C6-C10=107.9346
C1-C8-C10= 80.9966 C2-C10-C8= 76.8314 C3-C10-C8= 89.7047
C4-C8-C10= 89.3148 C5-C10-C8= 61.7184 C6-C10-C8= 70.8872
C7-C8-C10= 76.233 C2-C10-C9=113.5398 C3-C10-C9=108.814
C4-C9-C10= 86.6211 C5-C10-C9= 73.2869 C6-C10-C9=103.6982
C7-C9-C10= 76.2806 C8-C9-C10=104.267 C2-C1-C11=103.2127
C3-C1-C11=122.6868 C3-C2-C11=126.4821 C4-C1-C11=104.0741
C4-C2-C11= 60.495 C3-C4-C11= 96.1902 C5-C1-C11=132.8103
C5-C2-C11= 97.1353 C5-C4-C11=134.7088 C1-C11-C6= 72.4159
C2-C6-C11= 71.077 C3-C6-C11=100.784 C4-C11-C6= 72.4098
C1-C11-C7= 95.4182 C2-C11-C7= 72.6617 C4-C11-C7= 72.3935
C6-C7-C11=103.0208 C1-C11-C8= 72.1837 C2-C11-C8= 72.7128
C3-C8-C11= 84.5395 C8-C4-C11= 71.1468 C5-C8-C11= 95.7349
C8-C6-C11= 60.4857 C8-C7-C11=103.5594 C9-C4-C11= 94.9591
C9-C6-C11= 97.2273 C9-C7-C11=132.731 C9-C8-C11=132.7291
C10-C2-C11=101.3277 C10-C4-C11= 85.2553 C10-C6-C11=126.78
C10-C7-C11=122.083 C10-C8-C11= 96.0849 C2-C1-O12= 81.9853
C1-C3-O12= 72.71 C2-C3-O12=100.6399 C1-C4-O12= 92.4512
C2-C4-O12= 80.6091 C3-C4-O12= 60.7192 C1-C5-O12= 93.2998
C2-C5-O12=101.5936 C3-C5-O12=108.3797 C4-C5-O12=107.8797
C6-C1-O12=104.9569 C6-C3-O12=133.7882 C6-C4-O12=107.493
C7-C1-O12=122.8306 C7-C4-O12=140.0934 C8-C1-O12= 89.6044
C8-C3-O12= 91.4536 C8-C4-O12=142.9908 C8-C5-O12=144.3952
C9-C3-O12=107.7157 C9-C4-O12=107.8055 C9-C5-O12=179.4503
C10-C3-O12=142.5859 C10-C4-O12= 91.4701 C10-C5-O12=144.8595
C11-C1-O12=159.74 C11-C4-O12=130.304 C1-C5-C13=113.9142
C2-C5-C13=106.5515 C3-C5-C13= 90.0543 C4-C5-C13= 89.6322
C1-C8-C13=127.1664 C2-C8-C13=104.7707 C3-C8-C13= 74.3798
C4-C8-C13=101.461 C5-C8-C13= 69.77 C6-C8-C13=100.0183
C7-C8-C13=131.4088 C3-C9-C13=110.384 C4-C9-C13=109.6424
C5-C9-C13= 90.4944 C6-C9-C13=161.1308 C7-C9-C13=159.2651
C8-C9-C13=121.6317 C2-C10-C13=128.0142 C3-C10-C13=102.0047
C4-C10-C13= 74.1084 C5-C10-C13= 69.861 C6-C10-C13=131.5207
C7-C10-C13= 95.7697 C10-C8-C13= 62.6118 C10-C9-C13=122.6053
C11-C8-C13=157.9513 O12-C5-C13=150.8091 C3-C9-N14=119.8301
C4-C9-N14=118.742 C5-C9-N14=101.3615 C6-C9-N14=164.4785
C7-C9-N14=157.2956 C8-C9-N14=124.6385 C10-C9-N14=126.2585
C5-C13-N14=144.7823 C8-C13-N14=148.941 C9-C13-N14=155.3937

C10-C13-N14=150.7135 C1-C3-O15= 97.0111 C2-C3-O15=132.4794
C1-C4-O15=135.1865 C2-C4-O15= 98.5418 C4-C3-O15= 60.8791
C1-C5-O15=148.1249 C2-C5-O15=142.1329 C3-C5-O15=112.6855
C4-C5-O15=113.3449 C6-C3-O15=117.03 C6-C4-O15= 96.2937
C7-C4-O15=115.1568 C1-C8-O15= 87.5987 C2-C8-O15= 79.1117
C8-C3-O15= 65.0621 C8-C4-O15= 88.5941 C8-C5-O15= 89.7699
C6-C8-O15= 96.8733 C7-C8-O15=135.2955 C3-O15-C9= 62.9468
C4-O15-C9= 62.9152 C5-O15-C9= 79.7326 C6-C9-O15=110.2378
C7-C9-O15=117.9588 C8-C9-O15= 91.4476 C2-C10-O15= 91.5896
C10-C3-O15= 88.2439 C4-O15-C10= 65.1107 C10-C5-O15= 89.2235
C6-C10-O15=124.427 C7-C10-O15= 99.8509 C8-C10-O15= 65.5819
C10-C9-O15= 90.6672 C11-C4-O15=149.5252 C11-C8-O15=124.2804
C1-O12-O15= 88.2233 C3-O15-O12= 61.0366 C4-O12-O15= 61.3797
O12-C5-O15=112.4395 C8-O15-O12= 92.9665 C9-O15-O12=114.5883
C10-O15-O12= 93.3002 C3-O15-C13= 95.3587 C4-O15-C13= 94.6896
C5-O15-C13=116.9568 C8-C13-O15= 75.2005 C9-C13-O15= 84.4644
C10-C13-O15= 74.3877 O12-O15-C13=151.8013 C3-O15-N14=113.5464
C4-O15-N14=112.4015 C5-O15-N14=137.7784 C8-O15-N14= 79.789
N14-C9-O15= 69.1716 C10-O15-N14= 80.6389 O12-O15-N14=172.5237
N14-C13-O15=120.1392 C2-C1-H16=114.8234 C3-C1-H16=117.1499
C3-C2-H16=110.8895 C4-C1-H16=113.8636 C2-H16-C4= 65.246
C3-C4-H16= 86.5054 C5-C1-H16=105.693 C5-C2-H16= 76.8585
C3-C5-H16= 83.1865 C5-C4-H16=101.5674 C6-C1-H16=150.6693
C6-C2-H16=127.4661 C6-C4-H16= 83.8376 C7-C1-H16=159.9435
C7-C2-H16= 89.6561 C7-C4-H16= 90.2652 C8-C1-H16=149.4937
C8-C2-H16= 82.9352 C8-C4-H16=128.0632 C8-C5-H16= 77.1923
C9-C4-H16=136.6413 C9-C5-H16=106.717 C10-C2-H16=133.3492
C10-C4-H16=106.8811 C10-C5-H16= 97.1346 C11-C1-H16=117.6195
C2-H16-C11= 65.4557 C4-H16-C11= 65.9635 C5-H16-C11= 89.2804
C6-C11-H16= 94.2711 C7-C11-H16=120.5423 C8-C11-H16= 93.7888
C1-H16-O12= 82.4009 C2-H16-O12= 74.1533 C3-O12-H16= 72.5478
O12-C4-H16= 76.2741 C5-O12-H16= 78.3019 C11-H16-O12=118.1417
C13-C5-H16=133.4353 O15-C4-H16=132.093 O15-C5-H16=158.9769
O15-O12-H16=108.7242 C1-C2-H17=115.6224 C1-H17-C3= 67.0956
C3-C2-H17=119.3202 C4-C1-H17=124.4112 C4-C2-H17=148.8855
C4-C3-H17= 92.3527 C5-C1-H17= 90.4395 C5-C2-H17=135.9195
C5-C3-H17=120.3188 C1-H17-C6= 65.3179 C6-C2-H17=118.1017
C6-C3-H17= 61.0459 C4-C6-H17= 80.7131 C7-C1-H17= 94.0365
C7-C2-H17=135.0787 C7-C6-H17=117.3198 C8-C1-H17=114.0103
C8-C2-H17=166.7637 C8-C3-H17= 99.0048 C8-C6-H17=113.9764
C9-C3-H17=120.8442 C9-C6-H17=124.2777 C10-C2-H17=132.5124
C10-C3-H17=103.2271 C10-C6-H17=102.9884 C11-C1-H17=104.6091
C11-C2-H17=113.6559 C11-C6-H17= 79.7497 O12-C1-H17= 88.5991
O12-C3-H17=101.1644 O15-C3-H17=151.275 H16-C1-H17= 92.7806
H16-C2-H17= 93.305 C3-H17-H16= 81.241 C4-H16-H17= 90.0539
C5-H16-H17= 74.7937 C6-H17-H16= 90.3641 C11-H16-H17= 78.0891
O12-H16-H17= 84.5802 C1-C2-H18=123.0451 C1-C3-H18=140.2134
C2-C3-H18=119.9959 C4-C2-H18= 91.1015 C4-C3-H18=149.5138
C1-C5-H18= 93.8717 C2-H18-C5= 66.9285 C5-C3-H18=113.3909
C4-C5-H18=126.6696 C6-C2-H18=102.2121 C6-C3-H18=132.064
C7-C2-H18=122.9818 C8-C2-H18= 97.6823 C8-C3-H18=164.8337
C8-C5-H18=111.8188 C9-C3-H18=134.1573 C9-C5-H18= 89.9228
C2-C10-H18= 61.5783 C10-C3-H18=115.8936 C4-C10-H18= 80.8001
C5-H18-C10= 68.6164 C6-C10-H18=103.6576 C7-C10-H18=120.9917

C8-C10-H18=114.1153 C9-C10-H18=123.9298 C11-C2-H18=150.1401
C1-O12-H18= 75.2917 C2-H18-O12= 77.9698 O12-C3-H18= 89.1512
C4-O12-H18= 82.9308 O12-C5-H18= 90.1466 C10-H18-O12=101.2771
C13-C5-H18= 97.9589 C13-C10-H18=106.3521 C2-H18-O15= 89.7709
O15-C3-H18=102.8266 C4-O15-H18= 78.0699 O15-C5-H18=104.1145
C8-O15-H18= 86.1979 C9-O15-H18= 78.8009 O15-C10-H18= 67.0301
O15-O12-H18= 69.7701 C13-O15-H18=104.1398 N14-O15-H18=117.2946
H16-C2-H18=116.382 H16-C5-H18= 96.0865 H16-O12-H18= 88.7338
C1-H17-H18= 88.3106 H17-C2-H18= 95.358 H17-C3-H18= 95.7403
C5-H18-H17= 87.1536 C6-H17-H18= 76.2242 C10-H18-H17= 77.1298
O12-H18-H17= 87.5808 O15-H18-H17=112.5418 H16-H17-H18= 96.4187
C2-C1-H19=125.92 C3-C1-H19= 90.0057 C1-C4-H19=115.3654
C2-C4-H19=151.8249 C3-C4-H19=149.8696 C1-H19-C5= 67.5927
C2-C5-H19= 93.0202 C3-C5-H19=128.1268 C5-C4-H19=111.8618
C6-C1-H19=113.0356 C6-C4-H19=161.1284 C7-C1-H19= 91.8249
C7-C4-H19=128.6898 C1-H19-C8= 66.6904 C2-C8-H19= 82.0895
C3-C8-H19= 81.4356 C8-C4-H19=112.053 C5-H19-C8= 69.9149
C6-C8-H19=114.9165 C7-C8-H19=116.7394 C9-C4-H19=128.3144
C9-C5-H19= 88.3399 C9-C8-H19=121.9111 C10-C4-H19=158.6493
C10-C5-H19=111.5951 C10-C8-H19=114.1781 C11-C1-H19=102.5355
C2-C11-H19= 77.0283 C11-C4-H19=109.6339 C5-H19-C11= 89.6905
C6-C11-H19= 92.1157 C7-C11-H19= 85.499 C11-C8-H19= 79.162
C1-H19-O12= 73.0372 C3-O12-H19= 82.6943 O12-C4-H19= 90.1333
O12-C5-H19= 91.3356 C8-H19-O12=102.159 C11-H19-O12=102.8289
C13-C5-H19= 94.7306 C13-C8-H19=103.5049 C1-H19-O15= 93.5063
C3-O15-H19= 79.4026 O15-C4-H19= 98.8668 O15-C5-H19=102.0088
C8-H19-O15= 68.3623 C9-O15-H19= 78.2407 C10-O15-H19= 86.8223
C11-H19-O15=108.4764 O15-O12-H19= 68.1012 C13-O15-H19=101.8229
N14-O15-H19=113.9111 H16-C1-H19= 93.1934 C2-H16-H19= 90.36
H16-C4-H19= 94.1793 C5-H19-H16= 76.6707 C8-H19-H16= 91.8154
C11-H16-H19= 76.5875 O12-H19-H16= 67.0673 O15-H19-H16=105.2136
H17-C1-H19=145.4769 H17-H16-H19=114.9756 H18-C5-H19=151.0241
H18-O12-H19=106.6772 H18-O15-H19= 96.8014 C1-C2-H20=117.5724
C3-C2-H20=103.1728 C4-C2-H20=114.0626 C5-C2-H20=123.5727
C1-C6-H20=135.629 C2-C6-H20=117.6097 C3-C6-H20=131.7605
C4-C6-H20=167.4975 C1-C7-H20= 93.7933 C2-H20-C7= 65.4564
C4-C7-H20=113.1829 C7-C6-H20=116.1854 C8-C2-H20= 80.9202
C8-C6-H20=149.4859 C8-C7-H20=124.0959 C9-C6-H20=135.2829
C9-C7-H20= 89.4657 C10-C2-H20= 61.217 C3-C10-H20=102.2968
C4-C10-H20= 98.646 C5-C10-H20=121.5979 C10-C6-H20=118.3205
C7-H20-C10= 67.6909 C8-C10-H20= 91.9735 C9-C10-H20=117.8414
C11-C2-H20= 80.2245 C11-C6-H20=114.5137 C11-C7-H20=104.7691
C13-C10-H20=144.2674 O15-C10-H20=148.5549 H16-C2-H20=136.1643
C1-H17-H20= 86.1817 H17-C2-H20= 93.3196 C3-H17-H20= 77.1181
H17-C6-H20= 93.0496 C7-H20-H17= 85.9844 C10-H20-H17= 77.3569
H16-H17-H20=109.9746 H18-C2-H20=106.0301 H18-C10-H20=106.8675
H18-H17-H20= 89.2422 C1-C6-H21= 89.3235 C2-C6-H21=127.2083
C3-C6-H21=133.7089 C4-C6-H21= 83.1995 C1-C7-H21=158.6272
C2-C7-H21=151.0576 C4-C7-H21=149.903 C6-C7-H21=116.0462
C1-C8-H21= 89.7024 C2-C8-H21= 83.5306 C3-C8-H21=106.7006
C4-C8-H21=127.1899 C5-C8-H21=137.1404 C6-H21-C8= 64.8466
C8-C7-H21=114.6377 C3-C9-H21= 97.8452 C4-C9-H21= 77.7046
C5-C9-H21=108.2387 C9-C6-H21= 77.1647 C9-C7-H21=107.0572
C9-C8-H21=100.4564 C10-C6-H21=112.2842 C10-C7-H21=119.0333

C10-C8-H21= 87.1972 C10-C9-H21= 85.9966 C1-C11-H21=121.0145
C2-C11-H21= 94.9519 C4-C11-H21= 94.4347 C6-H21-C11= 65.3209
C11-C7-H21=116.3976 C8-H21-C11= 65.8639 C9-H21-C11= 88.7284
C13-C8-H21=122.7247 C13-C9-H21=150.1526 N14-C9-H21=142.1381
O15-C8-H21=151.789 O15-C9-H21=137.0784 H16-C11-H21=146.1305
H17-C6-H21=135.046 H19-C8-H21=133.682 H19-C11-H21=102.8176
C2-H20-H21= 90.2013 H20-C6-H21= 93.8792 H20-C7-H21= 93.7804
C8-H21-H20= 89.373 C9-H21-H20= 73.3702 C10-H20-H21= 82.2254
C11-H21-H20= 78.1059 H17-H20-H21=109.2457 C1-C4-H22=116.6107
C2-C4-H22=115.1545 C3-C4-H22=114.7936 C5-C4-H22=120.7976
C6-C4-H22= 82.1803 C1-C7-H22= 91.8607 C2-C7-H22=113.145
C4-H22-C7= 66.2999 C6-C7-H22=125.6608 C1-C8-H22=129.5808
C2-C8-H22=161.7022 C3-C8-H22=159.4134 C4-C8-H22=113.7291
C5-C8-H22=128.5232 C6-C8-H22=151.2352 C7-C8-H22=115.0861
C3-C9-H22=111.8651 C4-H22-C9= 69.265 C5-C9-H22= 88.6357
C6-C9-H22= 94.3529 C7-H22-C9= 66.3751 C9-C8-H22=112.6607
C10-C4-H22= 81.8988 C10-C7-H22= 89.8907 C10-C8-H22=149.3872
C10-C9-H22=130.8731 C1-C11-H22= 85.4954 C2-C11-H22= 92.3696
C11-C4-H22= 79.1298 C6-C11-H22= 76.985 C11-C7-H22=102.5436
C11-C8-H22=110.0251 C9-H22-C11= 88.4314 O12-C4-H22=149.4005
C4-H22-C13= 79.803 C5-C13-H22= 69.7027 C7-H22-C13= 96.3225
C13-C8-H22= 92.0116 C13-C9-H22=101.4013 C10-C13-H22= 76.3415
C11-H22-C13=115.84 N14-C9-H22=101.1554 N14-C13-H22=126.8443
O15-C4-H22= 92.7104 O15-C8-H22=109.6094 O15-C9-H22= 95.4558
O15-C13-H22= 85.8932 H16-C4-H22=134.2509 H16-C11-H22=102.5551
C1-H19-H22= 88.3747 H19-C4-H22= 85.93 C5-H19-H22= 91.7004
C7-H22-H19= 87.9397 H19-C8-H22= 87.0029 C9-H22-H19= 91.3023
C11-H19-H22= 66.2074 O12-H19-H22=124.9304 C13-H22-H19= 91.7659
O15-H19-H22= 80.3615 H16-H19-H22=112.0443 H20-C7-H22=144.9768
C4-H22-H21= 91.3232 C6-H21-H22= 89.8515 H21-C7-H22= 93.3363
H21-C8-H22= 93.6095 C9-H22-H21= 76.1106 C11-H21-H22= 76.8067
C13-H22-H21=103.7896 H19-H22-H21=111.3511 H20-H21-H22=114.1291
C1-C3-H23=121.6659 C2-C3-H23=103.9812 C4-C3-H23=114.3976
C5-C3-H23=122.0063 C1-C6-H23=122.7762 C2-C6-H23=101.97
C6-C3-H23= 61.9226 C4-C6-H23= 97.6069 C7-C6-H23=123.4574
C8-C3-H23= 81.1684 C8-C6-H23= 91.3405 C3-H23-C9= 68.3392
C4-C9-H23=112.3087 C5-C9-H23= 90.1805 C6-H23-C9= 65.3581
C7-C9-H23= 95.8605 C8-C9-H23=129.5349 C2-C10-H23=132.3971
C3-C10-H23=117.5515 C4-C10-H23=165.4572 C5-C10-H23=134.4036
C6-C10-H23=120.0539 C7-C10-H23=139.6125 C8-C10-H23=149.1775
C9-C10-H23=114.0518 C11-C6-H23=150.2535 O12-C3-H23=151.3328
C3-H23-C13= 77.9824 C5-C13-H23= 69.9522 C6-H23-C13= 93.5448
C8-C13-H23= 75.0955 C13-C9-H23=104.809 C13-C10-H23= 95.9732
N14-C9-H23=104.7597 N14-C13-H23=129.2215 O15-C3-H23= 94.1664
O15-C9-H23= 97.4107 O15-C10-H23=115.0796 O15-C13-H23= 85.9229
H17-C3-H23=107.326 H17-C6-H23=106.1617 C2-H18-H23= 78.2574
H18-C3-H23= 91.0945 C5-H18-H23= 89.9363 C6-H23-H18= 77.56
C9-H23-H18= 89.9237 H18-C10-H23= 92.1652 O12-H18-H23=123.3374
C13-H23-H18= 90.8507 O15-H18-H23= 79.0249 H17-H18-H23= 90.8769
C2-H20-H23= 76.5298 C3-H23-H20= 76.3152 H20-C6-H23= 94.5288
C7-H20-H23= 88.8077 C9-H23-H20= 85.6099 H20-C10-H23= 95.5669
C13-H23-H20=114.3049 H17-H20-H23= 89.7961 H18-H23-H20= 90.0848
H21-C6-H23=117.4465 H21-C9-H23= 98.3209 H21-H20-H23= 97.4147
H22-C9-H23=153.7719 H22-C13-H23= 95.1148 C2-C1-H24=129.7676

C3-C1-H24=139.5472 C4-C1-H24= 91.9623 C2-C4-H24= 83.1617
C3-C4-H24=119.5184 C5-C1-H24=128.4345 C5-C4-H24=157.6181
C6-C1-H24= 94.2882 C6-C4-H24= 75.0426 C1-H24-C7= 62.2771
C2-C7-H24= 94.1571 C4-C7-H24= 71.6852 C6-C7-H24=129.6121
C8-C1-H24= 71.6718 C2-C8-H24= 74.9181 C3-C8-H24=104.2807
C4-C8-H24= 73.2604 C5-C8-H24=105.8691 C6-C8-H24= 83.0123
C8-C7-H24= 91.5284 C9-C4-H24=105.0688 C9-C7-H24=128.7197
C9-C8-H24=155.5591 C10-C4-H24=104.9461 C10-C7-H24=138.9836
C10-C8-H24=119.4433 C1-C11-H24=113.042 C2-C11-H24=150.8627
C4-C11-H24= 94.1735 C6-C11-H24=150.6643 C7-C11-H24=112.8112
C8-C11-H24= 93.8442 O12-C1-H24=141.0301 O12-C4-H24=139.8431
C13-C8-H24=173.9852 O15-C4-H24=161.6431 O15-C8-H24=131.2227
H16-C1-H24=102.8007 C2-H16-H24= 88.0549 C4-H16-H24= 67.5381
C5-H16-H24= 97.0245 C7-H24-H16= 85.3538 C8-H24-H16= 78.8531
H16-C11-H24= 99.6724 O12-H16-H24=122.3271 H17-C1-H24=130.0639
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C5-H19-H24=110.8826 C7-H24-H19= 77.7345 H19-C8-H24= 70.4813
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H19-H16-H24= 67.5836 H20-C7-H24=130.3449 C1-H24-H21= 85.6838
C4-H24-H21= 79.3672 C6-H21-H24= 88.1079 H21-C7-H24=101.5068
C8-H21-H24= 67.5396 C9-H21-H24= 96.8658 H21-C11-H24= 99.0473
H16-H24-H21=108.4342 H19-H24-H21= 95.6594 H20-H21-H24=102.0221
C1-H24-H22= 77.8097 H22-C4-H24= 70.321 H22-C7-H24= 81.3245
H22-C8-H24= 87.6224 C9-H22-H24=109.5799 C11-H24-H22= 83.9236
C13-H22-H24=135.8638 H16-H24-H22= 95.3403 H22-H19-H24= 65.3734
H22-H21-H24= 67.8703 C2-C1-H25= 90.6293 C3-C1-H25=122.2449
C3-C2-H25=148.9889 C4-C1-H25=130.394 C4-C2-H25= 83.601
C5-C1-H25=150.2492 C5-C2-H25=120.2787 C6-C1-H25= 71.0286
C2-C6-H25= 73.2422 C3-C6-H25=113.4484 C4-C6-H25= 75.4527
C1-H25-C7= 62.2732 C2-C7-H25= 71.1072 C4-C7-H25= 94.3758
C6-C7-H25= 90.7458 C8-C1-H25= 94.3249 C8-C2-H25= 75.2283
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C9-C7-H25=150.2977 C10-C2-H25=113.8214 C10-C6-H25=149.3023
C10-C7-H25=122.138 C1-C11-H25=113.3067 C2-C11-H25= 93.2875
C4-C11-H25=150.2465 C6-C11-H25= 93.1182 C7-C11-H25=112.4743
C8-C11-H25=149.9574 O12-C1-H25=171.5854 H16-C1-H25=103.5947
C2-H16-H25= 66.428 C4-H16-H25= 88.1703 C5-H16-H25=106.7501
C6-H25-H16= 79.1288 C7-H25-H16= 85.0452 H16-C11-H25=100.6314
O12-H16-H25=134.9772 H17-C1-H25= 83.006 H17-C2-H25= 91.6809
C3-H17-H25=103.2801 H17-C6-H25= 71.7395 C7-H25-H17= 78.5022
C11-H25-H17= 83.4468 H17-H16-H25= 68.8929 H18-C2-H25=172.8052
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H19-H16-H25=100.0696 C1-H25-H20= 78.1875 H20-C2-H25= 71.9908
H20-C6-H25= 92.3362 H20-C7-H25= 83.2838 C10-H20-H25=103.4187
C11-H25-H20= 83.6869 H16-H25-H20= 96.1633 H20-H17-H25= 64.2486
C1-H25-H21= 85.4472 C2-H25-H21= 79.8931 C6-H21-H25= 66.6338
H21-C7-H25=102.1503 C8-H21-H25= 88.4486 C9-H21-H25=106.4006
H21-C11-H25= 99.4399 H16-H25-H21=107.7741 H17-H25-H21= 97.0713
H20-H21-H25= 69.1986 H22-C7-H25=128.3181 H22-C11-H25=155.3543
H22-H21-H25=100.6416 H23-C6-H25=172.9321 H23-H20-H25=127.4908
C1-H24-H25= 66.4238 C2-H25-H24= 96.924 C4-H24-H25= 96.3123
C6-H25-H24= 96.967 C7-H25-H24= 66.3695 C8-H24-H25= 96.4543
H24-C11-H25=109.3086 H16-H24-H25= 71.0747 H17-H25-H24=115.0241
H19-H24-H25=115.764 H20-H25-H24=115.2277 H21-H24-H25= 70.6249

H22-H24-H25=115.6742 C1-C5-H26=119.6504 C2-C5-H26=127.8976
C3-C5-H26=121.9478 C4-C5-H26=122.4941 C8-C5-H26=151.3025
C9-C5-H26=152.5831 C10-C5-H26=150.4833 C1-O12-H26=157.3311
C3-O12-H26=124.2756 C4-O12-H26=125.6868 C5-O12-H26=107.4633
C13-C5-H26=122.895 C3-O15-H26= 81.3468 C4-O15-H26= 81.4078
O15-C5-H26= 84.5158 C8-O15-H26=114.7667 C9-O15-H26=138.634
C10-O15-H26=114.7583 O12-H26-O15= 81.1894 C13-O15-H26=175.8172
N14-O15-H26=163.2732 H16-C5-H26= 98.9701 H16-O12-H26=159.1046
H18-C5-H26= 96.838 H18-O12-H26=111.3534 H18-O15-H26= 73.6635
H19-C5-H26= 97.9215 H19-O12-H26=111.5262 H19-O15-H26= 75.1031
C1-C7-O27=128.6946 C2-C7-O27=108.2213 C4-C7-O27= 96.2456
C6-C7-O27= 81.8541 C1-C8-O27=136.2267 C2-C8-O27=104.9039
C3-C8-O27= 93.5124 C4-C8-O27=147.346 C5-C8-O27=112.3819
C6-C8-O27= 75.8359 C7-C8-O27= 84.3459 C3-C9-O27=139.5743
C4-C9-O27=140.0534 C5-C9-O27=172.4674 C6-C9-O27= 93.2269
C7-C9-O27= 85.2606 C8-C9-O27=103.9075 C2-C10-O27=129.73
C3-C10-O27=148.1818 C4-C10-O27= 94.0778 C5-C10-O27=113.0604
C6-C10-O27= 92.8441 C7-C10-O27= 68.0655 C8-C10-O27= 61.4412
C10-C9-O27=103.7873 C11-C7-O27=165.8153 C11-C8-O27=122.3129
C5-C13-O27=104.5621 C7-O27-C13= 95.1823 C8-O27-C13= 64.9737
C13-C9-O27= 97.0349 C10-O27-C13= 65.255 C7-O27-N14=115.5041
C8-O27-N14= 83.4027 N14-C9-O27= 86.1688 C10-O27-N14= 84.0546
N14-C13-O27=110.6513 O15-C8-O27= 94.4531 O15-C9-O27=155.3218
O15-C10-O27= 95.1688 O15-C13-O27=129.2084 O15-N14-O27= 86.8493
H18-C10-O27=160.5186 H19-C8-O27=157.5784 H20-C7-O27= 85.4292
H20-C10-O27= 92.4498 C6-H21-O27= 74.8386 C7-H21-O27= 85.64
H21-C8-O27= 68.7121 C9-O27-H21= 81.0904 C10-O27-H21= 76.2271
C11-H21-O27=122.6488 C13-O27-H21=115.6261 N14-O27-H21=133.9211
H20-H21-O27= 82.5926 C4-H22-O27=103.6291 C7-H22-O27= 68.0333
H22-C8-O27= 90.7169 H22-C9-O27= 90.089 C10-O27-H22= 80.1897
C11-H22-O27= 98.1695 C13-O27-H22= 67.8745 N14-O27-H22= 80.1397
H19-H22-O27=127.9209 H22-H21-O27= 63.1819 C3-H23-O27=103.8013
C6-H23-O27= 73.7587 C7-O27-H23= 76.9369 C8-O27-H23= 80.9414
H23-C9-O27= 87.685 H23-C10-O27= 88.3573 C13-O27-H23= 70.7664
N14-O27-H23= 83.6045 H18-H23-O27=127.2786 H20-H23-O27= 81.2196
H21-O27-H23= 93.0745 H22-O27-H23=103.3373 H24-C7-O27=144.2259
H24-C8-O27=131.7426 H24-H21-O27=127.7317 H24-H22-O27=116.0073
H25-C7-O27=166.8569 H25-H21-O27=138.36 C3-C9-H28=153.3262
C4-C9-H28=148.8743 C5-C9-H28=163.972 C6-C9-H28=116.3643
C7-C9-H28=106.2859 C8-C9-H28=114.2212 C10-C9-H28=118.5098
C5-C13-H28=128.6937 C8-C13-H28= 80.6951 C13-C9-H28= 73.6207
C10-C13-H28= 82.5949 C9-H28-N14= 64.8657 N14-C13-H28= 86.471
O15-C9-H28=131.9014 O15-C13-H28=153.3491 O15-N14-H28=105.1312
H21-C9-H28= 85.6139 H22-C9-H28= 92.3709 H22-C13-H28= 75.622
H23-C9-H28= 95.8561 H23-C13-H28= 76.9509 C7-O27-H28=155.4263
C8-O27-H28=126.1037 C9-O27-H28=113.6792 C10-O27-H28=133.2456
C13-H28-O27= 80.1124 N14-H28-O27=107.4436 H21-O27-H28=147.1632
H22-O27-H28=108.405 H23-O27-H28=119.5503 C2-H20-O29=140.1762
C6-H20-O29=102.9482 C7-H20-O29= 84.7683 C10-H20-O29= 87.1063
H17-H20-O29=164.0477 C6-H21-O29= 79.8146 C7-H21-O29=115.2398
C8-H21-O29=111.0045 C9-H21-O29= 80.2495 C11-H21-O29=142.9725
H20-H21-O29= 64.8773 H22-H21-O29=116.7642 H23-H20-O29= 77.0532
H24-H21-O29=166.8907 H25-H20-O29=117.4185 H25-H21-O29=129.2529
C7-O27-O29= 83.047 C8-O27-O29=116.4001 C9-O27-O29=126.9072

```
   C10-O27-O29= 92.9593    C13-O27-O29=154.0119    N14-O27-O29=154.2743
   H20-O29-O27= 76.3655    H21-O27-O29= 69.0591    H22-O27-O29=124.6316
   H23-O27-O29= 83.6483    H28-O27-O29=115.1465    H20-O29-H30=157.8172
   H21-O29-H30=136.7895    O27-O29-H30=125.7953      C1-C6-H31=130.0015
     C2-C6-H31=153.8685      C3-C6-H31=111.8316      C4-C6-H31=102.0507
     C1-C7-H31=141.7846      C2-C7-H31=110.4936      C4-C7-H31=115.2168
     C6-C7-H31= 75.8951      C8-C6-H31= 70.0239      C8-C7-H31= 82.7575
     C3-C9-H31=120.2183      C4-C9-H31=131.8725      C5-C9-H31=152.9981
     C6-C9-H31= 73.6559      C7-C9-H31= 72.5172      C8-C9-H31=100.8537
    C2-C10-H31=123.0798     C3-C10-H31=161.7817     C4-C10-H31=106.4025
    C5-C10-H31=131.8357     C6-C10-H31= 79.4837     C7-C10-H31= 65.2868
    C8-C10-H31= 73.0275     C10-C9-H31= 85.5416     C11-C6-H31=110.5793
    C11-C7-H31=173.6642     C13-C9-H31=114.4598    C13-C10-H31= 75.4693
    N14-C9-H31=103.8153     O15-C9-H31=167.6711    O15-C10-H31=116.7787
    H17-C6-H31=168.9917    H18-C10-H31=172.7553     C2-H20-H31=109.7998
    H20-C6-H31= 86.1292     H20-C7-H31= 71.4996     C9-H31-H20= 74.1321
   H20-C10-H31= 73.2437    H17-H20-H31=133.8985     C6-H21-H31= 75.1553
    C7-H21-H31= 98.3653     C8-H21-H31= 80.9544     C9-H31-H21= 74.0447
   C10-H31-H21= 75.835     C11-H21-H31=136.1318    H20-H21-H31= 73.4842
    H22-C7-H31= 82.9022     H22-C9-H31= 95.8923    H22-H21-H31= 85.0983
    C3-H23-H31=114.3495     C6-H23-H31= 68.7083     C7-H31-H23= 75.4113
    H23-C9-H31= 74.1495    H23-C10-H31= 80.64      C13-H23-H31= 70.0156
   H18-H23-H31=139.422     H20-H23-H31= 67.9363    H21-H31-H23= 96.1589
    H24-C7-H31=154.4789    H24-H21-H31=148.3251     H25-C6-H31=119.2509
    H25-C7-H31=146.6639    H25-H20-H31=107.9348    H25-H21-H31=141.2413
    C6-H31-O27= 87.6373     C7-O27-H31= 81.1638     C8-O27-H31=114.5191
    C9-O27-H31=125.5774    C10-O27-H31= 91.9971    C13-O27-H31=153.9847
   N14-O27-H31=155.7311    H20-H31-O27=108.2489    H21-H31-O27= 90.7597
   H22-O27-H31=122.8645    H23-O27-H31= 83.3598     C6-H31-H28=117.7444
    C7-H31-H28=107.8726     C9-H28-H31= 73.5429    C10-H31-H28= 91.5075
   C13-H28-H31=109.3852    N14-H28-H31=135.0667    H20-H31-H28=137.4116
   H21-H31-H28=115.2877    H23-H31-H28= 91.8315    H28-O27-H31=116.9081
    C6-H31-O29= 94.9248     C7-H31-O29=104.7244     C9-H31-O29=147.7885
   C10-H31-O29=115.1984    H20-O29-H31= 75.4064    H21-H31-O29= 92.2278
   H23-H31-O29=105.0097    O27-H31-O29=176.9092    H28-H31-O29=146.1643
    C6-H31-H30=114.6163     C7-H31-H30=120.4379     C9-H31-H30=166.928
   C10-H31-H30=133.2203    H20-H31-H30= 93.9572    H21-H31-H30=103.7097
   H23-H31-H30=118.7599    O27-H31-H30=157.7464    H28-H31-H30=127.1575
   H30-O29-H31=126.7379     C2-H20-H32=156.8441     C6-H20-H32=119.5184
    C7-H20-H32= 97.5739    C10-H20-H32=101.8115    H17-H20-H32=175.7602
   H21-H20-H32= 74.6397    H23-H20-H32= 87.9801    H25-H20-H32=120.2754
   H20-H32-O29=117.1836    H21-O29-H32= 83.289     O27-O29-H32=122.4181
   H20-H32-H30=151.2279    H30-O29-H32=111.7612     C6-H31-H32= 73.4247
    C7-H31-H32= 87.0515     C9-H31-H32=126.3321    C10-H31-H32= 94.8411
   H20-H32-H31= 80.3348    H21-H31-H32= 79.7963    H23-H31-H32= 88.7505
   O27-H31-H32=160.6753    H28-H31-H32=164.7196    H31-O29-H32=121.495
   H30-H32-H31= 70.9943
Stoichiometry    C12H15NO4
Framework group  C1[X(C12H15NO4)]
Deg. of freedom   90
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
```

```
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0       -1.457841   -1.776787   -0.435589
   2          6             0       -0.897859   -1.600025    1.005763
   3          6             0       -1.079771   -0.100159    1.387506
   4          6             0       -1.419227   -0.323416   -0.955235
   5          6             0       -1.851510    0.552060    0.231054
   6          6             0        0.636336   -1.353254    0.756784
   7          6             0        0.762534   -1.428758   -0.793476
   8          6             0        0.119776   -0.075073   -1.214292
   9          6             0        0.628029    0.903251   -0.157769
  10          6             0        0.451088    0.161011    1.155695
  11          6             0       -0.304379   -2.469936   -1.178044
  12          8             0       -3.270598    0.337746    0.449348
  13          6             0        0.418569    2.335063   -0.281953
  14          7             0        0.735972    3.430200   -0.457313
  15          8             0       -1.540902    1.879040    0.069291
  16          1             0       -2.432964   -2.233502   -0.489477
  17          1             0       -1.181483   -2.363338    1.713278
  18          1             0       -1.460120    0.165574    2.358571
  19          1             0       -2.014014   -0.131026   -1.834098
  20          1             0        1.338163   -1.950489    1.322257
  21          1             0        1.757438   -1.594761   -1.180989
  22          1             0        0.344726    0.245193   -2.219976
  23          1             0        1.015772    0.576614    1.974846
  24          1             0       -0.465031   -2.531542   -2.248852
  25          1             0       -0.077603   -3.458464   -0.791735
  26          1             0       -3.699224    1.205815    0.447240
  27          8             0        2.265233    0.917742   -0.384593
  28          1             0        2.619197    1.792118   -0.617362
  29          8             0        3.982767   -0.730879    0.612317
  30          1             0        4.943093   -0.650166    0.553367
  31          1             0        2.914613    0.250214   -0.004539
  32          1             0        3.719158   -1.506690    1.125095
---------------------------------------------------------------------
 Rotational constants (GHZ):      0.7031891      0.5383322      0.3789078
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,O-16,C-
12,N-14,
 O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,O-16,H-1,O-16,H-1,H-
1,H-1
 Standard basis: 3-21+G* (6D, 7F)
 There are   251 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    131072 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
   251 basis functions      368 primitive gaussians
    63 alpha electrons       63 beta electrons
       nuclear repulsion energy      1372.7634045579 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   251 RedAO= T  NBF=   251
 NBsUse=   251 1.00D-04 NBFU=   251
```

```
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -812.510184372     A.U. after   18 cycles
            Convg  =    0.3258D-08             -V/T =  2.0025
            S**2   =   0.0000
 Range of M.O.s used for correlation:     1   251
 NBasis=   251 NAE=    63 NBE=    63 NFC=     0 NFV=     0
 NROrb=    251 NOA=    63 NOB=    63 NVA=   188 NVB=   188

 **** Warning!!: The largest alpha MO coefficient is  0.11936804D+03

          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   3 vectors were produced by pass 12.
   1 vectors were produced by pass 13.
 Inv2:  IOpt= 1 Iter= 1 AM= 6.55D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  40 with in-core refinement.
 PrsmSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 G2DrvN: will do    8 atoms at a time, making    4 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  33 IRICut=      33 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
          There are  99 degrees of freedom in the 1st order CPHF.
    96 vectors were produced by pass  0.
 AX will form  32 AO Fock derivatives at one time.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
```

```
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  96 vectors were produced by pass  1.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  96 vectors were produced by pass  2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  96 vectors were produced by pass  3.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  96 vectors were produced by pass  4.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  96 vectors were produced by pass  5.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  96 vectors were produced by pass  6.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  46 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
 Inv2:  IOpt= 1 Iter= 1 AM= 4.91D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 721 with in-core refinement.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.

 ******************************************************************

            Population analysis using the SCF density.

 ******************************************************************

 Alpha  occ. eigenvalues --  -20.59917 -20.58956 -20.43155 -20.34998 -
15.47498
 Alpha  occ. eigenvalues --  -11.32790 -11.24066 -11.23688 -11.20772 -
11.20507
 Alpha  occ. eigenvalues --  -11.20163 -11.19852 -11.17839 -11.17609 -
11.17061
 Alpha  occ. eigenvalues --  -11.16798 -11.16380  -1.48312  -1.45583  -
1.34268
 Alpha  occ. eigenvalues --   -1.25814  -1.22827  -1.20762  -1.10572  -
1.08687
 Alpha  occ. eigenvalues --   -1.03306  -0.96352  -0.91347  -0.89324  -
0.85923
 Alpha  occ. eigenvalues --   -0.83626  -0.82849  -0.79113  -0.76528  -
0.75105
```

```
 Alpha  occ. eigenvalues --   -0.72629  -0.71396  -0.68051  -0.67064  -
0.65325
 Alpha  occ. eigenvalues --   -0.63781  -0.62447  -0.61613  -0.61029  -
0.59645
 Alpha  occ. eigenvalues --   -0.57905  -0.54252  -0.53876  -0.51925  -
0.51529
 Alpha  occ. eigenvalues --   -0.50735  -0.48777  -0.48069  -0.47743  -
0.47144
 Alpha  occ. eigenvalues --   -0.45328  -0.44690  -0.44075  -0.42714  -
0.41702
 Alpha  occ. eigenvalues --   -0.40628  -0.32510  -0.32185
 Alpha virt. eigenvalues --    0.03115   0.06309   0.06604   0.07353
0.08803
 Alpha virt. eigenvalues --    0.09289   0.09856   0.10433   0.11091
0.11931
 Alpha virt. eigenvalues --    0.12690   0.13101   0.14235   0.14774
0.14989
 Alpha virt. eigenvalues --    0.15312   0.16541   0.17426   0.18112
0.18465
 Alpha virt. eigenvalues --    0.18943   0.19362   0.19731   0.19938
0.20379
 Alpha virt. eigenvalues --    0.20503   0.21205   0.22286   0.22749
0.23489
 Alpha virt. eigenvalues --    0.23831   0.24502   0.24749   0.25114
0.25614
 Alpha virt. eigenvalues --    0.25934   0.26305   0.26854   0.27416
0.27929
 Alpha virt. eigenvalues --    0.27992   0.28286   0.28850   0.29234
0.29873
 Alpha virt. eigenvalues --    0.30375   0.30732   0.31125   0.31474
0.32782
 Alpha virt. eigenvalues --    0.33210   0.34010   0.34659   0.35239
0.35469
 Alpha virt. eigenvalues --    0.36134   0.37225   0.37822   0.38264
0.39392
 Alpha virt. eigenvalues --    0.39757   0.40646   0.40972   0.41998
0.42229
 Alpha virt. eigenvalues --    0.42533   0.43296   0.43910   0.44360
0.45220
 Alpha virt. eigenvalues --    0.45975   0.46755   0.47593   0.47765
0.48442
 Alpha virt. eigenvalues --    0.49092   0.50009   0.51005   0.51280
0.51419
 Alpha virt. eigenvalues --    0.51904   0.53735   0.54192   0.54399
0.55939
 Alpha virt. eigenvalues --    0.56339   0.57144   0.57421   0.58354
0.59417
 Alpha virt. eigenvalues --    0.60407   0.61529   0.62658   0.62806
0.63068
 Alpha virt. eigenvalues --    0.64809   0.65489   0.65844   0.67018
0.68314
 Alpha virt. eigenvalues --    0.69081   0.72156   0.74147   0.81339
0.93834
```

```
 Alpha virt. eigenvalues --    1.10444   1.12439   1.13005   1.14989
1.16171
 Alpha virt. eigenvalues --    1.16690   1.17160   1.18177   1.18989
1.19829
 Alpha virt. eigenvalues --    1.20657   1.20826   1.22397   1.23110
1.23945
 Alpha virt. eigenvalues --    1.24236   1.26619   1.27666   1.28837
1.30195
 Alpha virt. eigenvalues --    1.31477   1.32508   1.33871   1.36988
1.38489
 Alpha virt. eigenvalues --    1.39527   1.41989   1.42600   1.45530
1.46542
 Alpha virt. eigenvalues --    1.48967   1.50476   1.51597   1.52952
1.53917
 Alpha virt. eigenvalues --    1.55700   1.56395   1.57789   1.58995
1.61309
 Alpha virt. eigenvalues --    1.61467   1.64073   1.64782   1.68934
1.73277
 Alpha virt. eigenvalues --    1.73630   1.75413   1.76648   1.79397
1.80505
 Alpha virt. eigenvalues --    1.82023   1.88028   1.91018   1.93230
2.00644
 Alpha virt. eigenvalues --    2.01768   2.03921   2.05609   2.09875
2.18331
 Alpha virt. eigenvalues --    2.19480   2.24103   2.28034   2.31920
2.34702
 Alpha virt. eigenvalues --    2.38010   2.40054   2.46541   2.50363
2.55815
 Alpha virt. eigenvalues --    2.56088   2.60608   2.82852   2.92407
3.14607
 Alpha virt. eigenvalues --    3.18548   3.30310   3.39092   3.54298
3.72627
 Alpha virt. eigenvalues --    3.81697   3.93035   4.16603
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   15.473488  -5.087939   0.870291  -8.300441   4.062221   3.111829
  2  C   -5.087939  19.468639 -12.132861  -0.974327   6.651230  -9.417865
  3  C    0.870291 -12.132861  33.613537  13.316938 -29.792929   9.528365
  4  C   -8.300441  -0.974327  13.316938  30.430658 -29.048568   0.456753
  5  C    4.062221   6.651230 -29.792929 -29.048568  62.229296  -4.508679
  6  C    3.111829  -9.417865   9.528365   0.456753  -4.508679  19.128165
  7  C   -1.219229   2.735208  -4.018181   0.097523   3.082651  -5.455560
  8  C    5.202443   0.076895  -8.003574 -15.742750  13.847701  -0.720355
  9  C   -3.434477  -5.410129  16.200230  14.325085 -21.735900   8.976509
 10  C    1.230571  11.200616 -25.510979 -13.783926  22.689377 -15.866938
 11  C   -3.918221   0.930487   0.379977   1.806594  -2.577309  -0.540040
 12  O   -0.006362  -0.114304   0.737226   0.625443  -1.935075   0.034715
 13  C   -1.874943  -1.602772   8.911631  10.117328 -12.495419   0.749285
 14  N   -0.003049  -0.007015  -0.116295  -0.125330   0.077795   0.125835
 15  O   -0.259122  -0.009273   0.917564   1.168432  -3.093835   0.012751
 16  H    0.539069  -0.101232   0.052163  -0.155765  -0.038443   0.039345
 17  H   -0.096232   0.585308  -0.150212   0.030824  -0.020565  -0.128590
 18  H    0.023480  -0.101094   0.599685   0.047379  -0.182589   0.048470
 19  H   -0.034766   0.007852   0.062270   0.568462  -0.160367   0.000981
```

20	H	0.000269	-0.049460	0.070612	0.003551	0.000004	0.549127
21	H	-0.025768	0.052192	-0.008960	0.045310	-0.003542	-0.139862
22	H	0.059675	0.001423	-0.033676	-0.196886	0.080099	-0.001667
23	H	-0.009234	0.098906	-0.144916	-0.017095	0.050030	-0.173538
24	H	-0.082799	0.026284	0.003980	0.035336	-0.024703	0.021448
25	H	-0.074773	0.011431	-0.015107	0.024187	0.011014	0.010429
26	H	0.006888	0.016025	-0.087893	-0.085604	0.210398	-0.004321
27	O	0.014648	0.075579	-0.233585	-0.167269	0.154585	-0.066012
28	H	0.002382	0.000794	-0.006635	-0.010707	0.006469	-0.001585
29	O	0.002395	0.024754	-0.038894	0.000130	0.002370	0.108975
30	H	0.000163	-0.001200	0.000189	-0.000250	0.000109	-0.006685
31	H	-0.002204	0.002385	0.000346	0.004203	-0.005475	0.015682
32	H	-0.000093	0.000878	0.002513	0.000259	-0.000362	0.006993

		7	8	9	10	11	12
1	C	-1.219229	5.202443	-3.434477	1.230571	-3.918221	-0.006362
2	C	2.735208	0.076895	-5.410129	11.200616	0.930487	-0.114304
3	C	-4.018181	-8.003574	16.200230	-25.510979	0.379977	0.737226
4	C	0.097523	-15.742750	14.325085	-13.783926	1.806594	0.625443
5	C	3.082651	13.847701	-21.735900	22.689377	-2.577309	-1.935075
6	C	-5.455560	-0.720355	8.976509	-15.866938	-0.540040	0.034715
7	C	16.931619	-4.065221	-1.934747	7.852142	-3.802078	-0.011130
8	C	-4.065221	42.580805	-38.552723	25.508020	1.024204	-0.164734
9	C	-1.934747	-38.552723	103.001705	-52.406224	-0.290694	0.318263
10	C	7.852142	25.508020	-52.406224	70.295212	0.634111	-0.233715
11	C	-3.802078	1.024204	-0.290694	0.634111	13.815283	0.081187
12	O	-0.011130	-0.164734	0.318263	-0.233715	0.081187	8.940076
13	C	-4.920239	-13.685246	-17.082505	-22.836961	-0.793936	0.100272
14	N	0.149726	0.076011	1.341097	-0.015961	0.014187	0.001473
15	O	0.072123	-0.032792	0.053390	-0.402149	0.103628	0.025718
16	H	-0.037178	0.049914	0.018913	-0.017497	-0.006771	0.004825
17	H	-0.005135	0.022553	-0.025574	0.118107	0.031988	0.002745
18	H	-0.003808	0.014927	-0.005728	-0.067759	0.001885	-0.001275
19	H	0.014342	-0.115638	0.016497	0.021778	0.023012	0.000347
20	H	-0.154794	0.085260	-0.095769	-0.076345	0.044519	0.000016
21	H	0.545838	-0.165417	0.012878	0.027457	-0.006651	0.000007
22	H	-0.028914	0.736962	-0.323680	0.171319	-0.012798	-0.000089
23	H	0.040661	0.109625	-0.362711	0.848780	-0.002016	-0.000122
24	H	-0.129654	0.050181	-0.027312	0.013548	0.424017	0.000039
25	H	-0.108435	0.058365	-0.027637	0.012772	0.418718	-0.000044
26	H	0.001889	0.002694	-0.021006	0.011746	-0.004126	0.173723
27	O	0.204484	0.795666	-2.382679	1.346556	0.029686	0.002636
28	H	0.015193	0.009377	-0.015404	0.020452	0.000592	-0.000001
29	O	-0.085039	0.141751	-0.180905	0.070389	-0.025538	0.000000
30	H	0.008920	-0.002907	-0.002118	0.009377	0.000512	0.000000
31	H	-0.021765	-0.002661	0.027568	-0.016369	-0.000418	0.000000
32	H	-0.001715	-0.003842	0.002152	-0.001470	0.002324	0.000000

		13	14	15	16	17	18
1	C	-1.874943	-0.003049	-0.259122	0.539069	-0.096232	0.023480
2	C	-1.602772	-0.007015	-0.009273	-0.101232	0.585308	-0.101094
3	C	8.911631	-0.116295	0.917564	0.052163	-0.150212	0.599685
4	C	10.117328	-0.125330	1.168432	-0.155765	0.030824	0.047379
5	C	-12.495419	0.077795	-3.093835	-0.038443	-0.020565	-0.182589
6	C	0.749285	0.125835	0.012751	0.039345	-0.128590	0.048470
7	C	-4.920239	0.149726	0.072123	-0.037178	-0.005135	-0.003808

8	C	-13.685246	0.076011	-0.032792	0.049914	0.022553	0.014927
9	C	-17.082505	1.341097	0.053390	0.018913	-0.025574	-0.005728
10	C	-22.836961	-0.015961	-0.402149	-0.017497	0.118107	-0.067759
11	C	-0.793936	0.014187	0.103628	-0.006771	0.031988	0.001885
12	O	0.100272	0.001473	0.025718	0.004825	0.002745	-0.001275
13	C	62.029044	-1.931769	0.007071	0.005982	-0.001098	-0.016761
14	N	-1.931769	7.942405	0.095355	-0.000021	0.000008	-0.000273
15	O	0.007071	0.095355	9.733430	-0.000157	0.000286	0.002240
16	H	0.005982	-0.000021	-0.000157	0.362499	-0.000471	0.000001
17	H	-0.001098	0.000008	0.000286	-0.000471	0.375870	-0.000089
18	H	-0.016761	-0.000273	0.002240	0.000001	-0.000089	0.356792
19	H	-0.051167	0.000027	0.001085	0.000027	-0.000008	-0.000015
20	H	-0.019128	-0.000048	0.000089	-0.000015	-0.000619	-0.000097
21	H	0.014548	-0.000587	-0.000037	-0.000017	-0.000015	0.000000
22	H	-0.101385	0.000143	0.000619	-0.000014	0.000001	0.000000
23	H	-0.085291	-0.001122	0.001364	0.000001	-0.000094	-0.000548
24	H	0.005788	-0.000043	-0.000008	-0.000301	-0.000034	0.000000
25	H	-0.003488	0.000006	-0.000001	-0.000416	0.000127	0.000000
26	H	-0.002283	-0.000321	0.002796	-0.000025	0.000001	0.000456
27	O	-0.167856	-0.000042	0.059946	0.000025	0.000038	-0.000189
28	H	-0.018823	0.009453	0.000545	0.000000	0.000000	0.000000
29	O	-0.029222	-0.000690	0.000476	0.000000	-0.000004	0.000019
30	H	-0.003735	0.000001	0.000000	0.000000	0.000000	0.000000
31	H	0.008449	0.004466	0.000481	0.000000	0.000000	0.000001
32	H	-0.000998	0.000025	-0.000001	0.000000	0.000000	0.000000

		19	20	21	22	23	24
1	C	-0.034766	0.000269	-0.025768	0.059675	-0.009234	-0.082799
2	C	0.007852	-0.049460	0.052192	0.001423	0.098906	0.026284
3	C	0.062270	0.070612	-0.008960	-0.033676	-0.144916	0.003980
4	C	0.568462	0.003551	0.045310	-0.196886	-0.017095	0.035336
5	C	-0.160367	0.000004	-0.003542	0.080099	0.050030	-0.024703
6	C	0.000981	0.549127	-0.139862	-0.001667	-0.173538	0.021448
7	C	0.014342	-0.154794	0.545838	-0.028914	0.040661	-0.129654
8	C	-0.115638	0.085260	-0.165417	0.736962	0.109625	0.050181
9	C	0.016497	-0.095769	0.012878	-0.323680	-0.362711	-0.027312
10	C	0.021778	-0.076345	0.027457	0.171319	0.848780	0.013548
11	C	0.023012	0.044519	-0.006651	-0.012798	-0.002016	0.424017
12	O	0.000347	0.000016	0.000007	-0.000089	-0.000122	0.000039
13	C	-0.051167	-0.019128	0.014548	-0.101385	-0.085291	0.005788
14	N	0.000027	-0.000048	-0.000587	0.000143	-0.001122	-0.000043
15	O	0.001085	0.000089	-0.000037	0.000619	0.001364	-0.000008
16	H	0.000027	-0.000015	-0.000017	-0.000014	0.000001	-0.000301
17	H	-0.000008	-0.000619	-0.000015	0.000001	-0.000094	-0.000034
18	H	-0.000015	-0.000097	0.000000	0.000000	-0.000548	0.000000
19	H	0.359036	0.000000	-0.000015	-0.000162	0.000000	0.000131
20	H	0.000000	0.415875	-0.000173	-0.000019	0.000262	-0.000033
21	H	-0.000015	-0.000173	0.395087	0.000499	0.000003	-0.000265
22	H	-0.000162	-0.000019	0.000499	0.362301	-0.000018	0.000090
23	H	0.000000	0.000262	0.000003	-0.000018	0.366418	0.000000
24	H	0.000131	-0.000033	-0.000265	0.000090	0.000000	0.435092
25	H	-0.000053	0.000162	-0.000396	-0.000036	0.000000	-0.017326
26	H	0.000415	0.000000	0.000000	0.000000	0.000000	0.000000
27	O	-0.000050	0.004782	0.004863	0.008580	0.011054	-0.000024
28	H	0.000001	-0.000004	0.000056	0.000110	0.000097	0.000000

29	O	0.000001	-0.002603	0.002075	0.000045	0.000588	0.000002
30	H	0.000000	0.000041	0.000022	0.000000	0.000005	0.000000
31	H	0.000000	-0.000264	-0.000505	0.000062	-0.000288	0.000001
32	H	0.000000	0.001101	-0.000067	0.000000	-0.000008	0.000000

		25	26	27	28	29	30
1	C	-0.074773	0.006888	0.014648	0.002382	0.002395	0.000163
2	C	0.011431	0.016025	0.075579	0.000794	0.024754	-0.001200
3	C	-0.015107	-0.087893	-0.233585	-0.006635	-0.038894	0.000189
4	C	0.024187	-0.085604	-0.167269	-0.010707	0.000130	-0.000250
5	C	0.011014	0.210398	0.154585	0.006469	0.002370	0.000109
6	C	0.010429	-0.004321	-0.066012	-0.001585	0.108975	-0.006685
7	C	-0.108435	0.001889	0.204484	0.015193	-0.085039	0.008920
8	C	0.058365	0.002694	0.795666	0.009377	0.141751	-0.002907
9	C	-0.027637	-0.021006	-2.382679	-0.015404	-0.180905	-0.002118
10	C	0.012772	0.011746	1.346556	0.020452	0.070389	0.009377
11	C	0.418718	-0.004126	0.029686	0.000592	-0.025538	0.000512
12	O	-0.000044	0.173723	0.002636	-0.000001	0.000000	0.000000
13	C	-0.003488	-0.002283	-0.167856	-0.018823	-0.029222	-0.003735
14	N	0.000006	-0.000321	-0.000042	0.009453	-0.000690	0.000001
15	O	-0.000001	0.002796	0.059946	0.000545	0.000476	0.000000
16	H	-0.000416	-0.000025	0.000025	0.000000	0.000000	0.000000
17	H	0.000127	0.000001	0.000038	0.000000	-0.000004	0.000000
18	H	0.000000	0.000456	-0.000189	0.000000	0.000019	0.000000
19	H	-0.000053	0.000415	-0.000050	0.000001	0.000001	0.000000
20	H	0.000162	0.000000	0.004782	-0.000004	-0.002603	0.000041
21	H	-0.000396	0.000000	0.004863	0.000056	0.002075	0.000022
22	H	-0.000036	0.000000	0.008580	0.000110	0.000045	0.000000
23	H	0.000000	0.000000	0.011054	0.000097	0.000588	0.000005
24	H	-0.017326	0.000000	-0.000024	0.000000	0.000002	0.000000
25	H	0.442652	0.000000	-0.000041	0.000000	0.000025	0.000000
26	H	0.000000	0.318686	-0.000013	0.000000	0.000000	0.000000
27	O	-0.000041	-0.000013	8.878350	0.225134	-0.069563	0.004283
28	H	0.000000	0.000000	0.225134	0.206774	0.001760	0.000000
29	O	0.000025	0.000000	-0.069563	0.001760	8.553732	0.221870
30	H	0.000000	0.000000	0.004283	0.000000	0.221870	0.269144
31	H	0.000000	0.000000	0.186728	-0.005580	0.032303	-0.000622
32	H	0.000000	0.000000	0.003783	-0.000023	0.239451	-0.016527

		31	32
1	C	-0.002204	-0.000093
2	C	0.002385	0.000878
3	C	0.000346	0.002513
4	C	0.004203	0.000259
5	C	-0.005475	-0.000362
6	C	0.015682	0.006993
7	C	-0.021765	-0.001715
8	C	-0.002661	-0.003842
9	C	0.027568	0.002152
10	C	-0.016369	-0.001470
11	C	-0.000418	0.002324
12	O	0.000000	0.000000
13	C	0.008449	-0.000998
14	N	0.004466	0.000025
15	O	0.000481	-0.000001
16	H	0.000000	0.000000

17	H	0.000000	0.000000
18	H	0.000001	0.000000
19	H	0.000000	0.000000
20	H	-0.000264	0.001101
21	H	-0.000505	-0.000067
22	H	0.000062	0.000000
23	H	-0.000288	-0.000008
24	H	0.000001	0.000000
25	H	0.000000	0.000000
26	H	0.000000	0.000000
27	O	0.186728	0.003783
28	H	-0.005580	-0.000023
29	O	0.032303	0.239451
30	H	-0.000622	-0.016527
31	H	0.152417	-0.000643
32	H	-0.000643	0.276771

Total atomic charges:

		1
1	C	-0.170161
2	C	-0.957416
3	C	1.027177
4	C	1.504526
5	C	-1.531593
6	C	0.106041
7	C	0.250504
8	C	-3.135494
9	C	6.023635
10	C	-4.846036
11	C	-1.786314
12	O	-0.581857
13	C	1.775626
14	N	-0.635446
15	O	-0.462014
16	H	0.285559
17	H	0.260882
18	H	0.284889
19	H	0.285977
20	H	0.223703
21	H	0.251441
22	H	0.277414
23	H	0.269207
24	H	0.266565
25	H	0.257866
26	H	0.459876
27	O	-0.924085
28	H	0.559571
29	O	-0.970652
30	H	0.519407
31	H	0.621701
32	H	0.489500

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.115398

```
  2  C   -0.696534
  3  C    1.312067
  4  C    1.790503
  5  C   -1.531593
  6  C    0.329743
  7  C    0.501945
  8  C   -2.858081
  9  C    6.023635
 10  C   -4.576828
 11  C   -1.261883
 12  O   -0.121981
 13  C    1.775626
 14  N   -0.635446
 15  O   -0.462014
 16  H    0.000000
 17  H    0.000000
 18  H    0.000000
 19  H    0.000000
 20  H    0.000000
 21  H    0.000000
 22  H    0.000000
 23  H    0.000000
 24  H    0.000000
 25  H    0.000000
 26  H    0.000000
 27  O    0.257188
 28  H    0.000000
 29  O    0.038256
 30  H    0.000000
 31  H    0.000000
 32  H    0.000000
 Sum of Mulliken charges=   0.00000
 Electronic spatial extent (au):  <R**2>=  3182.3661
 Charge=     0.0000 electrons
 Dipole moment (Debye):
    X=    12.5435    Y=    -8.9880    Z=     1.1225  Tot=    15.4720
 Quadrupole moment (Debye-Ang):
   XX=   -74.9171   YY=  -126.9457   ZZ=   -97.9084
   XY=    -3.2146   XZ=     7.3368   YZ=    -0.8073
 Octapole moment (Debye-Ang**2):
  XXX=   233.6842  YYY=  -117.9952  ZZZ=     5.0804  XYY=    20.4934
  XXY=   -15.3804  XXZ=    19.6143  XZZ=    11.5663  YZZ=    -4.3105
  YYZ=    17.8293  XYZ=   -15.6279
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -1061.7866 YYYY= -2026.2147 ZZZZ=  -549.3082 XXXY=  -203.0503
 XXXZ=   132.5061 YYYX=   -64.8454 YYYZ=    25.5162 ZZZX=    14.6083
 ZZZY=    -4.3128 XXYY=  -522.1977 XXZZ=  -398.6344 YYZZ=  -366.8616
 XXYZ=   -45.4784 YYXZ=    21.4289 ZZXY=   -18.1803
 N-N= 1.372763404558D+03 E-N=-4.649772587169D+03  KE= 8.104477311531D+02
  Exact polarizability: 141.838   7.482 146.360  -3.567  -2.084 110.008
 Approx polarizability: 125.424   6.854 130.481  -3.142  -4.165 106.685
 Full mass-weighted force constant matrix:
 Low frequencies --- -180.6412   -0.8503   -0.6846    0.0005    0.0009
0.0011
```

```
 Low frequencies ---    0.7906   25.6617   76.5236
 ******    1 imaginary frequencies (negative Signs) ******
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                      1                      2                      3
                     ?A                     ?A                     ?A
 Frequencies --  -180.6412                25.6617                76.5236
 Red. masses --     6.8199                 4.4967                 1.3166
 Frc consts  --     0.1311                 0.0017                 0.0045
 IR Inten    --    34.0722                 2.2989                 2.2395
 Raman Activ --     2.7756                 0.1620                 0.6337
 Depolar     --     0.6995                 0.7406                 0.7409
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.02  -0.04   0.01     0.04  -0.01   0.01     0.02   0.00
0.00
   2   6     0.04  -0.01   0.00    -0.03   0.03   0.03     0.03   0.00
0.00
   3   6    -0.06  -0.03   0.02    -0.07   0.03   0.00     0.02   0.00
0.00
   4   6    -0.08  -0.04   0.02     0.04  -0.02  -0.01     0.01   0.00
0.01
   5   6    -0.11  -0.06   0.03    -0.02   0.00  -0.05     0.01   0.00
0.01
   6   6     0.01   0.10  -0.02    -0.02   0.04   0.10     0.02   0.01  -
0.01
   7   6    -0.01   0.11  -0.03     0.05   0.01   0.11     0.01   0.01  -
0.01
   8   6    -0.10   0.08  -0.02     0.05   0.00   0.05     0.01   0.01
0.00
   9   6    -0.17   0.11  -0.01    -0.01   0.03   0.06     0.01   0.01  -
0.01
  10   6    -0.08   0.09   0.00    -0.06   0.05   0.06     0.02   0.01  -
0.01
  11   6     0.05   0.04  -0.01     0.08  -0.01   0.08     0.02   0.01
0.00
  12   8    -0.11  -0.14   0.04    -0.03  -0.02  -0.11     0.01  -0.02
0.02
  13   6     0.38   0.14  -0.09    -0.03   0.02   0.03    -0.01   0.01  -
0.01
  14   7     0.10   0.18  -0.05    -0.03   0.02   0.03    -0.02   0.01  -
0.03
  15   8    -0.14  -0.10   0.03    -0.03   0.00  -0.06     0.00   0.00
0.01
  16   1     0.05  -0.10   0.03     0.05  -0.02  -0.02     0.02   0.00
0.01
  17   1     0.11  -0.04   0.00    -0.05   0.03   0.03     0.04   0.00
0.00
  18   1    -0.07  -0.06   0.02    -0.12   0.04  -0.02     0.03   0.00
0.01
  19   1    -0.11  -0.07   0.03     0.08  -0.04  -0.04     0.00   0.00
0.01
```

20	1	0.07	0.16	-0.04	-0.04	0.07	0.15	0.02	0.02	0.00
21	1	-0.01	0.17	-0.04	0.06	0.02	0.14	0.01	0.02	-0.03
22	1	-0.13	0.09	-0.02	0.09	-0.01	0.06	0.00	0.01	-0.01
23	1	-0.09	0.12	-0.02	-0.10	0.07	0.08	0.03	0.01	-0.01
24	1	0.04	0.03	0.00	0.13	-0.03	0.07	0.01	0.01	0.00
25	1	0.13	0.06	-0.01	0.08	0.00	0.10	0.02	0.01	-0.01
26	1	-0.13	-0.15	0.05	-0.04	-0.02	-0.15	0.01	-0.02	0.03
27	8	0.12	-0.14	-0.02	0.00	0.06	0.14	0.00	0.02	-0.01
28	1	0.31	-0.28	-0.18	0.01	0.07	0.20	0.00	0.00	-0.07
29	8	0.09	-0.12	0.06	0.05	-0.17	-0.32	-0.10	-0.05	0.03
30	1	0.09	-0.09	0.06	0.05	-0.12	-0.31	-0.09	0.20	0.59
31	1	0.05	-0.16	0.01	0.01	-0.03	-0.03	-0.01	0.02	0.02
32	1	0.12	-0.11	0.09	0.09	-0.33	-0.54	-0.20	-0.43	-0.59

	4			5			6		
	?A			?A			?A		
Frequencies --	90.2845			129.6470			197.6047		
Red. masses --	2.2069			8.6390			5.8703		
Frc consts --	0.0106			0.0856			0.1351		
IR Inten --	1.8120			1.8366			37.3256		
Raman Activ --	0.5343			2.0753			0.1476		
Depolar --	0.7274			0.7497			0.4908		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.04	0.00	-0.01	0.00	-0.06	0.09	0.06	-0.12	0.02
2 6	-0.05	-0.01	-0.01	0.03	0.06	0.07	0.08	-0.08	0.00
3 6	-0.03	-0.01	0.00	0.03	0.09	-0.05	-0.03	-0.09	0.01
4 6	-0.02	0.00	0.00	-0.03	-0.09	-0.02	-0.08	-0.11	0.02
5 6	-0.02	0.01	-0.01	-0.01	-0.01	-0.09	-0.02	-0.06	0.01
6 6	-0.04	-0.03	0.01	0.02	0.04	0.01	0.06	0.05	-0.04
7 6	-0.04	-0.02	0.01	-0.01	-0.03	0.01	0.02	0.07	-0.05
8 6	-0.02	-0.01	0.01	-0.05	-0.06	-0.05	-0.09	0.01	-0.02
9 6	-0.01	-0.03	0.01	-0.01	-0.01	-0.10	-0.13	0.03	-0.01

10	6	-0.03	-0.03	0.01	0.04	0.05	-0.07	-0.05	0.02	-0.01
11	6	-0.05	-0.01	0.00	0.00	-0.09	0.12	0.11	-0.02	-0.02
12	8	-0.02	0.04	-0.02	0.00	0.00	-0.02	-0.05	0.36	0.04
13	6	0.02	-0.02	0.01	0.05	0.02	0.13	-0.11	0.02	0.00
14	7	0.04	-0.03	0.01	0.11	0.07	0.56	-0.13	0.04	0.02
15	8	0.01	0.00	0.00	-0.03	-0.02	-0.24	0.21	-0.09	-0.07
16	1	-0.05	0.01	-0.02	0.01	-0.08	0.14	0.10	-0.22	0.04
17	1	-0.06	-0.01	-0.01	0.04	0.11	0.13	0.17	-0.10	0.01
18	1	-0.04	-0.01	0.00	0.04	0.16	-0.06	-0.04	-0.13	0.02
19	1	-0.01	0.01	-0.01	-0.05	-0.17	-0.02	-0.11	-0.16	0.03
20	1	-0.04	-0.03	0.01	0.03	0.07	0.03	0.12	0.09	-0.07
21	1	-0.04	-0.03	0.00	-0.02	-0.04	0.00	0.03	0.15	-0.07
22	1	-0.01	-0.01	0.01	-0.07	-0.11	-0.07	-0.14	0.05	-0.02
23	1	-0.03	-0.04	0.01	0.05	0.10	-0.10	-0.07	0.06	-0.02
24	1	-0.04	0.00	-0.01	-0.03	-0.18	0.13	0.08	-0.02	-0.02
25	1	-0.06	-0.01	-0.01	0.03	-0.05	0.19	0.20	0.00	-0.04
26	1	0.00	0.05	-0.02	-0.01	0.00	-0.10	0.20	0.48	-0.12
27	8	0.00	-0.04	0.02	-0.02	-0.04	-0.24	-0.03	0.00	0.01
28	1	-0.01	-0.06	-0.05	-0.02	-0.01	-0.15	-0.02	0.02	0.09
29	8	0.21	0.13	-0.01	-0.08	0.06	-0.03	0.08	-0.11	0.06
30	1	0.19	0.55	0.35	-0.08	0.14	0.16	0.08	-0.09	0.06
31	1	0.03	0.00	0.04	-0.02	-0.01	-0.17	-0.04	0.01	0.00
32	1	0.35	-0.23	-0.48	-0.12	-0.01	-0.15	0.11	-0.12	0.06

	7	8	9
	?A	?A	?A
Frequencies --	218.9917	250.6819	295.4949
Red. masses --	6.7315	8.1699	3.7128
Frc consts --	0.1902	0.3025	0.1910
IR Inten --	0.7989	4.1365	12.7553
Raman Activ --	0.2470	0.4605	1.7082
Depolar --	0.3769	0.6261	0.7480

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.05	-0.07	-0.02	0.00	-0.04	-0.04	0.02	0.02	-0.10
2	6	0.00	-0.08	0.00	0.00	-0.01	-0.04	-0.07	0.00	-0.04
3	6	-0.08	-0.10	0.03	0.02	0.01	-0.03	-0.03	0.01	-0.01
4	6	0.00	-0.04	0.02	-0.06	-0.05	-0.01	0.03	0.04	-0.02
5	6	-0.02	-0.04	0.03	-0.02	-0.01	-0.02	0.00	0.02	-0.01
6	6	0.00	-0.01	0.05	0.00	-0.01	-0.05	-0.05	-0.04	0.08
7	6	0.04	0.04	0.05	0.00	0.03	-0.05	0.05	0.03	0.10
8	6	-0.02	0.01	0.06	-0.03	0.02	0.00	0.04	0.03	0.10
9	6	-0.03	0.00	0.07	0.01	-0.01	0.03	0.04	-0.01	0.11
10	6	-0.07	-0.02	0.08	-0.02	-0.02	0.00	0.01	-0.04	0.10
11	6	0.11	0.00	0.00	0.02	0.01	-0.07	0.09	0.07	-0.05
12	8	-0.06	0.12	-0.13	0.04	0.01	0.40	0.02	0.03	0.14
13	6	0.14	0.01	0.02	0.04	-0.02	-0.02	0.02	-0.01	0.07
14	7	0.28	-0.05	-0.08	0.24	-0.08	-0.05	-0.15	0.02	-0.04
15	8	0.10	-0.05	0.14	-0.07	-0.03	-0.35	-0.02	0.00	-0.11
16	1	0.07	-0.12	-0.06	0.02	-0.09	-0.03	0.04	0.00	-0.17
17	1	0.02	-0.12	-0.03	0.01	0.01	-0.03	-0.15	0.01	-0.07
18	1	-0.11	-0.15	0.04	-0.01	-0.01	-0.04	-0.08	-0.02	-0.02
19	1	0.00	-0.05	0.02	-0.04	-0.05	-0.02	0.09	0.08	-0.05
20	1	0.00	0.00	0.06	0.00	-0.02	-0.06	-0.11	-0.09	0.11
21	1	0.06	0.10	0.07	0.00	0.06	-0.06	0.07	0.07	0.15
22	1	0.00	0.03	0.07	-0.05	0.06	0.00	0.11	0.05	0.12
23	1	-0.11	-0.02	0.10	-0.01	-0.04	0.01	-0.03	-0.07	0.15
24	1	0.15	0.02	-0.01	0.01	0.05	-0.07	0.18	0.15	-0.07
25	1	0.14	0.00	-0.01	0.05	0.00	-0.12	0.05	0.03	-0.11
26	1	0.07	0.19	-0.01	-0.07	-0.05	-0.33	-0.05	-0.01	-0.40

27	8	-0.09	-0.05	-0.07	-0.05	0.05	0.29	0.00	-0.14	-0.18
28	1	-0.12	-0.07	-0.17	-0.05	0.09	0.41	0.01	-0.23	-0.51
29	8	-0.27	0.24	-0.15	-0.10	0.09	-0.04	0.00	0.00	-0.02
30	1	-0.27	0.29	-0.15	-0.11	0.17	-0.20	0.01	0.00	0.08
31	1	-0.04	-0.03	-0.05	-0.07	-0.03	0.21	0.04	-0.06	-0.10
32	1	-0.26	0.25	-0.13	0.05	0.00	-0.09	-0.05	0.08	0.08

	10			11			12		
	?A			?A			?A		
Frequencies --	305.6351			318.6936			347.2210		
Red. masses --	2.8151			6.9251			1.1529		
Frc consts --	0.1549			0.4144			0.0819		
IR Inten --	82.6803			58.3979			117.2727		
Raman Activ --	2.1981			5.2529			1.8527		
Depolar --	0.3907			0.7470			0.7419		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.04	0.03	0.02	0.07	0.00	-0.03	0.00	0.01	0.01
2 6	0.06	0.04	0.00	0.03	0.03	-0.02	0.01	0.00	0.01
3 6	0.04	0.04	0.00	-0.03	0.03	-0.01	-0.01	-0.01	0.02
4 6	0.02	0.02	0.00	-0.03	0.02	-0.01	0.02	0.01	0.01
5 6	0.03	0.03	-0.01	-0.05	0.02	0.00	0.00	0.00	0.03
6 6	0.06	0.05	-0.02	0.03	0.07	0.03	0.01	0.01	-0.01
7 6	0.02	0.04	-0.04	0.06	0.11	0.03	0.00	-0.01	-0.01
8 6	-0.01	0.02	-0.02	-0.05	0.04	0.02	0.01	-0.01	-0.02
9 6	0.03	-0.01	-0.02	-0.10	-0.03	0.01	-0.01	0.00	-0.03
10 6	0.00	0.04	-0.01	-0.02	0.04	0.02	-0.01	0.01	-0.02
11 6	0.03	0.02	0.01	0.14	0.07	-0.01	-0.01	-0.01	0.01
12 8	0.03	-0.02	-0.04	-0.03	-0.06	0.02	0.00	0.00	0.01
13 6	-0.05	-0.02	0.00	-0.24	-0.08	0.05	-0.01	0.00	-0.02
14 7	-0.05	-0.01	0.02	0.32	-0.24	-0.03	0.01	0.00	0.01
15 8	-0.01	0.05	0.01	-0.12	0.09	0.04	0.00	0.01	0.06
16 1	0.04	0.02	0.04	0.11	-0.08	-0.06	0.00	0.03	0.02

17	1	0.09	0.04	0.01	0.02	0.03	-0.02	0.03	-0.02	0.00
18	1	0.03	0.03	0.00	-0.04	-0.01	0.00	0.00	-0.01	0.02
19	1	-0.01	0.00	0.01	-0.03	0.00	-0.01	0.01	0.01	0.02
20	1	0.08	0.07	-0.04	0.03	0.08	0.03	0.02	0.03	-0.01
21	1	0.01	0.04	-0.06	0.07	0.20	0.04	0.00	-0.02	-0.02
22	1	-0.02	0.04	-0.02	-0.03	0.08	0.04	0.00	-0.02	-0.03
23	1	0.02	0.07	-0.04	-0.04	0.10	0.00	-0.01	0.03	-0.03
24	1	0.01	0.01	0.01	0.19	0.09	-0.02	-0.02	-0.03	0.01
25	1	0.05	0.03	0.02	0.17	0.08	-0.02	-0.02	0.00	0.03
26	1	0.02	-0.02	0.13	-0.09	-0.09	0.20	-0.14	-0.07	-0.97
27	8	-0.15	-0.23	0.08	-0.15	0.05	-0.20	-0.01	0.00	-0.01
28	1	-0.01	-0.33	-0.03	-0.27	0.18	0.05	0.00	0.02	0.08
29	8	-0.05	-0.01	0.01	0.15	-0.16	0.08	0.00	-0.01	0.00
30	1	-0.10	0.41	-0.29	0.16	-0.16	0.19	0.00	0.04	-0.01
31	1	-0.26	-0.31	0.19	-0.13	0.11	-0.20	-0.03	-0.02	-0.01
32	1	0.45	-0.13	0.08	0.12	-0.12	0.13	0.05	-0.02	0.01

	13			14			15		
	?A			?A			?A		
Frequencies --	352.2206			396.1941			401.5173		
Red. masses --	3.9318			6.7061			1.2488		
Frc consts --	0.2874			0.6202			0.1186		
IR Inten --	7.3608			107.5126			214.6790		
Raman Activ --	1.8312			2.9719			1.7065		
Depolar --	0.7117			0.4966			0.6890		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.02	0.00	0.13	-0.08	0.01	-0.03	0.00	0.00	0.00
2 6	0.08	-0.02	0.08	-0.12	0.00	0.00	0.00	0.00	0.00
3 6	0.05	0.00	0.08	-0.04	-0.01	0.02	0.00	0.00	0.00
4 6	-0.01	-0.02	0.11	0.01	0.00	-0.04	0.00	0.00	0.01
5 6	0.01	-0.02	0.01	0.15	-0.07	-0.02	-0.01	0.00	0.00
6 6	0.06	-0.02	-0.03	-0.11	0.04	0.03	0.00	-0.01	0.01

7	6	-0.06	0.05	-0.06	-0.07	0.05	0.05	0.01	0.00	0.01
8	6	-0.06	0.07	0.08	-0.05	0.04	0.00	0.01	0.00	0.01
9	6	0.01	0.01	0.12	-0.13	0.09	0.01	0.01	-0.01	0.00
10	6	0.08	-0.04	0.08	-0.09	0.04	0.04	0.01	0.00	0.00
11	6	-0.12	0.11	-0.09	-0.05	0.03	0.03	0.00	0.01	-0.02
12	8	-0.01	-0.05	-0.19	0.22	-0.23	0.03	-0.02	0.01	0.00
13	6	-0.01	0.00	0.10	-0.05	0.11	-0.01	0.01	-0.01	0.00
14	7	0.02	-0.03	-0.06	0.05	0.10	-0.02	-0.01	0.00	0.00
15	8	0.01	-0.04	-0.18	0.37	-0.10	-0.04	-0.02	0.00	0.00
16	1	-0.03	0.04	0.19	-0.08	0.04	-0.09	0.01	-0.01	0.00
17	1	0.14	-0.02	0.11	-0.13	-0.01	-0.02	-0.01	0.00	0.00
18	1	0.05	0.00	0.09	-0.15	0.04	-0.04	0.01	0.00	0.01
19	1	-0.04	-0.05	0.13	-0.05	0.08	0.02	0.01	0.00	0.00
20	1	0.10	-0.06	-0.13	-0.11	0.04	0.04	0.00	0.00	0.03
21	1	-0.09	0.05	-0.14	-0.06	0.04	0.09	0.01	0.01	0.01
22	1	-0.12	0.17	0.10	0.00	0.03	0.01	0.01	-0.01	0.01
23	1	0.11	-0.11	0.09	-0.07	0.03	0.03	0.01	-0.01	0.01
24	1	-0.28	0.34	-0.08	-0.01	0.00	0.02	0.00	0.06	-0.02
25	1	-0.07	0.02	-0.34	-0.04	0.04	0.05	0.00	-0.01	-0.06
26	1	-0.05	-0.07	-0.33	-0.04	-0.36	0.02	0.00	0.02	0.00
27	8	-0.01	0.01	0.00	-0.11	0.03	-0.08	0.03	-0.01	-0.05
28	1	-0.05	-0.03	-0.22	-0.09	0.12	0.28	0.02	0.06	0.19
29	8	0.01	-0.01	0.00	0.00	-0.03	0.04	-0.01	0.05	0.09
30	1	0.02	-0.11	0.03	-0.04	0.15	-0.23	-0.03	-0.28	-0.67
31	1	0.03	0.05	-0.01	-0.18	0.01	-0.04	-0.02	0.05	0.12
32	1	-0.08	0.03	0.00	0.30	-0.19	-0.04	0.12	-0.38	-0.49
			16			17			18	
			?A			?A			?A	

Frequencies --	422.7973			443.4232			470.7800		
Red. masses --	1.4848			1.9109			1.8149		
Frc consts --	0.1564			0.2214			0.2370		
IR Inten --	144.3338			76.9391			122.1812		
Raman Activ --	0.7698			1.5700			3.6341		
Depolar --	0.5364			0.5387			0.7008		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.01	-0.01	0.02	-0.02	0.00	-0.02	0.00	0.03	0.00
2 6	0.00	-0.01	0.03	0.00	-0.01	-0.03	0.00	0.03	-0.01
3 6	-0.01	0.00	0.02	0.02	-0.02	0.00	-0.01	0.02	0.01
4 6	0.01	-0.01	0.03	0.00	0.01	-0.01	-0.02	0.03	0.00
5 6	-0.01	-0.01	0.02	-0.01	0.01	-0.01	-0.01	0.01	0.00
6 6	-0.01	-0.01	0.05	0.01	-0.04	-0.05	0.00	0.05	-0.02
7 6	0.02	-0.03	0.05	-0.02	0.02	-0.05	-0.01	0.07	-0.04
8 6	0.03	-0.03	0.02	-0.02	0.05	0.02	-0.03	0.04	-0.01
9 6	0.01	-0.01	-0.04	0.02	0.02	0.08	-0.01	-0.04	0.02
10 6	0.00	0.01	-0.01	0.05	-0.07	0.03	-0.01	0.01	0.02
11 6	-0.01	0.06	-0.09	0.01	-0.08	0.10	0.03	0.02	0.04
12 8	-0.02	0.01	0.00	-0.01	0.02	-0.02	-0.01	-0.03	-0.01
13 6	0.01	-0.01	-0.06	0.03	0.04	0.09	0.00	-0.08	0.01
14 7	-0.01	0.01	0.02	0.00	0.02	-0.06	-0.06	-0.08	0.00
15 8	-0.02	-0.01	-0.01	-0.05	0.01	-0.03	0.05	-0.01	-0.01
16 1	0.01	-0.01	0.01	-0.02	0.02	-0.02	0.01	0.01	0.00
17 1	-0.02	0.00	0.03	-0.01	-0.02	-0.04	0.02	0.02	-0.02
18 1	0.01	0.01	0.02	0.02	-0.04	0.00	-0.02	0.01	0.01
19 1	0.02	-0.01	0.02	0.00	0.03	-0.02	-0.04	0.04	0.01
20 1	0.00	0.02	0.07	0.01	-0.09	-0.11	0.00	0.02	-0.05
21 1	0.03	-0.04	0.08	-0.03	0.02	-0.07	-0.02	0.10	-0.06
22 1	0.03	-0.09	0.00	-0.01	0.12	0.05	-0.03	0.10	0.01
23 1	-0.01	0.04	-0.01	0.06	-0.14	0.07	-0.01	0.02	0.01

```
  24   1    -0.04   0.32  -0.10     0.04  -0.38   0.12     0.03  -0.10
0.05
  25   1    -0.05  -0.04  -0.33     0.05   0.04   0.38     0.06   0.07
0.15
  26   1     0.01   0.03   0.09     0.01   0.04  -0.03    -0.06  -0.05
0.01
  27   8     0.04   0.02  -0.06     0.03   0.05  -0.07     0.08  -0.10  -
0.02
  28   1     0.08   0.16   0.54     0.05   0.14   0.30     0.07   0.11
0.74
  29   8    -0.04  -0.03  -0.01    -0.04  -0.05   0.01     0.01   0.06  -
0.03
  30   1    -0.07   0.44   0.08    -0.09   0.43  -0.10     0.04  -0.20
0.21
  31   1    -0.07  -0.12  -0.11    -0.08  -0.05  -0.07     0.09  -0.16  -
0.13
  32   1     0.30   0.01   0.22     0.41  -0.10   0.17    -0.35   0.14  -
0.09
                     19                    20                    21
                     ?A                    ?A                    ?A
 Frequencies --   509.8955              545.8766              569.2250
 Red. masses --     2.5968                3.8407                4.0490
 Frc consts  --     0.3978                0.6743                0.7730
 IR Inten    --    16.9586                3.2825                2.9101
 Raman Activ --     5.6134                0.3154                0.9161
 Depolar     --     0.7498                0.3840                0.5969
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01  -0.02   0.00     0.00   0.13  -0.09     0.00   0.15  -
0.01
   2   6     0.01  -0.05  -0.01    -0.02  -0.06  -0.05     0.16   0.03  -
0.07
   3   6     0.03  -0.04   0.02    -0.01  -0.09   0.21    -0.05  -0.07  -
0.07
   4   6     0.05  -0.01   0.01     0.08   0.12   0.12     0.06   0.05  -
0.10
   5   6     0.04   0.01   0.00     0.02  -0.01   0.17    -0.07  -0.08  -
0.07
   6   6     0.02  -0.06   0.00    -0.01   0.00  -0.02     0.15   0.08
0.03
   7   6     0.01  -0.06   0.01     0.03   0.01   0.00     0.03  -0.09
0.01
   8   6     0.02  -0.03   0.02     0.05   0.01   0.00     0.11   0.01
0.04
   9   6     0.01   0.04   0.01    -0.05  -0.01  -0.06     0.01   0.02
0.06
  10   6     0.00  -0.03   0.03    -0.03  -0.01   0.02    -0.05   0.10
0.05
  11   6    -0.02  -0.05  -0.02     0.01   0.01   0.06    -0.20   0.00
0.04
  12   8     0.05   0.04  -0.01    -0.02   0.01  -0.05    -0.12   0.01
0.08
  13   6     0.05   0.12  -0.03    -0.04  -0.03  -0.21    -0.01  -0.01
0.05
```

```
  14   7     0.02   0.14  -0.03     0.02  -0.01   0.08     0.02  -0.03  -
0.01
  15   8    -0.09   0.04  -0.02    -0.03  -0.05  -0.14     0.05  -0.13  -
0.01
  16   1    -0.01   0.02   0.00    -0.03   0.20  -0.16    -0.08   0.29
0.17
  17   1     0.01  -0.06  -0.02     0.01  -0.21  -0.21     0.17  -0.06  -
0.15
  18   1     0.01  -0.07   0.02     0.08  -0.26   0.29    -0.14  -0.13  -
0.09
  19   1     0.04   0.00   0.01     0.03   0.36   0.21     0.16   0.03  -
0.18
  20   1     0.00  -0.06   0.03    -0.02   0.01   0.00     0.16   0.17
0.11
  21   1     0.00  -0.09  -0.02     0.03  -0.01   0.00    -0.04  -0.25  -
0.12
  22   1     0.04  -0.04   0.02    -0.01  -0.02  -0.02     0.22   0.04
0.07
  23   1     0.01  -0.06   0.04     0.08   0.01  -0.06    -0.17   0.17
0.10
  24   1    -0.02  -0.02  -0.02     0.11  -0.22   0.06    -0.18   0.00
0.04
  25   1    -0.05  -0.06  -0.03    -0.06   0.09   0.31    -0.37  -0.02
0.08
  26   1     0.11   0.07   0.03     0.06   0.05   0.16    -0.03   0.05
0.11
  27   8    -0.19  -0.05  -0.03     0.00   0.01   0.00    -0.04   0.00  -
0.04
  28   1    -0.14   0.11   0.61     0.00  -0.05  -0.20    -0.05   0.01
0.01
  29   8     0.07   0.02   0.01    -0.01   0.00   0.00     0.00  -0.01
0.01
  30   1     0.12  -0.37   0.22    -0.01   0.02  -0.03     0.00  -0.01
0.00
  31   1    -0.18  -0.12  -0.17     0.01   0.04   0.03    -0.04  -0.01  -
0.05
  32   1    -0.35   0.08  -0.11     0.03  -0.01   0.01     0.00   0.00
0.00
                     22                    23                    24
                     ?A                    ?A                    ?A
 Frequencies --   587.9513              621.7303              635.4651
 Red. masses --     6.8552                5.7767                6.0147
 Frc consts  --     1.3962                1.3156                1.4310
 IR Inten    --    66.1997               16.6345              126.7055
 Raman Activ --     0.1775                3.0717               29.1488
 Depolar     --     0.7452                0.7440                0.1480
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.01  -0.04     0.09  -0.02   0.15    -0.02   0.08
0.00
   2   6    -0.05   0.05   0.00    -0.11  -0.07   0.15    -0.04   0.06
0.04
   3   6     0.03   0.07  -0.02    -0.17   0.01   0.07     0.05   0.02
0.00
```

4	6	-0.08	0.04	0.07	0.24	-0.02	0.07	0.01	0.00	-0.08
5	6	-0.12	0.02	0.06	0.00	-0.04	0.01	0.09	-0.14	-0.05
6	6	-0.03	-0.05	0.00	-0.17	0.06	-0.09	-0.04	0.04	0.03
7	6	0.00	0.04	0.02	0.02	0.04	-0.16	-0.04	0.11	0.02
8	6	-0.03	0.03	0.03	0.21	0.11	-0.15	-0.04	0.04	-0.06
9	6	0.37	-0.03	-0.08	0.14	0.02	-0.05	0.00	-0.09	-0.01
10	6	0.10	-0.02	-0.08	-0.19	-0.04	-0.10	0.02	0.01	0.02
11	6	0.10	0.03	0.01	0.00	0.01	0.00	-0.01	0.12	0.05
12	8	-0.31	-0.08	0.01	-0.02	0.02	0.07	0.18	0.10	-0.03
13	6	0.15	-0.03	-0.04	-0.02	0.02	0.16	0.28	-0.19	-0.03
14	7	-0.03	0.03	0.00	0.01	-0.01	-0.05	-0.09	-0.12	0.03
15	8	0.20	-0.10	-0.02	-0.03	-0.04	-0.02	-0.15	-0.22	0.06
16	1	0.05	-0.08	-0.08	0.02	0.15	-0.03	-0.02	0.08	-0.04
17	1	-0.11	0.09	0.02	0.01	-0.10	0.17	-0.08	0.06	0.02
18	1	0.21	0.07	0.05	-0.13	0.17	0.05	-0.03	0.18	-0.08
19	1	-0.04	0.08	0.05	0.21	-0.19	0.05	-0.05	0.03	-0.03
20	1	-0.07	-0.12	-0.02	-0.06	0.16	-0.13	-0.02	0.00	-0.04
21	1	0.02	0.08	0.04	0.07	-0.14	0.03	-0.03	0.10	0.04
22	1	-0.12	-0.07	-0.03	0.11	0.21	-0.15	0.03	0.06	-0.04
23	1	0.10	-0.10	-0.02	-0.17	-0.17	-0.05	0.06	0.06	-0.03
24	1	0.15	-0.05	0.01	-0.27	-0.02	0.05	-0.01	0.12	0.05
25	1	0.11	0.06	0.09	0.18	0.03	-0.04	0.02	0.13	0.05
26	1	-0.40	-0.12	-0.02	0.08	0.07	0.22	0.52	0.27	-0.11
27	8	-0.21	0.08	0.01	-0.01	-0.02	-0.06	-0.16	0.12	0.01
28	1	-0.26	0.12	0.06	-0.02	-0.01	-0.05	-0.23	0.14	-0.02
29	8	0.05	-0.04	0.03	0.01	-0.01	0.01	0.01	-0.02	0.02
30	1	0.06	-0.09	0.05	0.01	-0.02	0.00	0.01	0.01	-0.02

31	1	-0.20	0.03	-0.04	-0.02	-0.02	-0.01	-0.11	0.12	-0.10
32	1	0.01	-0.04	0.02	0.00	-0.01	-0.01	0.08	-0.05	0.02

	25			26			27		
	?A			?A			?A		
Frequencies --	656.9817			665.2218			692.5623		
Red. masses --	4.9493			6.1620			5.9287		
Frc consts --	1.2586			1.6066			1.6754		
IR Inten --	5.4774			10.2563			9.0945		
Raman Activ --	3.0607			6.5024			6.3298		
Depolar --	0.7442			0.7179			0.4954		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.03	0.06	-0.10	0.05	0.03	-0.04	-0.04	-0.14	-0.13
2 6	-0.05	0.07	0.00	0.06	0.02	-0.05	-0.03	0.19	-0.09
3 6	0.14	0.06	0.06	-0.06	0.02	0.11	-0.02	0.18	0.13
4 6	-0.02	0.02	-0.01	-0.01	0.04	0.05	0.05	-0.08	0.06
5 6	0.00	-0.13	0.09	0.00	0.16	0.10	0.02	-0.05	0.09
6 6	-0.04	0.00	0.03	0.05	0.07	0.01	-0.10	0.18	-0.09
7 6	0.02	-0.05	0.11	0.09	-0.14	-0.01	-0.02	-0.09	-0.13
8 6	0.00	-0.03	-0.08	-0.03	-0.12	-0.11	0.02	-0.04	0.10
9 6	-0.07	0.06	-0.09	-0.19	-0.10	-0.03	0.09	0.03	0.11
10 6	0.11	0.02	-0.17	-0.11	0.03	-0.04	0.04	0.22	0.16
11 6	0.02	0.03	0.00	0.03	-0.08	-0.06	-0.01	-0.25	-0.18
12 8	-0.05	0.03	-0.04	0.01	-0.04	-0.01	0.01	0.02	-0.02
13 6	-0.13	0.13	0.29	0.28	-0.09	0.30	-0.02	-0.02	-0.03
14 7	0.07	0.02	-0.11	-0.12	-0.07	-0.08	0.01	-0.03	0.02
15 8	-0.05	-0.18	-0.01	0.08	0.14	-0.08	-0.03	-0.09	0.04
16 1	-0.02	0.04	-0.14	0.05	0.01	0.03	-0.06	-0.10	-0.10
17 1	-0.14	0.07	-0.03	0.12	-0.07	-0.12	0.16	0.20	-0.01
18 1	0.32	0.12	0.11	0.01	-0.14	0.18	-0.12	0.10	0.11
19 1	-0.09	0.20	0.08	-0.11	0.12	0.13	0.10	0.13	0.08
20 1	-0.10	0.02	0.13	0.03	0.20	0.17	-0.26	0.08	0.00

21	1	0.04	-0.07	0.17	0.09	-0.12	-0.02	0.01	-0.06	-0.08
22	1	0.03	-0.20	-0.12	-0.04	-0.16	-0.12	-0.07	0.15	0.13
23	1	0.22	0.07	-0.28	-0.03	0.17	-0.17	0.15	0.11	0.14
24	1	0.15	0.10	-0.02	0.06	0.02	-0.08	-0.02	-0.25	-0.18
25	1	-0.10	-0.01	-0.02	-0.12	-0.14	-0.13	0.04	-0.24	-0.19
26	1	0.18	0.15	-0.07	-0.23	-0.16	0.10	0.13	0.08	-0.03
27	8	0.04	-0.07	0.04	-0.08	0.09	0.00	0.00	0.00	-0.02
28	1	0.16	-0.10	0.13	-0.18	0.12	-0.03	0.00	0.01	0.01
29	8	0.00	0.02	-0.01	-0.01	-0.01	0.01	0.00	0.00	0.00
30	1	0.01	-0.05	0.04	-0.01	0.04	-0.04	0.00	0.03	-0.02
31	1	-0.02	-0.12	0.04	-0.01	0.13	-0.10	0.00	-0.03	-0.05
32	1	-0.09	0.04	-0.03	0.07	-0.03	0.01	0.03	-0.01	0.02

	28			29			30		
	?A			?A			?A		
Frequencies --	715.2907			823.9653			829.5155		
Red. masses --	4.9665			3.3446			6.0660		
Frc consts --	1.4972			1.3379			2.4593		
IR Inten --	49.1170			8.0906			3.5998		
Raman Activ --	3.0286			1.7340			19.2832		
Depolar --	0.7441			0.3585			0.0077		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.10	-0.08	-0.06	0.08	0.03	-0.05	-0.07	0.01	0.08
2 6	0.05	-0.15	-0.07	-0.03	-0.04	0.11	-0.06	0.11	-0.22
3 6	-0.06	-0.14	-0.07	0.04	0.06	-0.14	-0.01	0.03	-0.19
4 6	-0.09	0.03	0.09	0.09	0.10	0.11	0.03	-0.10	0.25
5 6	0.05	-0.02	0.05	-0.02	-0.02	0.01	-0.02	-0.01	0.03
6 6	0.02	0.15	0.07	0.08	-0.09	0.10	-0.02	0.03	-0.23
7 6	-0.11	0.05	0.10	-0.04	-0.04	-0.04	0.18	-0.03	0.00
8 6	-0.08	0.00	0.02	-0.09	0.10	0.14	0.04	-0.12	0.26
9 6	0.33	0.02	-0.09	-0.06	0.02	0.01	-0.06	0.02	0.04
10 6	-0.09	0.13	-0.05	-0.08	0.03	-0.13	-0.09	-0.04	-0.17

11	6	-0.05	0.00	0.02	0.00	-0.13	-0.11	0.00	0.17	0.12
12	8	0.13	0.00	-0.03	0.03	0.00	-0.01	0.07	0.01	-0.01
13	6	-0.02	0.01	0.12	0.02	-0.03	-0.01	0.02	-0.01	0.01
14	7	0.00	-0.01	-0.03	-0.01	-0.03	0.01	0.00	-0.01	0.00
15	8	-0.06	0.04	-0.03	0.00	-0.03	0.00	0.00	-0.03	0.02
16	1	-0.08	-0.12	-0.01	0.01	0.20	-0.09	-0.02	-0.10	0.01
17	1	0.15	-0.20	-0.09	-0.31	0.11	0.16	0.09	0.18	-0.11
18	1	-0.05	-0.28	-0.03	0.22	0.24	-0.12	0.11	-0.07	-0.12
19	1	-0.13	0.19	0.16	0.14	0.16	0.09	0.25	-0.07	0.12
20	1	0.12	0.29	0.09	0.24	0.11	0.12	-0.22	0.03	0.01
21	1	-0.12	0.07	0.05	-0.04	0.14	-0.12	0.12	-0.10	-0.11
22	1	-0.18	-0.21	-0.07	-0.21	0.16	0.13	-0.26	-0.12	0.20
23	1	-0.29	0.20	0.06	-0.32	0.16	-0.05	-0.17	-0.20	-0.05
24	1	0.13	-0.01	-0.01	0.01	-0.27	-0.10	-0.05	0.16	0.13
25	1	-0.05	0.01	0.05	-0.01	-0.07	0.05	-0.05	0.15	0.11
26	1	0.15	0.01	-0.01	0.05	0.01	0.00	0.05	-0.01	-0.02
27	8	0.05	0.00	-0.01	0.00	0.01	0.00	-0.01	0.00	-0.01
28	1	0.02	0.03	-0.01	0.04	-0.01	0.00	-0.02	0.00	0.02
29	8	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	1	0.01	0.00	0.01	0.00	-0.01	0.00	0.00	0.00	0.00
31	1	0.03	-0.04	0.04	-0.01	-0.01	-0.02	-0.01	0.04	0.04
32	1	0.01	0.00	0.02	-0.01	0.00	0.00	0.00	0.00	0.00

	31	32	33
	?A	?A	?A
Frequencies --	847.9042	886.0196	895.4016
Red. masses --	3.6515	3.2108	2.2251
Frc consts --	1.5467	1.4851	1.0511
IR Inten --	4.0794	4.0519	17.9026
Raman Activ --	1.5058	13.5425	1.6760
Depolar --	0.1065	0.0411	0.3557

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z

1	6	0.11	0.12	0.04	0.17	0.11	0.09	-0.04	0.05	-0.06
2	6	-0.03	0.13	-0.03	0.16	0.07	-0.09	0.04	-0.04	0.11
3	6	-0.11	0.02	0.00	-0.05	-0.02	-0.02	-0.07	0.10	0.07
4	6	-0.12	0.01	0.04	0.05	0.05	0.01	-0.06	0.05	-0.04
5	6	0.01	-0.03	0.02	-0.02	-0.01	-0.03	-0.01	-0.02	-0.05
6	6	0.07	-0.12	0.09	-0.19	0.00	-0.04	0.05	0.08	-0.08
7	6	0.13	-0.08	-0.14	-0.11	0.00	0.12	0.01	-0.04	0.02
8	6	-0.11	-0.05	-0.10	-0.11	0.01	0.03	-0.03	-0.09	0.06
9	6	0.11	-0.03	-0.04	0.01	0.00	-0.02	0.03	-0.02	0.04
10	6	-0.08	-0.03	0.12	0.02	-0.06	-0.05	-0.05	-0.11	-0.03
11	6	0.04	0.03	0.00	0.03	-0.11	-0.04	0.04	0.01	-0.02
12	8	0.06	0.00	-0.01	0.02	0.00	0.01	0.02	0.00	0.00
13	6	-0.06	0.06	0.01	0.00	0.00	-0.01	-0.01	0.02	-0.02
14	7	0.03	0.06	-0.01	0.00	0.00	0.00	0.01	0.03	0.00
15	8	-0.02	-0.07	0.01	0.00	-0.02	0.00	0.00	-0.02	0.01
16	1	0.17	-0.01	0.13	0.08	0.29	0.37	-0.02	0.00	-0.07
17	1	-0.26	0.15	-0.10	0.26	-0.07	-0.21	0.21	-0.19	0.02
18	1	-0.27	-0.04	-0.04	-0.10	-0.09	-0.02	-0.11	0.47	-0.04
19	1	-0.30	-0.01	0.16	0.01	-0.11	0.00	-0.01	0.15	-0.05
20	1	-0.08	-0.24	0.16	-0.29	-0.12	-0.05	0.23	0.31	-0.06
21	1	0.09	-0.01	-0.27	0.01	0.24	0.34	0.00	0.05	-0.03
22	1	-0.26	-0.04	-0.14	-0.08	-0.10	0.00	0.01	-0.15	0.05
23	1	-0.22	0.06	0.18	0.12	-0.22	-0.04	0.06	-0.41	0.04
24	1	-0.12	-0.01	0.02	0.01	0.01	-0.04	0.19	-0.01	-0.04
25	1	-0.10	0.01	0.03	-0.03	-0.15	-0.11	-0.07	0.01	0.03
26	1	0.09	0.01	-0.01	0.02	0.00	0.01	0.02	0.00	0.00
27	8	0.04	0.00	-0.01	0.01	0.00	0.00	0.01	-0.02	-0.01

28	1	-0.06	0.05	0.00	-0.03	0.02	0.03	-0.17	0.08	0.04
29	8	0.00	-0.01	0.00	0.00	0.00	-0.01	0.00	-0.01	-0.01
30	1	0.00	0.03	0.00	0.00	0.01	0.01	0.00	0.02	0.03
31	1	0.05	0.09	0.17	0.01	0.07	0.14	0.08	0.19	0.25
32	1	0.02	0.00	0.02	0.00	0.01	0.01	0.00	0.02	0.04

	34	35	36
	?A	?A	?A
Frequencies --	901.9626	926.6470	939.1968
Red. masses --	1.2045	2.4134	2.0393
Frc consts --	0.5773	1.2210	1.0598
IR Inten --	247.0834	60.5501	4.8633
Raman Activ --	0.9872	1.3842	4.3490
Depolar --	0.3820	0.5379	0.6124

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	0.02	0.00	-0.01	-0.07	0.04	-0.06	-0.05	0.03
2	6	0.01	0.00	0.00	0.02	0.03	-0.01	0.07	0.10	0.05
3	6	-0.03	0.02	0.01	0.05	-0.01	-0.05	-0.03	-0.01	-0.05
4	6	-0.05	0.01	0.00	-0.15	0.07	-0.03	0.00	0.11	-0.01
5	6	-0.01	0.00	0.00	-0.01	0.00	0.07	0.01	0.00	0.05
6	6	0.00	0.03	0.00	-0.04	0.03	0.00	0.04	-0.08	-0.08
7	6	0.02	-0.04	0.01	0.08	-0.07	0.04	-0.09	0.02	0.03
8	6	-0.01	0.03	0.00	0.08	0.17	-0.05	0.07	-0.07	-0.01
9	6	0.02	0.02	0.02	0.00	0.02	0.07	-0.02	-0.01	-0.01
10	6	-0.01	-0.05	-0.02	-0.05	-0.05	-0.06	-0.08	0.00	0.04
11	6	0.01	0.00	0.01	-0.01	-0.06	0.02	0.07	-0.01	-0.01
12	8	0.02	0.00	0.00	0.03	0.00	-0.03	0.00	0.00	0.00
13	6	-0.02	0.00	-0.02	0.01	-0.02	-0.05	-0.01	0.01	0.02
14	7	0.00	-0.01	0.01	0.00	-0.01	0.02	0.00	0.01	-0.01
15	8	0.00	-0.01	0.00	0.00	-0.02	-0.01	0.00	-0.03	-0.01
16	1	0.05	-0.04	0.02	0.05	-0.23	0.16	-0.05	-0.08	0.13
17	1	0.03	-0.06	-0.05	0.06	0.10	0.08	0.11	0.29	0.27

18	1	-0.04	0.08	-0.01	0.21	-0.07	0.03	-0.06	-0.12	-0.03
19	1	-0.07	0.00	0.01	-0.29	0.22	0.09	-0.01	0.38	0.05
20	1	0.00	0.12	0.09	-0.08	0.15	0.18	0.08	-0.26	-0.34
21	1	0.00	-0.11	-0.02	0.11	-0.20	0.18	-0.09	0.01	0.04
22	1	-0.04	0.06	0.00	0.23	0.38	0.04	0.24	-0.24	-0.03
23	1	0.06	-0.18	-0.01	-0.12	-0.18	0.05	-0.24	0.08	0.10
24	1	0.02	0.03	0.00	-0.05	0.10	0.02	0.13	0.03	-0.02
25	1	-0.05	-0.02	-0.01	-0.06	-0.14	-0.13	0.25	0.01	-0.06
26	1	0.00	-0.01	0.00	0.00	-0.02	-0.02	0.03	0.02	0.01
27	8	0.00	0.03	0.03	-0.01	-0.02	-0.02	0.00	0.01	0.00
28	1	0.25	-0.12	-0.13	-0.12	0.05	0.04	0.06	-0.03	-0.05
29	8	0.00	0.02	0.03	0.00	-0.01	-0.01	0.00	0.00	0.01
30	1	0.00	-0.03	-0.07	0.00	0.01	0.03	0.00	-0.01	-0.02
31	1	-0.05	-0.44	-0.76	0.02	0.18	0.29	0.00	-0.11	-0.22
32	1	0.02	-0.05	-0.07	-0.01	0.02	0.03	0.01	-0.02	-0.03

	37			38			39		
	?A			?A			?A		
Frequencies --	979.5182			1005.9099			1012.7043		
Red. masses --	2.2655			2.6416			2.5774		
Frc consts --	1.2807			1.5749			1.5574		
IR Inten --	9.2861			7.3317			12.0662		
Raman Activ --	4.9754			5.8801			4.7543		
Depolar --	0.5112			0.1479			0.1366		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	-0.01	0.01	0.13	0.01	-0.07	0.17	-0.08	-0.08
2 6	-0.12	0.09	-0.04	0.07	-0.01	-0.05	0.00	0.05	0.02
3 6	0.03	-0.05	-0.03	0.14	0.10	-0.01	-0.09	-0.02	0.04
4 6	0.10	-0.01	-0.02	-0.02	-0.11	0.01	0.03	0.04	-0.03
5 6	0.04	0.00	0.05	0.03	-0.02	0.07	-0.05	0.01	0.01
6 6	0.10	0.14	0.00	-0.05	0.01	0.04	0.01	-0.02	-0.03
7 6	-0.05	0.04	0.03	-0.13	0.03	0.00	-0.15	-0.13	-0.02

```
    8   6    -0.07  -0.03  -0.05     0.05  -0.06  -0.04    -0.04   0.04
0.06
    9   6     0.01  -0.02   0.03     0.00  -0.04   0.06     0.00   0.00
0.00
   10   6    -0.01  -0.12   0.02    -0.13  -0.03   0.03     0.05   0.04  -
0.05
   11   6     0.00  -0.07   0.05    -0.06   0.08  -0.02     0.00   0.10
0.12
   12   8    -0.04   0.00   0.00    -0.03  -0.01  -0.01     0.04   0.01
0.00
   13   6    -0.01   0.01  -0.02    -0.01   0.02  -0.01     0.01   0.00
0.00
   14   7     0.01   0.02   0.00     0.01   0.03   0.00     0.00   0.00
0.00
   15   8     0.00   0.00  -0.01     0.00   0.03   0.00     0.00   0.00
0.00
   16   1    -0.02   0.12  -0.04     0.19  -0.12  -0.03     0.34  -0.39  -
0.31
   17   1    -0.36   0.26   0.04    -0.04  -0.06  -0.16    -0.06   0.07
0.03
   18   1     0.08  -0.28   0.05     0.38   0.19   0.06    -0.11  -0.15
0.07
   19   1     0.03   0.00   0.03    -0.12  -0.20   0.07     0.08   0.08  -
0.06
   20   1     0.29   0.34  -0.03     0.04   0.03  -0.06     0.06  -0.01  -
0.08
   21   1    -0.07   0.14  -0.06    -0.13  -0.09   0.06    -0.26  -0.36  -
0.18
   22   1    -0.04  -0.06  -0.05     0.19  -0.08  -0.02     0.00   0.06
0.08
   23   1     0.00  -0.29   0.09    -0.37  -0.03   0.19     0.18   0.02  -
0.12
   24   1    -0.08   0.29   0.03    -0.04  -0.16   0.00    -0.08   0.26
0.12
   25   1     0.01  -0.19  -0.29    -0.07   0.18   0.25    -0.04   0.04  -
0.03
   26   1     0.04   0.04   0.00     0.05   0.04  -0.02    -0.07  -0.05
0.03
   27   8     0.01  -0.01   0.01     0.01  -0.01   0.00     0.00   0.00
0.00
   28   1    -0.14   0.05  -0.01    -0.24   0.08  -0.04     0.00   0.01
0.02
   29   8     0.00   0.00   0.00    -0.01   0.00   0.01     0.00   0.00
0.00
   30   1    -0.01   0.01  -0.01    -0.01   0.03  -0.03     0.00   0.00
0.02
   31   1     0.11   0.03  -0.08     0.18   0.04  -0.18    -0.03   0.06
0.15
   32   1     0.01   0.00   0.01     0.04  -0.02   0.00    -0.01   0.01
0.01
                     40                    41                    42
                     ?A                    ?A                    ?A
 Frequencies --  1018.3235             1024.6478             1032.1390
 Red. masses --     2.5846                2.4603                3.2044
```

Frc consts --		1.5791			1.5219			2.0113		
IR Inten --		29.6680			5.8540			10.2595		
Raman Activ --		1.6696			2.9737			2.1371		
Depolar --		0.7430			0.6297			0.4981		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	0.08	0.07	-0.02	-0.09	-0.01	0.01	-0.05	-0.06
2	6	-0.08	0.03	0.03	0.07	0.08	-0.05	-0.01	0.03	-0.10
3	6	0.04	-0.08	0.11	-0.10	0.02	0.01	-0.08	0.14	0.10
4	6	-0.09	-0.03	-0.14	0.01	0.00	0.02	0.01	-0.11	0.00
5	6	-0.09	0.04	0.02	-0.02	0.00	0.01	-0.06	0.03	0.04
6	6	0.00	-0.01	-0.03	0.02	0.02	0.17	0.17	-0.10	-0.04
7	6	-0.02	0.03	-0.05	-0.02	0.10	-0.04	0.00	0.10	0.14
8	6	0.04	-0.06	0.13	0.09	0.00	0.04	0.03	0.11	-0.01
9	6	0.05	0.02	0.03	-0.03	-0.04	-0.06	0.02	0.07	-0.07
10	6	-0.05	0.06	-0.09	0.05	-0.13	-0.06	-0.07	-0.06	-0.01
11	6	0.04	-0.03	-0.05	-0.08	0.03	-0.08	-0.09	-0.08	0.04
12	8	0.08	0.02	-0.02	0.03	0.00	0.00	0.06	0.01	-0.01
13	6	0.00	0.00	0.01	0.00	0.02	0.01	0.01	-0.03	0.01
14	7	0.00	0.00	0.00	0.01	0.03	-0.01	-0.01	-0.04	0.00
15	8	0.00	-0.02	-0.01	0.00	-0.02	0.00	0.00	-0.02	0.01
16	1	0.03	0.04	0.22	0.01	-0.18	0.19	-0.02	-0.01	0.02
17	1	-0.30	-0.04	-0.13	0.03	0.16	0.03	-0.07	-0.09	-0.25
18	1	0.33	-0.24	0.27	-0.17	-0.13	0.02	-0.01	0.22	0.12
19	1	0.04	-0.19	-0.28	0.12	0.16	-0.02	0.01	-0.18	-0.02
20	1	0.09	0.14	0.03	-0.07	0.13	0.40	0.21	-0.28	-0.27
21	1	-0.01	0.19	-0.11	-0.06	0.15	-0.16	-0.01	0.16	0.08
22	1	0.28	-0.14	0.16	0.13	-0.11	0.02	0.10	-0.03	-0.05
23	1	-0.05	0.06	-0.08	0.28	-0.17	-0.20	-0.13	0.02	0.00
24	1	-0.13	-0.10	-0.02	-0.16	-0.34	-0.04	-0.03	0.12	0.02

```
  25   1     0.19   0.01  -0.02     0.16   0.19   0.21    -0.17  -0.15  -
0.11
  26   1    -0.20  -0.13   0.03    -0.03  -0.03   0.02    -0.13  -0.09
0.04
  27   8     0.00   0.00  -0.01    -0.01  -0.01   0.01    -0.01   0.03  -
0.02
  28   1     0.00   0.00  -0.01    -0.10   0.03   0.00     0.37  -0.12
0.01
  29   8     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.00  -
0.01
  30   1     0.00   0.00  -0.01     0.00   0.01   0.00     0.02  -0.05
0.04
  31   1     0.00  -0.03  -0.04     0.05   0.04  -0.01    -0.25  -0.07
0.21
  32   1     0.00   0.00   0.00     0.01   0.01   0.02    -0.05   0.02  -
0.01
                     43                    44                    45
                     ?A                    ?A                    ?A
 Frequencies --  1037.6615             1055.4519             1068.8056
 Red. masses --     1.7750                1.7164                1.7077
 Frc consts  --     1.1261                1.1265                1.1494
 IR Inten    --    18.9828               13.9579               26.5787
 Raman Activ --     4.2087                3.7228                8.6334
 Depolar     --     0.5499                0.4690                0.5757
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.06  -0.07     0.09   0.01   0.04    -0.07   0.00  -
0.03
   2   6     0.02   0.07   0.09    -0.05  -0.06  -0.01     0.07   0.06
0.02
   3   6    -0.03  -0.08  -0.03     0.01   0.01  -0.06     0.06  -0.02
0.04
   4   6    -0.04  -0.10   0.07    -0.06   0.05   0.04     0.07  -0.04  -
0.06
   5   6    -0.04   0.02   0.00     0.04   0.02   0.00     0.02   0.01
0.00
   6   6     0.00   0.03  -0.04    -0.02   0.06   0.00    -0.03   0.00
0.05
   7   6    -0.01  -0.02   0.05    -0.03   0.01  -0.03    -0.02  -0.04  -
0.04
   8   6     0.04   0.02  -0.03     0.06  -0.09  -0.01    -0.07   0.00  -
0.01
   9   6     0.00   0.02   0.01    -0.03   0.07   0.01     0.02   0.05  -
0.01
  10   6     0.03  -0.01   0.01     0.05   0.00   0.05    -0.08  -0.06
0.00
  11   6    -0.01   0.03  -0.09    -0.01   0.00  -0.03     0.03   0.05
0.01
  12   8     0.04   0.01  -0.01    -0.02   0.00   0.00    -0.02   0.00
0.00
  13   6     0.00  -0.01  -0.01     0.01  -0.02   0.01     0.01  -0.02
0.00
  14   7     0.00  -0.01   0.00    -0.01  -0.04   0.00    -0.01  -0.03
0.00
```

15	8	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.02	0.00
16	1	-0.02	0.13	-0.14	0.15	-0.11	0.05	-0.11	0.08	0.00
17	1	-0.09	0.30	0.31	-0.19	-0.07	-0.08	0.20	0.10	0.10
18	1	-0.09	-0.30	0.00	-0.08	0.07	-0.12	0.19	-0.10	0.11
19	1	-0.09	-0.33	0.06	-0.15	0.11	0.12	0.13	-0.06	-0.11
20	1	0.18	0.08	-0.20	0.10	0.16	-0.05	-0.18	0.05	0.30
21	1	0.06	-0.14	0.27	0.00	0.05	0.02	-0.10	-0.13	-0.20
22	1	-0.03	0.07	-0.04	0.18	-0.23	-0.02	-0.16	0.01	-0.02
23	1	0.08	-0.11	0.02	0.05	-0.14	0.12	-0.19	-0.18	0.13
24	1	0.26	-0.25	-0.11	-0.16	-0.11	0.00	0.16	0.03	-0.01
25	1	-0.22	0.11	0.25	0.02	0.04	0.06	0.13	0.07	0.01
26	1	-0.10	-0.07	0.02	0.03	0.02	-0.01	0.01	0.01	0.00
27	8	-0.01	0.00	0.00	-0.03	0.03	-0.02	0.00	0.04	-0.02
28	1	0.05	-0.02	0.01	0.52	-0.18	0.05	0.46	-0.14	0.02
29	8	0.00	0.00	0.00	0.01	0.01	-0.01	0.01	0.01	-0.01
30	1	0.00	-0.02	0.02	0.02	-0.07	0.06	0.02	-0.04	0.05
31	1	-0.05	0.01	0.06	-0.37	-0.07	0.32	-0.31	-0.06	0.28
32	1	-0.02	0.01	-0.01	-0.07	0.04	0.00	-0.05	0.04	0.01

	46			47			48		
	?A			?A			?A		
Frequencies --	1074.0477			1100.0117			1162.1197		
Red. masses --	1.8553			2.7660			1.6986		
Frc consts --	1.2610			1.9720			1.3516		
IR Inten --	11.2129			142.7601			10.6147		
Raman Activ --	5.4932			10.9820			1.7952		
Depolar --	0.7439			0.6539			0.6762		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.06	-0.03	-0.06	0.01	0.03	0.02	0.00	0.06	-0.06
2 6	0.02	0.03	0.09	-0.02	0.07	-0.01	0.02	0.01	0.04
3 6	0.02	-0.05	0.02	-0.05	-0.04	0.08	-0.08	-0.02	-0.05
4 6	0.00	0.02	-0.07	-0.06	-0.07	-0.03	-0.03	-0.06	0.02

5	6	0.02	-0.02	0.01	0.19	-0.13	-0.02	-0.01	-0.03	0.07
6	6	-0.05	-0.02	-0.04	0.04	-0.06	-0.04	0.00	0.00	0.03
7	6	0.13	0.07	0.01	-0.02	-0.03	0.03	-0.03	0.04	-0.05
8	6	-0.05	-0.04	0.04	0.02	0.06	0.09	0.04	-0.03	-0.01
9	6	0.02	0.02	-0.02	0.01	0.03	-0.01	0.00	-0.02	0.07
10	6	-0.04	0.00	-0.01	-0.04	0.03	-0.08	0.07	0.00	-0.07
11	6	-0.11	-0.02	0.02	0.01	0.01	-0.04	0.02	-0.05	0.07
12	8	-0.02	-0.01	0.00	-0.11	-0.06	0.02	0.01	-0.01	0.00
13	6	0.01	-0.01	0.01	0.03	-0.02	0.00	0.00	0.00	-0.02
14	7	0.00	-0.01	0.00	-0.01	-0.02	0.00	0.00	0.01	0.00
15	8	0.00	0.04	-0.01	0.01	0.13	-0.01	0.01	0.04	-0.01
16	1	0.18	-0.27	-0.27	0.01	0.00	0.24	-0.10	0.30	-0.31
17	1	0.15	0.14	0.25	-0.23	0.04	-0.13	0.26	-0.03	0.10
18	1	0.05	-0.09	0.04	-0.28	0.01	-0.03	0.04	0.09	-0.03
19	1	0.06	0.17	-0.07	-0.17	0.03	0.07	-0.29	-0.16	0.17
20	1	-0.11	-0.07	-0.03	0.10	0.07	0.02	-0.21	-0.14	0.14
21	1	0.23	0.40	0.12	-0.04	-0.05	-0.02	-0.10	0.22	-0.30
22	1	-0.06	-0.12	0.01	0.10	0.07	0.11	0.38	-0.02	0.07
23	1	-0.06	-0.04	0.03	0.11	0.01	-0.18	-0.10	0.09	-0.01
24	1	-0.38	-0.05	0.06	0.08	-0.10	-0.04	0.01	0.22	0.05
25	1	-0.38	-0.06	0.06	0.04	0.06	0.08	-0.02	-0.15	-0.18
26	1	0.08	0.04	-0.01	0.62	0.32	-0.11	0.08	0.03	0.00
27	8	0.00	0.01	0.00	0.00	0.00	0.00	-0.01	0.01	0.00
28	1	0.06	-0.02	-0.01	0.00	0.00	0.00	0.06	-0.02	0.00
29	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	1	0.00	0.00	-0.01	0.00	-0.01	0.01	0.00	0.00	0.00
31	1	-0.02	-0.05	-0.06	0.00	0.00	0.02	-0.05	-0.02	0.02

```
  32   1     0.00  -0.01  -0.01     0.00   0.00   0.00     0.00   0.00
0.01
                     49                     50                     51
                     ?A                     ?A                     ?A
 Frequencies --  1197.3782              1200.7340              1224.3410
 Red. masses --     1.8626                 4.4187                 2.6032
 Frc consts  --     1.5734                 3.7535                 2.2992
 IR Inten    --    73.0106                21.0503                31.0104
 Raman Activ --     1.3231                 2.2857                 3.3967
 Depolar     --     0.2848                 0.4584                 0.6716
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.02  -0.03   0.03    -0.04  -0.06   0.03    -0.03   0.04  -
0.08
   2   6    -0.03  -0.02  -0.02     0.03  -0.03  -0.02     0.10   0.01
0.03
   3   6     0.03   0.01   0.01    -0.20   0.05  -0.03    -0.01  -0.02
0.00
   4   6     0.03   0.02   0.00     0.16  -0.03  -0.12    -0.02  -0.10  -
0.01
   5   6     0.12   0.11  -0.03     0.01   0.01   0.15     0.20   0.14
0.00
   6   6     0.04  -0.06  -0.05     0.00  -0.08   0.00    -0.08  -0.05
0.05
   7   6     0.00  -0.03   0.05     0.07  -0.01   0.04    -0.01   0.04  -
0.07
   8   6    -0.05   0.04  -0.01    -0.17  -0.09  -0.13     0.03  -0.03
0.04
   9   6     0.01   0.08   0.02     0.04   0.07   0.24     0.00  -0.05
0.02
  10   6    -0.06   0.05   0.00     0.13   0.10  -0.14    -0.03   0.01  -
0.05
  11   6    -0.01   0.02  -0.03    -0.04   0.10  -0.05     0.02  -0.02
0.08
  12   8    -0.03   0.02   0.00     0.01   0.00   0.00    -0.04   0.03
0.00
  13   6    -0.01  -0.01   0.00     0.00  -0.02  -0.05    -0.02   0.02
0.00
  14   7     0.00  -0.03   0.01     0.00  -0.02   0.02     0.01   0.02
0.00
  15   8    -0.03  -0.08   0.01     0.00   0.00  -0.02    -0.04  -0.08
0.01
  16   1     0.00   0.03  -0.19    -0.07  -0.04   0.38     0.00  -0.04
0.12
  17   1     0.16   0.07   0.16    -0.22   0.00  -0.08    -0.23   0.00  -
0.11
  18   1    -0.19  -0.06  -0.06     0.26   0.04   0.15    -0.20   0.01  -
0.09
  19   1    -0.25  -0.23   0.14    -0.14   0.19   0.12     0.02   0.23
0.04
  20   1    -0.16   0.07   0.34     0.20   0.08  -0.07     0.28   0.15  -
0.19
  21   1    -0.10   0.15  -0.26     0.15  -0.02   0.26     0.07   0.06
0.14
```

```
  22   1     0.36  -0.27  -0.02     0.05   0.04  -0.05    -0.17   0.35
0.12
  23   1     0.18  -0.14  -0.07    -0.15  -0.05   0.13     0.05   0.07  -
0.14
  24   1     0.03  -0.10  -0.02    -0.01  -0.19  -0.03    -0.03   0.22
0.07
  25   1    -0.03   0.06   0.10     0.06   0.22   0.21    -0.06  -0.12  -
0.14
  26   1    -0.25  -0.10   0.04    -0.02  -0.01   0.05    -0.42  -0.17
0.07
  27   8     0.01  -0.01   0.00     0.00  -0.01   0.00     0.00   0.01  -
0.01
  28   1    -0.17   0.06  -0.01     0.00   0.00   0.03     0.09  -0.03
0.00
  29   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  30   1    -0.01   0.03  -0.02     0.00  -0.01   0.01     0.00  -0.02
0.01
  31   1     0.12   0.03  -0.06     0.01   0.01  -0.01    -0.05  -0.02
0.03
  32   1     0.02   0.00   0.02     0.00   0.00  -0.01    -0.01   0.00  -
0.01
                     52                    53                    54
                     ?A                    ?A                    ?A
 Frequencies --  1233.8714             1254.4586             1263.0122
 Red. masses --     2.0428                2.5318                1.2190
 Frc consts  --     1.8324                2.3474                1.1457
 IR Inten    --     8.5051               14.6431                8.3799
 Raman Activ --     2.7268                1.5932               13.8740
 Depolar     --     0.6720                0.7497                0.7309
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.02   0.01  -0.05     0.02   0.01   0.03    -0.01  -0.01
0.03
   2   6     0.10  -0.05   0.00    -0.01  -0.09  -0.03     0.00  -0.06  -
0.02
   3   6     0.05   0.07  -0.03    -0.02   0.09  -0.07    -0.01   0.06  -
0.01
   4   6    -0.01  -0.02   0.01    -0.03  -0.01  -0.13     0.02   0.02  -
0.01
   5   6    -0.11  -0.07   0.03     0.04   0.03   0.22    -0.01   0.00
0.04
   6   6    -0.07  -0.11   0.01     0.00   0.03  -0.01    -0.04   0.01
0.00
   7   6     0.02   0.03  -0.03     0.03  -0.04   0.01     0.00  -0.01  -
0.02
   8   6     0.02  -0.01  -0.03    -0.06   0.02   0.10     0.00   0.00
0.00
   9   6     0.00   0.10   0.00    -0.01  -0.06  -0.12     0.00  -0.06  -
0.01
  10   6    -0.06   0.09   0.04     0.01  -0.03   0.05    -0.01   0.01
0.02
  11   6     0.00  -0.01   0.07    -0.01   0.03  -0.01     0.01   0.01
0.01
```

```
  12   8     0.03   0.00  -0.01    -0.01  -0.01  -0.02     0.00  -0.01
0.00
  13   6     0.02  -0.02   0.00    -0.01   0.01   0.02    -0.01   0.01
0.00
  14   7    -0.01  -0.03   0.01     0.01   0.02  -0.01     0.01   0.02
0.00
  15   8     0.02   0.04   0.00     0.00  -0.02  -0.02     0.00  -0.01
0.00
  16   1    -0.11   0.20   0.00    -0.12   0.34  -0.19     0.05  -0.15
0.25
  17   1    -0.31   0.14   0.04     0.18   0.12   0.27    -0.11   0.13
0.14
  18   1    -0.22  -0.19  -0.06    -0.25  -0.08  -0.11     0.01  -0.15
0.05
  19   1     0.01   0.06   0.01     0.02  -0.26  -0.23     0.10  -0.12  -
0.10
  20   1     0.21   0.28   0.08     0.10   0.05  -0.12     0.01   0.02  -
0.05
  21   1     0.00   0.02  -0.07     0.07  -0.22   0.19    -0.05   0.27  -
0.26
  22   1    -0.04  -0.18  -0.10     0.09   0.13   0.17     0.18   0.12
0.07
  23   1     0.42  -0.43  -0.02     0.03   0.04   0.01     0.10   0.03  -
0.08
  24   1    -0.08   0.16   0.07    -0.26  -0.10   0.04     0.49   0.10  -
0.07
  25   1     0.15  -0.05  -0.13     0.31   0.11   0.02    -0.52  -0.08
0.09
  26   1     0.07   0.02  -0.02     0.09   0.04   0.00     0.14   0.06  -
0.02
  27   8     0.00  -0.01   0.00     0.01   0.01   0.00     0.00   0.01
0.00
  28   1    -0.11   0.03   0.00     0.06  -0.01   0.00     0.09  -0.03  -
0.01
  29   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  30   1     0.00   0.00   0.00     0.00  -0.01   0.01     0.00  -0.01
0.00
  31   1     0.07   0.03  -0.03    -0.04  -0.01   0.03    -0.06  -0.02
0.03
  32   1     0.01   0.00   0.01    -0.01   0.00  -0.01     0.00   0.01
0.00
                     55                    56                    57
                     ?A                    ?A                    ?A
 Frequencies --  1276.8234             1311.3100             1319.8172
 Red. masses --     1.6748                1.6956                1.9780
 Frc consts  --     1.6087                1.7178                2.0300
 IR Inten    --    13.0878                4.2408               89.7525
 Raman Activ --     4.9777                0.7727                2.2181
 Depolar     --     0.6004                0.6456                0.3658
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.05   0.00  -0.04     0.10  -0.08  -0.04     0.01   0.02
0.00
```

2	6	-0.03	0.01	0.07	-0.01	-0.04	0.00	0.02	-0.06	-0.02
3	6	0.00	-0.07	-0.05	0.00	0.02	0.03	-0.07	0.06	0.02
4	6	0.00	-0.06	-0.04	-0.02	0.02	-0.01	-0.07	0.04	-0.01
5	6	0.02	-0.01	0.11	0.00	0.00	-0.10	0.08	0.08	-0.03
6	6	-0.01	0.04	-0.03	-0.02	0.03	-0.02	0.00	0.03	0.08
7	6	0.03	0.03	0.00	0.08	0.07	0.03	0.00	0.03	-0.04
8	6	0.01	0.02	0.03	-0.03	-0.04	0.03	0.05	-0.03	0.02
9	6	-0.02	0.09	-0.07	0.01	-0.07	0.02	-0.02	0.16	0.01
10	6	0.04	0.00	0.03	-0.04	0.00	0.00	0.03	-0.03	-0.05
11	6	-0.04	-0.01	0.00	-0.09	0.00	0.01	0.01	-0.04	0.01
12	8	0.00	0.02	-0.01	0.00	0.00	0.01	-0.02	-0.03	0.01
13	6	0.02	-0.02	0.01	-0.01	0.01	0.00	0.01	-0.02	-0.01
14	7	-0.01	-0.03	0.00	0.01	0.02	0.00	-0.01	-0.05	0.01
15	8	-0.01	0.02	-0.01	0.00	0.00	0.01	-0.01	-0.04	0.01
16	1	0.01	0.02	0.43	-0.16	0.46	0.19	0.03	-0.02	-0.11
17	1	-0.12	-0.09	-0.07	-0.10	0.14	0.17	0.02	0.10	0.16
18	1	-0.11	0.31	-0.19	0.21	-0.11	0.14	0.23	-0.28	0.23
19	1	0.12	0.19	-0.07	-0.29	0.18	0.20	0.12	-0.22	-0.20
20	1	-0.23	-0.17	0.02	-0.10	-0.15	-0.11	-0.02	-0.29	-0.24
21	1	-0.11	-0.17	-0.29	-0.06	-0.35	-0.17	-0.04	-0.23	-0.04
22	1	-0.09	-0.15	-0.05	0.01	0.05	0.07	-0.33	-0.18	-0.11
23	1	-0.09	-0.13	0.18	0.15	0.07	-0.17	-0.12	-0.07	0.08
24	1	0.31	0.04	-0.06	0.21	0.02	-0.03	0.08	0.05	-0.01
25	1	-0.07	-0.01	0.00	0.22	0.06	-0.01	-0.06	-0.08	-0.07
26	1	-0.25	-0.11	0.06	-0.04	-0.02	-0.01	0.29	0.13	-0.05
27	8	0.00	-0.02	0.01	0.00	0.01	-0.01	0.00	-0.03	0.01
28	1	-0.18	0.05	0.00	0.09	-0.02	0.00	-0.21	0.06	0.02

```
  29   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  30   1    -0.01   0.03  -0.02     0.00   0.00   0.00    -0.01   0.02  -
0.02
  31   1     0.11   0.03  -0.05    -0.06  -0.02   0.05     0.14   0.05  -
0.06
  32   1     0.01   0.00   0.01    -0.01   0.00   0.00     0.01  -0.01
0.00
                     58                     59                     60
                     ?A                     ?A                     ?A
 Frequencies --  1334.5026              1348.8239              1355.2685
 Red. masses --     1.7665                 1.5276                 1.5329
 Frc consts  --     1.8536                 1.6374                 1.6589
 IR Inten    --     5.4060                 2.6507                 2.1123
 Raman Activ --     2.0690                 2.8595                 0.6387
 Depolar     --     0.7136                 0.7259                 0.7497
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.02   0.01   0.01     0.02  -0.05  -0.05    -0.04  -0.04  -
0.01
   2   6    -0.02  -0.01  -0.02     0.02   0.03  -0.01     0.09  -0.02  -
0.07
   3   6     0.03  -0.06   0.00    -0.01  -0.04   0.04    -0.02  -0.08
0.05
   4   6    -0.03   0.06   0.00    -0.03   0.08   0.03     0.02   0.05
0.02
   5   6     0.00   0.01   0.08     0.01   0.03   0.01     0.00  -0.02  -
0.02
   6   6     0.07  -0.01   0.01    -0.07  -0.07  -0.06    -0.01   0.07
0.04
   7   6    -0.03   0.07   0.03     0.03   0.04   0.00     0.01  -0.06  -
0.04
   8   6     0.03  -0.08  -0.06     0.00   0.02  -0.01    -0.03   0.02
0.03
   9   6     0.02  -0.04   0.11     0.00  -0.03   0.02     0.00   0.02  -
0.04
  10   6    -0.08   0.05  -0.04     0.07  -0.03   0.01    -0.01   0.00
0.00
  11   6    -0.03  -0.03  -0.01    -0.05  -0.01   0.03     0.03   0.02
0.02
  12   8     0.00  -0.01  -0.01     0.00  -0.01   0.00     0.00   0.01
0.00
  13   6    -0.01   0.00  -0.01    -0.01   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.02   0.00     0.00   0.01   0.00     0.00  -0.01
0.00
  15   8     0.00   0.00  -0.01     0.00  -0.01   0.00     0.00   0.01
0.00
  16   1     0.08  -0.10  -0.04    -0.03   0.04   0.10    -0.08   0.03  -
0.03
  17   1     0.02   0.10   0.10    -0.05   0.09   0.02    -0.45   0.35
0.11
  18   1    -0.15   0.34  -0.18    -0.07   0.22  -0.04     0.13   0.51  -
0.04
```

19	1	0.21	-0.27	-0.24	0.12	-0.40	-0.17	-0.10	-0.26	0.03
20	1	-0.21	-0.22	0.14	0.19	0.49	0.20	-0.06	-0.22	-0.20
21	1	-0.04	-0.10	0.08	-0.01	-0.08	-0.05	0.10	0.08	0.11
22	1	-0.35	0.21	-0.05	-0.06	-0.24	-0.10	0.27	-0.07	0.07
23	1	0.36	-0.13	-0.26	-0.30	0.35	0.08	0.02	-0.09	0.02
24	1	0.07	-0.01	-0.03	0.14	0.05	0.00	-0.13	0.00	0.04
25	1	0.07	-0.01	-0.02	0.13	-0.01	-0.06	-0.04	0.00	0.00
26	1	0.04	0.02	0.00	0.12	0.05	-0.01	-0.09	-0.04	0.02
27	8	0.00	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.09	-0.02	0.00	0.01	-0.01	0.00	-0.02	0.01	0.00
29	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	1	0.00	0.00	0.01	0.00	-0.01	0.01	0.00	0.00	0.00
31	1	-0.06	0.00	0.06	-0.01	0.00	-0.01	0.02	0.00	-0.02
32	1	-0.01	0.01	0.00	0.00	0.00	0.00	0.00	-0.01	-0.01

	61	62	63
	?A	?A	?A
Frequencies --	1369.9557	1384.4007	1389.6328
Red. masses --	1.6284	1.6655	1.3896
Frc consts --	1.8007	1.8807	1.5810
IR Inten --	23.7801	3.5894	1.8123
Raman Activ --	1.8164	1.4305	2.7830
Depolar --	0.6961	0.6683	0.7459

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	0.02	0.03	-0.01	-0.06	-0.02	0.02	0.00	0.01
2	6	-0.01	-0.06	-0.05	-0.05	0.09	0.02	-0.08	0.01	-0.09
3	6	0.07	0.04	0.06	0.08	-0.02	-0.01	-0.03	-0.05	0.00
4	6	0.00	-0.03	-0.03	0.04	0.07	0.01	0.00	-0.02	-0.03
5	6	-0.02	-0.08	0.00	-0.03	0.00	0.02	0.01	-0.03	0.00
6	6	0.00	0.04	0.01	-0.05	0.01	0.11	-0.03	-0.06	0.05
7	6	-0.02	0.00	-0.03	0.05	0.00	-0.04	-0.02	-0.01	0.00
8	6	0.00	0.01	0.00	-0.05	-0.03	0.01	0.04	0.01	0.01

```
    9   6     0.03   0.06   0.09     0.01   0.05   0.02     0.00   0.02  -
0.01
   10   6     0.00  -0.10  -0.04    -0.04  -0.02  -0.04    -0.01   0.02
0.04
   11   6     0.03   0.00   0.00    -0.02   0.01   0.00     0.05   0.01
0.00
   12   8     0.01   0.03  -0.01     0.00   0.00   0.00     0.00   0.01
0.00
   13   6     0.01  -0.01  -0.02     0.00   0.00  -0.01     0.00   0.00
0.00
   14   7     0.00  -0.01   0.01     0.00  -0.01   0.00     0.00   0.00
0.00
   15   8     0.00   0.03   0.00     0.00   0.00  -0.01     0.00   0.01
0.00
   16   1     0.00   0.05   0.02    -0.04  -0.03   0.09    -0.03   0.12
0.16
   17   1    -0.02   0.22   0.24     0.29  -0.30  -0.27     0.50   0.15
0.28
   18   1    -0.46  -0.08  -0.11    -0.31  -0.08  -0.15     0.31   0.31
0.03
   19   1    -0.01   0.20   0.03    -0.14  -0.33   0.05    -0.11   0.09
0.06
   20   1    -0.05  -0.03   0.00     0.31  -0.12  -0.46     0.34   0.20  -
0.13
   21   1     0.02  -0.08   0.11     0.04  -0.11  -0.06    -0.05   0.05  -
0.09
   22   1    -0.09  -0.26  -0.10     0.22   0.01   0.08    -0.23  -0.03  -
0.06
   23   1    -0.13   0.51  -0.26     0.08   0.00  -0.14     0.18  -0.04  -
0.05
   24   1    -0.02   0.01   0.01     0.11  -0.02  -0.02    -0.10   0.01
0.02
   25   1    -0.16  -0.03   0.03    -0.03  -0.01  -0.02    -0.21  -0.02
0.06
   26   1    -0.26  -0.12   0.04     0.03   0.01   0.00    -0.11  -0.05
0.02
   27   8     0.00   0.00  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
   28   1     0.01   0.00   0.01    -0.01   0.01   0.00    -0.02   0.00
0.00
   29   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   30   1     0.00   0.00   0.00     0.00  -0.01   0.00     0.00  -0.01
0.01
   31   1     0.00   0.01   0.01     0.02   0.01   0.01     0.01   0.01
0.00
   32   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                      64                     65                     66
                      ?A                     ?A                     ?A
 Frequencies --   1396.8968              1418.7456              1424.6830
 Red. masses --      1.5358                 1.5820                 1.4771
 Frc consts  --      1.7657                 1.8761                 1.7665
 IR Inten    --     17.0345                 3.8000                 1.6528
```

Raman Activ	--	2.9033			8.1260			2.8121		
Depolar	--	0.6112			0.6918			0.7107		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	-0.04	0.05	0.06	-0.11	-0.07	0.00	0.03	0.02
2	6	-0.01	0.00	-0.04	-0.04	0.01	0.02	-0.01	-0.02	-0.04
3	6	0.03	0.02	0.07	0.02	0.01	0.02	0.02	-0.01	0.05
4	6	0.00	0.06	-0.03	-0.08	0.00	0.05	-0.03	-0.03	0.06
5	6	0.00	-0.06	-0.02	0.01	0.03	-0.01	0.00	0.00	-0.03
6	6	0.01	-0.03	0.01	0.04	0.02	0.00	-0.03	-0.02	0.03
7	6	-0.02	0.01	0.00	-0.04	-0.08	-0.02	0.03	0.07	0.05
8	6	0.05	-0.09	0.01	0.01	0.01	-0.04	-0.07	-0.01	-0.05
9	6	-0.02	0.03	-0.06	0.00	0.00	0.03	0.00	-0.03	0.00
10	6	0.05	0.03	-0.05	0.00	0.02	-0.03	0.03	0.04	-0.05
11	6	-0.04	0.01	0.00	0.04	0.07	0.03	0.05	-0.03	-0.03
12	8	0.00	0.02	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
13	6	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.00
15	8	0.00	0.02	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
16	1	-0.03	0.11	-0.17	-0.26	0.52	0.32	0.03	-0.01	-0.05
17	1	0.00	0.08	0.05	0.07	-0.07	-0.01	0.08	0.13	0.14
18	1	-0.27	-0.05	-0.02	-0.11	-0.09	-0.01	-0.17	0.04	-0.03
19	1	-0.23	-0.08	0.09	0.34	0.07	-0.22	0.39	0.20	-0.17
20	1	0.01	0.05	0.08	-0.09	-0.11	0.03	0.10	0.01	-0.10
21	1	0.02	0.19	0.04	0.11	0.36	0.17	-0.16	-0.41	-0.24
22	1	-0.21	0.49	0.14	0.04	0.00	-0.04	0.41	0.11	0.10
23	1	-0.35	-0.23	0.35	-0.06	-0.09	0.07	-0.19	-0.21	0.22
24	1	0.22	0.04	-0.04	-0.20	0.03	0.07	-0.21	-0.06	0.01
25	1	0.00	0.03	0.04	-0.15	0.05	0.08	-0.14	-0.06	0.01

26	1	-0.20	-0.09	0.04	0.08	0.03	-0.02	0.01	0.00	0.00
27	8	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
28	1	-0.04	0.01	0.00	0.01	-0.01	0.00	0.00	0.00	-0.01
29	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
31	1	0.03	0.00	-0.04	0.01	0.00	-0.02	-0.01	0.00	0.02
32	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	67			68			69		
	?A			?A			?A		
Frequencies --	1428.6008			1438.2700			1458.7959		
Red. masses --	1.4545			1.5311			1.4691		
Frc consts --	1.7490			1.8661			1.8419		
IR Inten --	1.4891			8.0994			14.3168		
Raman Activ --	0.1587			2.0010			1.0306		
Depolar --	0.6577			0.6942			0.5092		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	-0.06	0.09	-0.01	0.06	-0.10	-0.04	-0.05	-0.03
2	6	0.01	0.05	0.00	-0.06	-0.04	0.00	0.02	0.01	0.04
3	6	-0.02	-0.02	-0.02	0.01	0.00	0.01	0.00	0.02	-0.01
4	6	-0.02	0.00	-0.01	0.05	0.00	0.02	0.04	0.05	-0.04
5	6	0.01	0.00	0.01	-0.04	0.04	-0.03	-0.01	0.00	0.01
6	6	0.03	-0.04	0.00	0.05	-0.02	-0.02	0.01	0.00	-0.04
7	6	-0.03	0.08	-0.11	-0.04	0.04	-0.07	-0.02	0.07	0.03
8	6	-0.04	-0.01	0.03	-0.04	-0.05	0.02	0.03	-0.01	0.03
9	6	0.00	0.02	-0.02	0.00	0.05	-0.05	-0.01	-0.04	-0.01
10	6	-0.01	0.00	0.02	0.00	-0.01	0.01	0.01	0.01	0.00
11	6	0.01	0.00	0.00	0.00	-0.01	0.04	0.12	0.01	-0.02
12	8	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
14	7	0.00	-0.01	0.00	0.00	-0.01	0.00	0.00	0.01	0.00
15	8	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00

16	1	-0.09	0.22	-0.33	0.11	-0.25	0.52	-0.11	0.06	0.16
17	1	-0.01	-0.10	-0.17	0.20	0.09	0.25	-0.16	-0.09	-0.12
18	1	0.12	0.09	0.01	-0.04	-0.01	0.00	-0.05	-0.10	0.00
19	1	0.08	0.16	-0.04	-0.13	-0.10	0.12	-0.30	-0.25	0.12
20	1	-0.01	0.10	0.21	-0.11	0.02	0.24	-0.12	0.01	0.12
21	1	0.13	-0.32	0.47	0.12	-0.15	0.43	-0.14	-0.32	-0.10
22	1	0.19	-0.12	0.04	0.23	0.18	0.15	-0.23	-0.02	-0.02
23	1	0.10	-0.02	-0.04	-0.02	0.01	0.03	-0.04	-0.03	0.04
24	1	0.32	0.07	-0.05	-0.04	0.11	0.03	-0.45	-0.06	0.07
25	1	-0.37	-0.07	0.05	0.07	-0.02	-0.06	-0.49	-0.10	0.07
26	1	0.00	0.00	0.00	0.13	0.06	-0.02	0.00	0.00	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
28	1	-0.01	0.01	0.00	-0.05	0.02	0.00	0.01	0.00	0.00
29	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	1	0.00	0.00	0.00	0.00	0.01	-0.01	0.00	0.00	0.00
31	1	0.01	0.00	0.00	0.04	0.00	-0.02	-0.02	0.00	0.02
32	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	70			71			72		
	?A			?A			?A		
Frequencies --	1473.7872			1491.2873			1639.1571		
Red. masses --	1.8758			1.9704			1.1012		
Frc consts --	2.4005			2.5818			1.7433		
IR Inten --	96.8377			26.6733			4.8755		
Raman Activ --	4.6466			7.9140			9.7920		
Depolar --	0.4100			0.6457			0.6534		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.02	-0.03	0.03	0.01	0.00	0.03	-0.01	0.00	0.00
2 6	0.03	0.01	0.00	-0.01	-0.01	-0.03	0.00	0.00	0.00
3 6	0.02	-0.05	0.00	0.06	-0.05	0.05	0.00	0.00	0.00
4 6	0.01	-0.05	-0.01	0.04	-0.07	-0.06	0.00	0.01	0.00
5 6	-0.09	0.13	0.01	-0.10	0.15	0.00	0.00	0.00	0.00

6	6	-0.03	0.00	-0.03	0.00	0.01	0.03	0.00	0.00	0.00
7	6	-0.01	-0.01	0.06	0.00	-0.01	-0.04	0.01	0.00	0.00
8	6	0.00	-0.09	-0.02	0.03	0.08	0.04	0.00	0.01	0.00
9	6	0.03	0.13	-0.03	-0.02	-0.10	0.03	0.00	0.00	0.00
10	6	-0.01	-0.08	0.04	0.02	0.06	-0.06	0.00	0.00	0.00
11	6	0.02	0.01	-0.02	-0.02	0.00	0.00	0.00	-0.08	-0.05
12	8	0.01	-0.04	0.00	0.00	-0.04	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	-0.02	0.01	0.00	0.00	0.00	0.00
14	7	0.00	-0.03	0.00	0.01	0.02	0.00	0.00	0.00	0.00
15	8	0.01	-0.03	0.00	0.01	-0.03	0.00	0.00	0.00	0.00
16	1	-0.06	0.16	-0.15	0.01	0.00	-0.04	-0.01	-0.02	-0.01
17	1	-0.12	0.04	-0.04	0.03	0.07	0.08	0.00	-0.02	-0.02
18	1	-0.04	0.23	-0.09	-0.31	0.15	-0.14	0.00	-0.01	0.00
19	1	-0.04	0.26	0.07	-0.26	0.22	0.20	0.00	-0.03	-0.01
20	1	0.01	0.11	0.03	0.02	-0.09	-0.08	0.00	-0.02	-0.02
21	1	-0.10	0.08	-0.21	0.05	0.02	0.08	0.01	-0.01	-0.01
22	1	0.01	0.49	0.15	-0.22	-0.39	-0.16	0.00	-0.03	-0.01
23	1	0.03	0.35	-0.19	-0.16	-0.27	0.21	0.00	-0.01	0.00
24	1	-0.11	-0.02	0.00	0.14	0.03	-0.02	-0.10	0.69	-0.06
25	1	-0.08	0.03	0.09	-0.02	0.00	0.00	0.09	0.24	0.65
26	1	0.39	0.17	-0.07	0.40	0.17	-0.07	-0.01	0.00	0.00
27	8	0.00	-0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00
28	1	-0.09	0.03	0.01	0.04	-0.01	0.00	0.00	0.00	0.00
29	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	1	0.00	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
31	1	0.07	0.02	-0.02	-0.03	-0.01	0.01	0.00	0.00	0.00
32	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

		73			74			75		
		?A			?A			?A		
Frequencies --		1742.7261			1820.0872			2411.8782		
Red. masses --		1.0968			1.0856			12.6169		
Frc consts --		1.9626			2.1189			43.2427		
IR Inten --		185.3940			275.4771			169.6872		
Raman Activ --		2.3084			0.6102			199.2914		
Depolar --		0.6273			0.5425			0.1642		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.02	0.00
6	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	-0.01	0.00	0.01	0.02	-0.13	0.01
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.13	0.78	-0.11
14	7	0.00	0.00	0.00	0.00	0.00	0.00	-0.15	-0.56	0.09
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.01	0.00
16	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
18	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	1	0.02	0.01	-0.01	0.01	0.00	0.00	0.00	0.00	0.00
21	1	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
22	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01

```
  23   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.01  -
0.01
  24   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  25   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  26   1     0.00   0.00   0.00     0.00   0.00   0.00    -0.03  -0.02
0.01
  27   8     0.00   0.00   0.00     0.07   0.01   0.00     0.00   0.00
0.00
  28   1     0.02   0.00   0.00    -0.52   0.21  -0.14    -0.05  -0.01
0.01
  29   8     0.05  -0.05   0.03     0.01   0.01   0.00     0.00   0.00
0.00
  30   1    -0.07   0.59  -0.39     0.02  -0.05   0.03     0.00   0.00
0.00
  31   1     0.01  -0.03   0.01    -0.60  -0.52   0.15    -0.04  -0.02
0.01
  32   1    -0.67   0.16  -0.10    -0.05   0.02  -0.02     0.00   0.00
0.00
                     76                    77                    78
                     ?A                    ?A                    ?A
 Frequencies --  3117.8623             3203.6631             3246.7235
 Red. masses --     1.0695                1.0588                1.0897
 Frc consts  --     6.1258                6.4025                6.7677
 IR Inten    --  1603.1776               49.9834               38.3592
 Raman Activ --   118.3110              137.8001               61.8698
 Depolar     --     0.2346                0.2018                0.5836
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   2   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.01
0.01
   3   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00     0.00   0.00   0.00    -0.05   0.04  -
0.04
   7   6     0.00   0.00   0.00    -0.01   0.00   0.00     0.02   0.00  -
0.01
   8   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   9   6    -0.01   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.00
0.01
  11   6     0.00   0.00   0.00     0.01  -0.06  -0.03     0.01  -0.01
0.02
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

```
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.00   0.00   0.00    -0.05  -0.03  -0.01    -0.01   0.00
0.00
  17   1     0.00   0.00   0.00     0.00  -0.01   0.01     0.04   0.12  -
0.11
  18   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.01
  19   1     0.00   0.00   0.00    -0.01   0.00  -0.01     0.01   0.00
0.01
  20   1     0.04  -0.03   0.03     0.02  -0.01   0.01     0.57  -0.48
0.46
  21   1     0.01   0.00   0.00     0.10  -0.02  -0.04    -0.28   0.05
0.10
  22   1     0.00   0.00   0.00     0.00   0.00  -0.01     0.00   0.01  -
0.02
  23   1     0.00   0.00   0.00     0.00   0.00   0.00    -0.07  -0.04  -
0.09
  24   1     0.00   0.00   0.00     0.09   0.01   0.60    -0.03  -0.02  -
0.23
  25   1     0.00  -0.01   0.00    -0.16   0.71  -0.29    -0.04   0.18  -
0.07
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  27   8    -0.04   0.04  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.04   0.08  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
  29   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  30   1     0.02  -0.03   0.02     0.00   0.00   0.00     0.00   0.00
0.00
  31   1     0.61  -0.68   0.38     0.01  -0.01   0.00    -0.03   0.03  -
0.02
  32   1     0.02  -0.02   0.01     0.00   0.00   0.00     0.00   0.00
0.00
                     79                     80                     81
                     ?A                     ?A                     ?A
 Frequencies --  3248.5085              3273.2001              3287.5716
 Red. masses --     1.1039                 1.0877                 1.0889
 Frc consts  --     6.8633                 6.8662                 6.9339
 IR Inten    --    55.1916                66.1643                36.5372
 Raman Activ --   103.5347               100.5710                87.9671
 Depolar     --     0.7487                 0.4099                 0.4890
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.02   0.01
0.00
   2   6     0.00   0.00   0.00     0.00  -0.01   0.01    -0.02  -0.05
0.05
```

3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01
4	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	-0.01
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	-0.02	0.01	-0.01	-0.01	0.01	-0.01	0.01	-0.01	0.01
7	6	0.01	0.00	0.00	-0.07	0.01	0.03	0.00	0.00	0.00
8	6	0.00	0.00	0.00	0.00	0.01	-0.02	0.00	0.00	0.01
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	-0.01
11	6	-0.02	0.04	-0.08	0.00	0.01	0.01	0.00	0.00	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	-0.02	-0.01	0.00	0.04	0.02	0.00	-0.29	-0.14	-0.01
17	1	0.02	0.05	-0.04	0.05	0.12	-0.12	0.23	0.62	-0.57
18	1	0.00	0.00	0.00	-0.01	0.01	0.02	-0.05	0.03	0.14
19	1	-0.01	0.00	-0.01	-0.03	0.01	-0.04	0.09	-0.03	0.13
20	1	0.19	-0.16	0.15	0.17	-0.14	0.14	-0.12	0.10	-0.09
21	1	-0.06	0.01	0.02	0.82	-0.13	-0.32	-0.03	0.00	0.01
22	1	0.00	0.01	-0.02	-0.06	-0.08	0.27	0.04	0.05	-0.17
23	1	-0.02	-0.02	-0.03	-0.05	-0.03	-0.07	0.05	0.03	0.07
24	1	0.11	0.05	0.74	-0.01	0.00	-0.08	0.00	0.00	-0.01
25	1	0.12	-0.52	0.19	0.01	-0.06	0.02	0.00	0.01	0.00
26	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  30   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  31   1    -0.01   0.02  -0.01    -0.01   0.02  -0.01     0.01  -0.01
0.00
  32   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     82                     83                     84
                     ?A                     ?A                     ?A
 Frequencies --  3293.2524              3300.9616              3305.0456
 Red. masses --     1.0885                 1.0893                 1.0878
 Frc consts  --     6.9553                 6.9934                 7.0011
 IR Inten    --    16.7774                34.9690                28.1091
 Raman Activ --    81.7870                65.7799                80.1221
 Depolar     --     0.4807                 0.2453                 0.6344
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.00   0.00   0.00    -0.04  -0.02
0.00
   2   6    -0.01  -0.01   0.01     0.00   0.00   0.00     0.00  -0.01
0.01
   3   6     0.00   0.00   0.00    -0.01   0.01   0.02     0.00   0.00
0.00
   4   6     0.02  -0.01   0.04    -0.01   0.00  -0.02     0.03  -0.01
0.04
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00    -0.01   0.01  -0.01     0.00   0.00
0.00
   7   6     0.02   0.00  -0.01    -0.01   0.00   0.00    -0.01   0.00
0.00
   8   6     0.01   0.02  -0.06     0.00   0.00   0.00    -0.01  -0.01
0.04
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6    -0.01  -0.01  -0.01    -0.04  -0.03  -0.06    -0.01  -0.01  -
0.01
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.03   0.01   0.00    -0.05  -0.02   0.00     0.52   0.24
0.03
  17   1     0.06   0.15  -0.14    -0.02  -0.05   0.05     0.05   0.14  -
0.13
  18   1     0.00   0.00   0.00     0.09  -0.06  -0.23     0.01  -0.01  -
0.02
  19   1    -0.29   0.10  -0.44     0.12  -0.04   0.18    -0.31   0.10  -
0.47
```

```
  20   1    -0.05   0.04  -0.04     0.11  -0.10   0.09     0.01  -0.01
0.01
  21   1    -0.24   0.04   0.09     0.07  -0.01  -0.03     0.07  -0.01  -
0.03
  22   1    -0.15  -0.22   0.69     0.00   0.00   0.00     0.11   0.15  -
0.48
  23   1     0.10   0.07   0.14     0.48   0.35   0.70     0.09   0.06
0.13
  24   1     0.01   0.00   0.03     0.00   0.00  -0.01     0.00   0.00
0.00
  25   1     0.00   0.02  -0.01     0.00  -0.01   0.00    -0.01   0.02  -
0.01
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  29   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  30   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  31   1     0.00   0.00   0.00    -0.01   0.01  -0.01     0.00   0.00
0.00
  32   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     85                    86                    87
                     ?A                    ?A                    ?A
 Frequencies --  3316.7277             3331.6555             3812.9933
 Red. masses --     1.0901                1.0909                1.0707
 Frc consts  --     7.0657                7.1344                9.1715
 IR Inten    --    24.6226               18.7319              236.3494
 Raman Activ --   204.7657              235.7849               49.7286
 Depolar     --     0.1202                0.0896                0.2194
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.06  -0.03   0.00     0.01   0.01   0.00     0.00   0.00
0.00
   2   6     0.00  -0.01   0.01     0.00   0.01  -0.01     0.00   0.00
0.00
   3   6     0.01  -0.01  -0.02     0.03  -0.02  -0.07     0.00   0.00
0.00
   4   6    -0.03   0.01  -0.04     0.01   0.00   0.01     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   7   6     0.01   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   8   6     0.01   0.01  -0.02     0.00   0.00   0.01     0.00   0.00
0.00
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

10	6	0.00	0.00	0.00	-0.01	-0.01	-0.02	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	0.66	0.31	0.04	-0.13	-0.06	-0.01	0.00	0.00	0.00
17	1	0.04	0.12	-0.11	-0.05	-0.15	0.14	0.00	0.00	0.00
18	1	-0.09	0.06	0.22	-0.32	0.23	0.83	0.00	0.00	0.00
19	1	0.29	-0.10	0.44	-0.07	0.02	-0.10	0.00	0.00	0.00
20	1	-0.03	0.03	-0.03	0.04	-0.04	0.03	0.00	0.00	0.00
21	1	-0.10	0.02	0.04	0.03	-0.01	-0.01	0.00	0.00	0.00
22	1	-0.05	-0.08	0.24	0.01	0.02	-0.06	0.00	0.00	0.00
23	1	0.01	0.01	0.01	0.13	0.09	0.18	0.00	0.00	0.00
24	1	0.01	0.00	0.06	0.00	0.00	-0.01	0.00	0.00	0.00
25	1	-0.01	0.04	-0.01	0.00	-0.01	0.00	0.00	0.00	0.00
26	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	-0.02	-0.06	0.02
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.37	0.89	-0.25
29	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	1	0.00	0.00	0.00	0.00	0.00	0.00	-0.05	0.00	0.00
31	1	0.00	0.00	0.00	0.00	0.00	0.00	-0.04	0.03	-0.02
32	1	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.03	-0.02

	88	89	90
	?A	?A	?A
Frequencies --	3853.0486	3872.9755	3976.8009
Red. masses --	1.0398	1.0655	1.0887
Frc consts --	9.0951	9.4167	10.1447
IR Inten --	33.5272	95.4649	205.0695
Raman Activ --	112.5990	110.3947	38.9322
Depolar --	0.1288	0.2209	0.6038

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	8	0.00	0.00	0.00	-0.03	0.05	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
18	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
22	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
23	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
25	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
26	1	0.00	0.00	0.00	0.47	-0.88	0.00	0.00	0.00	0.00

```
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.02   0.05  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
  29   8    -0.03   0.03  -0.02     0.00   0.00   0.00     0.06   0.04  -
0.03
  30   1     0.67   0.09  -0.06     0.00   0.00   0.00    -0.72  -0.06
0.05
  31   1    -0.01   0.01  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
  32   1    -0.23  -0.57   0.38     0.00   0.00   0.00    -0.18  -0.55
0.36

 -------------------
 - Thermochemistry -
 -------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Atom  1 has atomic number  6 and mass  12.00000
 Atom  2 has atomic number  6 and mass  12.00000
 Atom  3 has atomic number  6 and mass  12.00000
 Atom  4 has atomic number  6 and mass  12.00000
 Atom  5 has atomic number  6 and mass  12.00000
 Atom  6 has atomic number  6 and mass  12.00000
 Atom  7 has atomic number  6 and mass  12.00000
 Atom  8 has atomic number  6 and mass  12.00000
 Atom  9 has atomic number  6 and mass  12.00000
 Atom 10 has atomic number  6 and mass  12.00000
 Atom 11 has atomic number  6 and mass  12.00000
 Atom 12 has atomic number  8 and mass  15.99491
 Atom 13 has atomic number  6 and mass  12.00000
 Atom 14 has atomic number  7 and mass  14.00307
 Atom 15 has atomic number  8 and mass  15.99491
 Atom 16 has atomic number  1 and mass   1.00783
 Atom 17 has atomic number  1 and mass   1.00783
 Atom 18 has atomic number  1 and mass   1.00783
 Atom 19 has atomic number  1 and mass   1.00783
 Atom 20 has atomic number  1 and mass   1.00783
 Atom 21 has atomic number  1 and mass   1.00783
 Atom 22 has atomic number  1 and mass   1.00783
 Atom 23 has atomic number  1 and mass   1.00783
 Atom 24 has atomic number  1 and mass   1.00783
 Atom 25 has atomic number  1 and mass   1.00783
 Atom 26 has atomic number  1 and mass   1.00783
 Atom 27 has atomic number  8 and mass  15.99491
 Atom 28 has atomic number  1 and mass   1.00783
 Atom 29 has atomic number  8 and mass  15.99491
 Atom 30 has atomic number  1 and mass   1.00783
 Atom 31 has atomic number  1 and mass   1.00783
 Atom 32 has atomic number  1 and mass   1.00783
 Molecular mass:   237.10011 amu.
 Principal axes and moments of inertia in atomic units:
                           1         2         3
     EIGENVALUES --  2566.50912 3352.46755 4763.00896
           X            0.99985  -0.01511   0.00818
```

```
          Y            0.01504   0.99985   0.00842
          Z           -0.00831  -0.00829   0.99993
 THIS MOLECULE IS AN ASYMMETRIC TOP.
 ROTATIONAL SYMMETRY NUMBER  1.
 WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
          MAY CAUSE SIGNIFICANT ERROR
 ROTATIONAL TEMPERATURES (KELVIN)      0.03375     0.02584     0.01818
 ROTATIONAL CONSTANTS (GHZ)            0.70319     0.53833     0.37891
    1 IMAGINARY FREQUENCIES IGNORED.
 Zero-point vibrational energy     721442.6 (Joules/Mol)
                                  172.42891 (Kcal/Mol)
 WARNING-- EXPLICIT CONSIDERATION OF  21 DEGREES OF FREEDOM AS
          VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
 VIBRATIONAL TEMPERATURES:     36.92   110.10   129.90   186.53   284.31
          (KELVIN)            315.08   360.67   425.15   439.74   458.53
                              499.57   506.76   570.03   577.69   608.31
                              637.98   677.34   733.62   785.39   818.98
                              845.93   894.53   914.29   945.24   957.10
                              996.44  1029.14  1185.50  1193.48  1219.94
                             1274.78  1288.28  1297.72  1333.23  1351.29
                             1409.30  1447.27  1457.05  1465.13  1474.23
                             1485.01  1492.95  1518.55  1537.76  1545.31
                             1582.66  1672.02  1722.75  1727.58  1761.54
                             1775.26  1804.88  1817.18  1837.05  1886.67
                             1898.91  1920.04  1940.65  1949.92  1971.05
                             1991.83  1999.36  2009.81  2041.25  2049.79
                             2055.43  2069.34  2098.87  2120.44  2145.62
                             2358.37  2507.38  2618.68  3470.13  4485.88
                             4609.33  4671.28  4673.85  4709.38  4730.06
                             4738.23  4749.32  4755.20  4772.00  4793.48
                             5486.02  5543.65  5572.32  5721.70

 Zero-point correction=                           0.274783
(Hartree/Particle)
 Thermal correction to Energy=                    0.288279
 Thermal correction to Enthalpy=                  0.289224
 Thermal correction to Gibbs Free Energy=         0.234678
 Sum of electronic and zero-point Energies=           -812.235401
 Sum of electronic and thermal Energies=              -812.221905
 Sum of electronic and thermal Enthalpies=            -812.220961
 Sum of electronic and thermal Free Energies=         -812.275507

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 180.898             55.648           114.802
 ELECTRONIC              0.000              0.000             0.000
 TRANSLATIONAL           0.889              2.981            42.292
 ROTATIONAL              0.889              2.981            32.083
 VIBRATIONAL           179.121             49.686            40.427
 VIBRATION  1            0.593              1.985             6.139
 VIBRATION  2            0.599              1.965             3.978
 VIBRATION  3            0.602              1.956             3.654
 VIBRATION  4            0.612              1.924             2.951
 VIBRATION  5            0.637              1.843             2.155
```

VIBRATION 6	0.647	1.812	1.967
VIBRATION 7	0.663	1.762	1.726
VIBRATION 8	0.690	1.682	1.442
VIBRATION 9	0.696	1.663	1.386
VIBRATION 10	0.705	1.638	1.317
VIBRATION 11	0.725	1.581	1.179
VIBRATION 12	0.729	1.571	1.156
VIBRATION 13	0.763	1.478	0.977
VIBRATION 14	0.767	1.467	0.957
VIBRATION 15	0.785	1.421	0.883
VIBRATION 16	0.803	1.375	0.816
VIBRATION 17	0.828	1.315	0.735
VIBRATION 18	0.865	1.228	0.634
VIBRATION 19	0.901	1.149	0.553
VIBRATION 20	0.925	1.098	0.506
VIBRATION 21	0.945	1.057	0.471

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.113906-107	-107.943454	-248.548988
TOTAL V=0	0.279947D+19	18.447076	42.475962
VIB (BOT)	0.346373-122	-122.460456	-281.975620
VIB (BOT) 1	0.807013D+01	0.906880	2.088169
VIB (BOT) 2	0.269267D+01	0.430184	0.990534
VIB (BOT) 3	0.227720D+01	0.357401	0.822946
VIB (BOT) 4	0.157261D+01	0.196621	0.452737
VIB (BOT) 5	0.100999D+01	0.004315	0.009936
VIB (BOT) 6	0.903633D+00	-0.044008	-0.101332
VIB (BOT) 7	0.778315D+00	-0.108844	-0.250623
VIB (BOT) 8	0.645213D+00	-0.190297	-0.438175
VIB (BOT) 9	0.620251D+00	-0.207433	-0.477632
VIB (BOT) 10	0.590316D+00	-0.228915	-0.527097
VIB (BOT) 11	0.532319D+00	-0.273828	-0.630512
VIB (BOT) 12	0.523065D+00	-0.281445	-0.648050
VIB (BOT) 13	0.451124D+00	-0.345704	-0.796014
VIB (BOT) 14	0.443416D+00	-0.353189	-0.813247
VIB (BOT) 15	0.414417D+00	-0.382562	-0.880882
VIB (BOT) 16	0.388794D+00	-0.410280	-0.944706
VIB (BOT) 17	0.358054D+00	-0.446052	-1.027073
VIB (BOT) 18	0.319488D+00	-0.495546	-1.141037
VIB (BOT) 19	0.288626D+00	-0.539665	-1.242624
VIB (BOT) 20	0.270586D+00	-0.567695	-1.307165
VIB (BOT) 21	0.257110D+00	-0.589881	-1.358252
VIB (V=0)	0.851283D+04	3.930074	9.049330
VIB (V=0) 1	0.858560D+01	0.933771	2.150087
VIB (V=0) 2	0.323870D+01	0.510371	1.175173
VIB (V=0) 3	0.283145D+01	0.452008	1.040787
VIB (V=0) 4	0.215018D+01	0.332476	0.765553
VIB (V=0) 5	0.162697D+01	0.211381	0.486722
VIB (V=0) 6	0.153274D+01	0.185469	0.427057
VIB (V=0) 7	0.142508D+01	0.153840	0.354229
VIB (V=0) 8	0.131627D+01	0.119346	0.274803
VIB (V=0) 9	0.129669D+01	0.112835	0.259813
VIB (V=0) 10	0.127361D+01	0.105037	0.241856
VIB (V=0) 11	0.123032D+01	0.090017	0.207272
VIB (V=0) 12	0.122360D+01	0.087639	0.201797

VIB (V=0) 13	0.117343D+01	0.069458	0.159934
VIB (V=0) 14	0.116829D+01	0.067552	0.155545
VIB (V=0) 15	0.114942D+01	0.060477	0.139254
VIB (V=0) 16	0.113337D+01	0.054373	0.125198
VIB (V=0) 17	0.111498D+01	0.047268	0.108838
VIB (V=0) 18	0.109336D+01	0.038762	0.089253
VIB (V=0) 19	0.107733D+01	0.032347	0.074482
VIB (V=0) 20	0.106852D+01	0.028783	0.066276
VIB (V=0) 21	0.106223D+01	0.026220	0.060373
ELECTRONIC	0.100000D+01	0.000000	0.000000
TRANSLATIONAL	0.143502D+09	8.156858	18.781860
ROTATIONAL	0.229163D+07	6.360144	14.644772

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000001093	0.000002618	-0.000003819
2	6	-0.000000519	0.000000799	0.000001015
3	6	-0.000001081	-0.000001813	-0.000002380
4	6	-0.000000543	0.000000871	-0.000000828
5	6	-0.000000126	-0.000001794	0.000004564
6	6	-0.000000799	-0.000005684	-0.000001238
7	6	-0.000005168	-0.000000623	0.000004152
8	6	-0.000003412	0.000001814	-0.000000978
9	6	0.000027319	0.000007762	-0.000023675
10	6	0.000002576	-0.000000441	0.000002081
11	6	0.000001861	-0.000000057	0.000000736
12	8	-0.000000600	-0.000000215	-0.000000482
13	6	-0.000012343	-0.000002982	0.000009065
14	7	0.000001171	-0.000000826	-0.000000823
15	8	0.000001020	0.000001222	-0.000004962
16	1	0.000000630	0.000001039	0.000000100
17	1	0.000000501	0.000000196	-0.000000727
18	1	0.000000510	-0.000000081	0.000000182
19	1	-0.000000372	0.000000233	0.000000069
20	1	0.000001056	-0.000000673	0.000001484
21	1	-0.000000198	-0.000000445	0.000000564
22	1	0.000000715	0.000000954	-0.000000015
23	1	0.000000959	0.000000338	-0.000001011
24	1	0.000000381	0.000000727	0.000001037
25	1	-0.000000444	-0.000000130	-0.000000048
26	1	0.000003207	0.000000615	-0.000000895
27	8	-0.000021589	-0.000004027	-0.000016188
28	1	0.000001716	0.000010229	0.000002281
29	8	0.000004539	0.000016598	-0.000013044
30	1	-0.000001050	-0.000007170	-0.000002080
31	1	-0.000000415	-0.000015669	0.000046285
32	1	-0.000000596	-0.000003386	-0.000000421

Cartesian Forces: Max 0.000046285 RMS 0.000007648

Internal Coordinate Forces (Hartree/Bohr or radian)

Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J

1	C	0.000001(	1)	0.000003(	33)	-0.000004(	65)
2	C	-0.000001(	2)	0.000001(	34)	0.000001(	66)
3	C	-0.000001(	3)	-0.000002(	35)	-0.000002(	67)
4	C	-0.000001(	4)	0.000001(	36)	-0.000001(	68)
5	C	0.000000(	5)	-0.000002(	37)	0.000005(	69)
6	C	-0.000001(	6)	-0.000006(	38)	-0.000001(	70)
7	C	-0.000005(	7)	-0.000001(	39)	0.000004(	71)
8	C	-0.000003(	8)	0.000002(	40)	-0.000001(	72)
9	C	0.000027(	9)	0.000008(	41)	-0.000024(	73)
10	C	0.000003(	10)	0.000000(	42)	0.000002(	74)
11	C	0.000002(	11)	0.000000(	43)	0.000001(	75)
12	O	-0.000001(	12)	0.000000(	44)	0.000000(	76)
13	C	-0.000012(	13)	-0.000003(	45)	0.000009(	77)
14	N	0.000001(	14)	-0.000001(	46)	-0.000001(	78)
15	O	0.000001(	15)	0.000001(	47)	-0.000005(	79)
16	H	0.000001(	16)	0.000001(	48)	0.000000(	80)
17	H	0.000001(	17)	0.000000(	49)	-0.000001(	81)
18	H	0.000001(	18)	0.000000(	50)	0.000000(	82)
19	H	0.000000(	19)	0.000000(	51)	0.000000(	83)
20	H	0.000001(	20)	-0.000001(	52)	0.000001(	84)
21	H	0.000000(	21)	0.000000(	53)	0.000001(	85)
22	H	0.000001(	22)	0.000001(	54)	0.000000(	86)
23	H	0.000001(	23)	0.000000(	55)	-0.000001(	87)
24	H	0.000000(	24)	0.000001(	56)	0.000001(	88)
25	H	0.000000(	25)	0.000000(	57)	0.000000(	89)
26	H	0.000003(	26)	0.000001(	58)	-0.000001(	90)
27	O	-0.000022(	27)	-0.000004(	59)	-0.000016(	91)
28	H	0.000002(	28)	0.000010(	60)	0.000002(	92)
29	O	0.000005(	29)	0.000017(	61)	-0.000013(	93)
30	H	-0.000001(	30)	-0.000007(	62)	-0.000002(	94)
31	H	0.000000(	31)	-0.000016(	63)	0.000046(	95)
32	H	-0.000001(	32)	-0.000003(	64)	0.000000(	96)

Internal Forces: Max 0.000046285 RMS 0.000007648

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number 1 out of a maximum of 106
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.

Eigenvalues ---	-0.00943	0.00011	0.00026	0.00114	0.00496
Eigenvalues ---	0.00653	0.00667	0.00822	0.00945	0.01203
Eigenvalues ---	0.01262	0.01537	0.02407	0.02543	0.02788
Eigenvalues ---	0.02981	0.03189	0.04088	0.04334	0.04502
Eigenvalues ---	0.04592	0.04736	0.04832	0.04891	0.05053
Eigenvalues ---	0.05120	0.05202	0.05280	0.05380	0.05483
Eigenvalues ---	0.05750	0.05818	0.05976	0.06575	0.06911
Eigenvalues ---	0.07181	0.07887	0.09650	0.10027	0.10821
Eigenvalues ---	0.12636	0.14288	0.14704	0.15182	0.16499
Eigenvalues ---	0.17651	0.19197	0.20054	0.20216	0.20975
Eigenvalues ---	0.23925	0.25608	0.26991	0.29309	0.30449
Eigenvalues ---	0.35333	0.36594	0.38227	0.38743	0.40007

```
    Eigenvalues ---    0.48970   0.49377   0.50320   0.51362   0.51946
    Eigenvalues ---    0.56612   0.57895   0.60330   0.62752   0.66331
    Eigenvalues ---    0.69929   0.72035   0.72584   0.81053   0.83418
    Eigenvalues ---    0.87646   0.89291   0.94600   0.95323   0.96469
    Eigenvalues ---    0.97703   0.99095   1.02101   1.05716   1.07636
    Eigenvalues ---    1.09493   1.12145   1.20845   1.27954   2.81059
Eigenvalue   1 out of range, new value =    0.009429 Eigenvector:
                           1
          X1          -0.03194
          Y1           0.00839
          Z1          -0.01632
          X2          -0.02113
          Y2           0.00483
          Z2           0.00900
          X3           0.03102
          Y3           0.01921
          Z3          -0.08107
          X4           0.03591
          Y4           0.01528
          Z4          -0.09160
          X5           0.04371
          Y5           0.02804
          Z5          -0.14257
          X6           0.07759
          Y6          -0.02286
          Z6           0.07022
          X7           0.09060
          Y7          -0.02006
          Z7           0.06457
          X8           0.13103
          Y8          -0.01725
          Z8          -0.01890
          X9           0.21503
          Y9          -0.00615
          Z9          -0.04717
          X10          0.13750
          Y10         -0.00179
          Z10         -0.00055
          X11          0.00206
          Y11         -0.00534
          Z11          0.05588
          X12         -0.02433
          Y12          0.04466
          Z12         -0.20178
          X13         -0.19441
          Y13         -0.10280
          Z13          0.42917
          X14          0.05050
          Y14         -0.05630
          Z14          0.24354
          X15          0.04032
          Y15          0.03844
          Z15         -0.20693
          X16         -0.07849
```

```
          Y16          0.02054
          Z16         -0.03269
          X17         -0.08397
          Y17         -0.00156
          Z17          0.03222
          X18          0.01442
          Y18          0.02559
          Z18         -0.08645
          X19          0.02624
          Y19          0.01799
          Z19         -0.11219
          X20          0.07848
          Y20         -0.03090
          Z20          0.13272
          X21          0.11818
          Y21         -0.02974
          Z21          0.09209
          X22          0.14099
          Y22         -0.01740
          Z22         -0.02819
          X23          0.13994
          Y23         -0.01325
          Z23          0.00918
          X24         -0.00108
          Y24         -0.00262
          Z24          0.03726
          X25         -0.03340
          Y25         -0.00710
          Z25          0.11115
          X26         -0.02356
          Y26          0.03734
          Z26         -0.19945
          X27         -0.18615
          Y27         -0.01781
          Z27          0.00477
          X28         -0.36488
          Y28         -0.08229
          Z28          0.05101
          X29         -0.14898
          Y29          0.05573
          Z29         -0.01085
          X30         -0.13345
          Y30          0.05503
          Z30         -0.00083
          X31         -0.15310
          Y31          0.01117
          Z31         -0.04190
          X32         -0.14358
          Y32          0.07003
          Z32         -0.00006
Angle between quadratic step and forces=  78.46 degrees.
Linear search not attempted -- first point.
TrRot=  0.000018 -0.000010 -0.000004  0.000000  0.000009  0.000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
```

			(Linear)	(Quad)	(Total)	
X1	-0.52541	0.00000	0.00000	-0.00028	-0.00030	-0.52571
Y1	-0.75996	0.00000	0.00000	0.00004	0.00003	-0.75993
Z1	-4.32288	0.00000	0.00000	0.00002	0.00002	-4.32286
X2	-0.97355	0.00000	0.00000	-0.00012	-0.00014	-0.97368
Y2	1.95860	0.00000	0.00000	0.00005	0.00004	1.95864
Z2	-3.29385	0.00000	0.00000	0.00006	0.00007	-3.29379
X3	1.31971	0.00000	0.00000	0.00008	0.00009	1.31980
Y3	2.62106	0.00000	0.00000	0.00003	0.00002	2.62108
Z3	-1.56929	0.00000	0.00000	-0.00025	-0.00027	-1.56955
X4	1.38817	0.00000	0.00000	-0.00010	-0.00010	1.38807
Y4	-1.79784	0.00000	0.00000	0.00000	-0.00001	-1.79785
Z4	-2.38026	0.00000	0.00000	-0.00022	-0.00023	-2.38050
X5	3.18321	0.00000	0.00000	0.00002	0.00002	3.18324
Y5	0.40786	0.00000	0.00000	-0.00004	-0.00005	0.40781
Z5	-1.79492	0.00000	0.00000	-0.00040	-0.00044	-1.79536
X6	-2.65356	0.00000	0.00000	0.00018	0.00019	-2.65337
Y6	1.48470	-0.00001	0.00000	0.00005	0.00004	1.48475
Z6	-0.88611	0.00000	0.00000	0.00027	0.00029	-0.88583
X7	-2.96915	-0.00001	0.00000	0.00009	0.00010	-2.96906
Y7	-1.44082	0.00000	0.00000	0.00010	0.00009	-1.44073
Z7	-0.85013	0.00000	0.00000	0.00034	0.00036	-0.84976
X8	-0.29630	0.00000	0.00000	0.00018	0.00020	-0.29610
Y8	-2.29081	0.00000	0.00000	0.00002	0.00001	-2.29081
Z8	0.03585	0.00000	0.00000	0.00005	0.00005	0.03589
X9	0.40352	0.00003	0.00000	0.00071	0.00075	0.40427
Y9	-0.33056	0.00001	0.00000	0.00006	0.00005	-0.33051
Z9	2.03440	-0.00002	0.00000	-0.00022	-0.00023	2.03417
X10	-0.33579	0.00000	0.00000	0.00039	0.00041	-0.33538
Y10	2.17903	0.00000	0.00000	0.00005	0.00004	2.17908
Z10	0.85317	0.00000	0.00000	0.00003	0.00003	0.85320
X11	-3.00262	0.00000	0.00000	-0.00021	-0.00023	-3.00285
Y11	-2.13131	0.00000	0.00000	0.00008	0.00007	-2.13124
Z11	-3.67615	0.00000	0.00000	0.00032	0.00034	-3.67581
X12	4.75580	0.00000	0.00000	-0.00008	-0.00010	4.75570
Y12	0.82298	0.00000	0.00000	-0.00011	-0.00012	0.82286
Z12	-4.00405	0.00000	0.00000	-0.00050	-0.00055	-4.00460
X13	2.62463	-0.00001	0.00000	-0.00030	-0.00026	2.62437
Y13	-0.62143	0.00000	0.00000	-0.00015	-0.00016	-0.62159
Z13	3.62022	0.00001	0.00000	0.00092	0.00089	3.62111
X14	3.69571	0.00000	0.00000	0.00030	0.00037	3.69607
Y14	-0.99387	0.00000	0.00000	0.00013	0.00011	-0.99376
Z14	5.48208	0.00000	0.00000	0.00050	0.00046	5.48254
X15	4.57947	0.00000	0.00000	0.00000	0.00002	4.57949
Y15	0.05210	0.00000	0.00000	-0.00002	-0.00004	0.05206
Z15	0.36149	0.00000	0.00000	-0.00054	-0.00058	0.36090
X16	0.12736	0.00000	0.00000	-0.00045	-0.00049	0.12687
Y16	-0.84794	0.00000	0.00000	0.00002	0.00001	-0.84793
Z16	-6.25084	0.00000	0.00000	-0.00004	-0.00004	-6.25088
X17	-1.62047	0.00000	0.00000	-0.00025	-0.00027	-1.62074
Y17	3.32374	0.00000	0.00000	0.00004	0.00003	3.32378
Z17	-4.66257	0.00000	0.00000	0.00011	0.00013	-4.66245
X18	2.20946	0.00000	0.00000	0.00011	0.00011	2.20957
Y18	4.44393	0.00000	0.00000	0.00001	-0.00001	4.44393

Z18	-1.71648	0.00000	0.00000	-0.00029	-0.00032	-1.71680
X19	2.40205	0.00000	0.00000	-0.00022	-0.00023	2.40182
Y19	-3.46809	0.00000	0.00000	-0.00005	-0.00006	-3.46816
Z19	-2.96002	0.00000	0.00000	-0.00026	-0.00028	-2.96031
X20	-4.36873	0.00000	0.00000	0.00020	0.00021	-4.36852
Y20	2.57895	0.00000	0.00000	0.00005	0.00005	2.57900
Z20	-0.69794	0.00000	0.00000	0.00041	0.00044	-0.69750
X21	-4.50973	0.00000	0.00000	0.00015	0.00017	-4.50956
Y21	-2.16261	0.00000	0.00000	0.00024	0.00024	-2.16237
Z21	0.27907	0.00000	0.00000	0.00048	0.00052	0.27959
X22	-0.18530	0.00000	0.00000	0.00018	0.00020	-0.18510
Y22	-4.20239	0.00000	0.00000	0.00005	0.00004	-4.20235
Z22	0.73752	0.00000	0.00000	0.00009	0.00008	0.73760
X23	-0.48376	0.00000	0.00000	0.00054	0.00058	-0.48318
Y23	3.71282	0.00000	0.00000	0.00004	0.00003	3.71286
Z23	2.18634	0.00000	0.00000	0.00005	0.00005	2.18639
X24	-2.90904	0.00000	0.00000	-0.00027	-0.00029	-2.90933
Y24	-4.15267	0.00000	0.00000	0.00008	0.00007	-4.15260
Z24	-4.00138	0.00000	0.00000	0.00033	0.00035	-4.00103
X25	-4.63443	0.00000	0.00000	-0.00032	-0.00034	-4.63478
Y25	-1.36229	0.00000	0.00000	0.00008	0.00007	-1.36222
Z25	-4.65184	0.00000	0.00000	0.00048	0.00052	-4.65132
X26	6.49955	0.00000	0.00000	-0.00008	-0.00010	6.49945
Y26	0.78370	0.00000	0.00000	-0.00012	-0.00014	0.78356
Z26	-3.45191	0.00000	0.00000	-0.00046	-0.00052	-3.45243
X27	-1.72713	-0.00002	0.00000	-0.00017	-0.00011	-1.72724
Y27	-0.75320	0.00000	0.00000	-0.00021	-0.00022	-0.75341
Z27	4.27900	-0.00002	0.00000	0.00069	0.00070	4.27970
X28	-1.00643	0.00000	0.00000	0.00050	0.00057	-1.00586
Y28	-1.22542	0.00001	0.00000	0.00168	0.00167	-1.22374
Z28	5.90033	0.00000	0.00000	0.00093	0.00094	5.90126
X29	-6.19124	0.00000	0.00000	-0.00025	-0.00019	-6.19143
Y29	1.20088	0.00002	0.00000	-0.00019	-0.00020	1.20069
Z29	4.48538	-0.00001	0.00000	-0.00079	-0.00074	4.48465
X30	-7.34036	0.00000	0.00000	-0.00402	-0.00395	-7.34430
Y30	1.09018	-0.00001	0.00000	-0.00563	-0.00563	1.08454
Z30	5.89828	0.00000	0.00000	-0.00429	-0.00423	5.89405
X31	-3.47509	0.00000	0.00000	-0.00033	-0.00027	-3.47536
Y31	-0.00675	-0.00002	0.00000	-0.00079	-0.00080	-0.00755
Z31	4.29924	0.00005	0.00000	0.00110	0.00113	4.30037
X32	-6.88737	0.00000	0.00000	0.00332	0.00336	-6.88400
Y32	2.19868	0.00000	0.00000	0.00472	0.00471	2.20339
Z32	3.12291	0.00000	0.00000	0.00100	0.00106	3.12397

Item		Value	Threshold	Converged?
Maximum	Force	0.000046	0.000450	YES
RMS	Force	0.000008	0.000300	YES
Maximum	Displacement	0.005634	0.001800	NO
RMS	Displacement	0.001086	0.001200	YES

Predicted change in Energy=-5.543406D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1\1\GINC-PELICAN\Freq\RHF\3-21+G*\C12H15N1O4\SINGH\25-Feb-2003\0\\#N R
HF/3-21+G* FREQ\\H2O added-freq calc of m1s8H2Onew3.out\\0,1\C,-0.2780
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.00004628,0.00000060,0.00000339,0.00000042\\\@

WE LOSE BECAUSE WE WIN

GAMBLERS,

RECOLLECTING WHICH,

TOSS THEIR DICE AGAIN....

EMILY DICKINSON BOLTS OF MELODY NO. 533

Job cpu time: 0 days 5 hours 4 minutes 8.3 seconds.

File lengths (MBytes): RWF= 283 Int=   0 D2E=   0 Chk=   7 Scr=
1

Normal termination of Gaussian 98.

```
%chk=H3O
#N RHF/3-21+G* Iop(2/15=1) OPTCYC=1000

Optimisation
Energy = -75.8999

1  1
 O                  0.329210    0.000000    3.082707
 H                  0.239252    0.000000    4.061710
 H                  1.222030    0.000000    2.671111
 H                 -0.473653    0.000000    2.515299
```

```
%chk=H3O
#N RHF/3-21+G* Iop(2/15=1) OPTCYC=1000

Optimisation
Energy = -75.8999

1  1
 O                  0.329210    0.000000    3.082707
 H                  0.239252    0.000000    4.061710
 H                  1.222030    0.000000    2.671111
 H                 -0.473653    0.000000    2.515299
```

```
%chk=H2O
#n rhf/3-21+g* opt optcyc=1000

H2Oopt str from STO-3G-opt
Energy = -75.6193

0  1
 O                -0.089119    0.000000   -0.063016
 H                -0.102601    0.000000    0.901296
 H                 0.815550    0.000000   -0.397165
```

```
%chk=hcn3
#N RHF/3-21+G* OPT OPTCYC=1000

OPTIMISATION 3-21+G*

0  1
 C                 -0.499515    0.035252    0.018531
 N                  0.636048   -0.044994   -0.023578
 H                 -1.548736    0.109412    0.057436
```

```
%chk=NaCN
#N RHF/3-21+G* OPT OPTCYC=1000

NaCN opt
Energy = -252.6985

0  1
 C                  0.000000   -0.492488   -0.064052
 N                  0.000000    0.656688    0.086052
 Na                 0.000000   -2.640070   -0.344567
```

```
%chk=NaOH
#N RHF/3-21+G* OPT OPTCYC=1000

NaOH opt
Energy = -235.9452

0  1
 O                -0.784599    0.000000    0.590507
 H                -1.551481    0.000000    1.166100
 Na                0.711395    0.000000   -0.535290
```

```
%chk=Na
#N RHF/3-21+G* OPT OPTCYC=1000

Na opt
Energy = -160.6757

1  1
 Na                 0.000000    0.000000    0.000000
```

```
%chk=mech1st8
#N RHF/3-21+G* opt=(gdiis,modredundant) optcyc=20

Scan of OH grp (O27) attaching to C9 on cage

-1  1
 C                 -1.601301    1.270867    0.786601
 C                 -1.549929    0.718636   -0.551276
 C                 -1.262395   -0.744580   -0.255801
 C                 -0.685252    0.274300    1.571816
 C                 -0.800205   -0.995890    1.054408
 C                 -0.192995    1.023373   -1.026483
 C                  0.488593    1.686384    0.214083
 C                  0.733350    0.529924    1.110353
 C                  1.209526   -0.546697    0.028206
 C                  0.083552   -0.539458   -1.047822
 C                 -0.698992    2.534221    0.780785
 O                 -1.477012   -1.802964    1.742027
 C                  2.358361   -1.537118   -0.218953
 N                  3.220619   -2.265632   -0.391927
 O                  0.543150   -1.494061    0.893105
 H                 -2.604909    1.341060    1.159381
 H                 -2.286943    0.931788   -1.307812
 H                 -2.069297   -1.407743   -0.489396
 H                 -0.891404    0.470701    2.598770
 H                  0.020034    1.706246   -1.824265
 H                  1.413646    2.183769   -0.001182
 H                  1.403037    0.570528    1.937393
 H                  0.246519   -1.160467   -1.902172
 H                 -0.519941    2.969492    1.745033
 H                 -1.038538    3.327233    0.149885
 H                 -1.081770   -2.605832    2.090633
 O                  2.614984    1.182323   -0.941372
 H                  2.888454    1.792772   -0.249463

9   27   2.43   S   6   -0.1
```

```
%nproc=2
%chk=mech1s10S2
% %nosave

# #N RHF/3-21+G* OPT=(MODREDUNDANT,GDIIS) OPTCYC=20

Scan of bond bet C15-H27-to see if H moves to O12

0   1
C                    -1.00743   1.917     0.31798
 C                    -1.53676   1.0696   -0.87477
 C                    -1.44997  -0.43541  -0.4551
 C                    -0.17624   0.86307   1.09281
 C                    -1.01567  -0.40305   1.00716
 C                    -0.25867   0.88651  -1.77612
 C                     0.83943   1.64862  -0.9917
 C                     1.09862   0.67713   0.1891
 C                     1.06921  -0.71797  -0.46001
 C                    -0.17622  -0.61678  -1.35113
 C                     0.06379   2.80678  -0.33794
 C                     0.89002  -1.79128   0.57288
 N                     1.67988  -2.74995   0.71482
 O                     2.2465   -0.93816  -1.23865
 O                    -0.23967  -1.59547   1.33176
 O                    -2.07379  -0.34382   1.93811
 H                    -1.76692   2.40347   0.90981
 H                    -2.44792   1.42356  -1.32999
 H                    -2.28732  -1.08635  -0.65336
 H                     0.0523    1.12393   2.11477
 H                    -0.32823   1.11558  -2.8275
 H                     1.72265   1.89437  -1.55947
 H                     2.02384   0.8561    0.717
 H                    -0.21241  -1.37563  -2.11553
 H                     0.65454   3.361     0.38322
 H                    -0.3528    3.49587  -1.06443
 H                     1.46485  -3.41601   1.4427
 H                     2.7045   -1.74666  -0.95011
 H                    -2.49112  -1.20531   2.08055

15   27 2.4960 S   5 -0.200
```

```
%nproc=2
%chk=mech1str5S
%nosave

#N RHF/3-21+G* opt=(TS,NOEIGENTEST,gdiis,modredundant) optcyc=20

Scan of H26 towards O12

0  1

 C                  0.034197   -0.425728   -2.091392
 C                 -0.022056    1.074359   -1.677193
 C                  0.928210    1.293737   -0.455750
 C                  0.552731   -1.088337   -0.800268
 C                  1.510178   -0.085754   -0.144147
 C                 -1.265821    1.123782   -0.709794
 C                 -1.773116   -0.325373   -0.679979
 C                 -0.695849   -1.035606    0.176509
 C                 -0.219879   -0.020197    1.257767
 C                 -0.322950    1.347684    0.510429
 C                 -1.464711   -0.808635   -2.110455
 O                  2.909942   -0.316813   -0.150271
 C                 -0.755639   -0.114359    2.597328
 N                 -1.160836   -0.176876    3.661713
 O                  1.228297   -0.251373    1.315007
 H                  0.580668   -0.676637   -2.987639
 H                 -0.015471    1.795249   -2.479016
 H                  1.663892    2.077901   -0.419383
 H                  1.045262   -2.046377   -0.858358
 H                 -1.996973    1.888791   -0.922173
 H                 -2.785935   -0.463748   -0.328825
 H                 -1.038894   -1.984339    0.560013
 H                 -0.537377    2.185422    1.152038
 H                 -1.627776   -1.869296   -2.263999
 H                 -2.018251   -0.249922   -2.857452
 H                  2.719025   -0.486872    1.216594
```

```
%nproc=2
%chk=mech1s1S
%nosave

#N RHF/3-21+G* opt=(gdiis,modredundant) optcyc=20

Scan-stretch of bond bet.C9-C13

-1   1
 C                  1.330212   -0.258299    1.628809
 C                  0.949797    1.189530    1.178773
 C                 -0.618258    1.259968    1.117161
 C                  0.039308   -1.046652    1.252221
 C                 -1.031732   -0.068617    1.706281
 C                  1.018479    1.102189   -0.388389
 C                  1.445223   -0.376335   -0.637898
 C                  0.127092   -1.118953   -0.342962
 C                 -0.996191   -0.221264   -0.859019
 C                 -0.534586    1.170825   -0.468116
 C                  2.346392   -0.690876    0.567528
 O                 -1.914966   -0.277277    2.522911
 C                 -0.260436   -0.021684   -2.922712
 N                 -0.045688    0.041216   -4.064126
 O                 -2.190183   -0.573563   -0.911711
 H                  1.617155   -0.353321    2.667968
 H                  1.478155    1.983112    1.686214
 H                 -1.131144    2.110249    1.534944
 H                 -0.056724   -2.015874    1.716322
 H                  1.592225    1.840657   -0.925570
 H                  1.854558   -0.572876   -1.611725
 H                  0.062404   -2.130748   -0.708073
 H                 -1.009427    1.967780   -1.010105
 H                  2.611732   -1.741329    0.635266
 H                  3.250264   -0.088424    0.583981
```

```
%nproc=2
%chk=mech1s1S
%nosave
#N RHF/3-21+G* opt=(gdiis,modredundant) optcyc=20

Scan-stretch of bond bet.C9-C13

-1  1
 C                 -1.802432    1.169539    0.210048
 C                 -1.545203    0.524186   -1.172138
 C                 -1.075342   -0.931950   -0.957393
 C                 -0.965717    0.288214    1.160155
 C                 -1.098191   -1.218693    0.617825
 C                 -0.068376    0.956870   -1.501029
 C                  0.340029    1.795172   -0.271936
 C                  0.514175    0.707570    0.817954
 C                  1.022220   -0.574309    0.135807
 C                  0.400908   -0.499128   -1.265005
 C                 -0.982441    2.470995    0.130106
 O                 -1.979447   -2.007753    1.117833
 C                  2.719468   -0.660638    0.092282
 N                  3.872092   -0.727928    0.066305
 O                  0.378714   -1.674183    0.804891
 H                 -2.864487    1.276276    0.486269
 H                 -2.315661    0.713602   -1.933536
 H                 -1.523294   -1.711685   -1.586732
 H                 -1.226084    0.401112    2.225323
 H                  0.134811    1.410643   -2.481413
 H                  1.205423    2.463140   -0.417595
 H                  1.103668    1.036668    1.691788
 H                  0.938642   -1.007170   -2.077831
 H                 -0.922660    3.010971    1.089090
 H                 -1.354789    3.185718   -0.622064

9   13   1.7    S   5    0.1
```

```
%nproc=2

# opt=(gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity optcyc=200

TS search from mech1s8@1.83A

-1  1

 C                 -0.429201   -0.445968   -2.222999
 C                 -0.439735    1.046958   -1.803430
 C                  0.795520    1.296123   -0.884210
 C                  0.445681   -1.076475   -1.118437
 C                  1.510998   -0.050310   -0.708119
 C                 -1.379737    1.061130   -0.536928
 C                 -1.792060   -0.427738   -0.391191
 C                 -0.491900   -1.062177    0.149400
 C                  0.215709   -0.027381    1.076564
 C                 -0.134723    1.314200    0.376062
 C                 -1.852437   -0.913834   -1.856148
 O                  2.791070   -0.184498   -1.309548
 C                  0.003886   -0.151348    2.568091
 N                  0.666044   -0.568739    3.482078
 O                  1.630287   -0.206981    0.715014
 H                 -0.095974   -0.637350   -3.234462
 H                 -0.645455    1.751135   -2.597043
 H                  1.450939    2.130626   -1.072616
 H                  0.862604   -2.045315   -1.350607
 H                 -2.190124    1.775723   -0.514229
 H                 -2.675239   -0.616399    0.203049
 H                 -0.609259   -2.027239    0.618430
 H                 -0.119859    2.172732    1.024533
 H                 -1.979844   -1.988903   -1.937860
 H                 -2.624410   -0.413397   -2.434431
 H                  3.449687   -0.372219   -0.624977
 O                 -1.444728    0.441314    2.799386
 H                 -2.010409    0.474014    2.014912
```

```
%chk=mech1s10ts2
# opt=(gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity optcyc=200

TS search for mech1str10 using input@1.2964A from m1s10S2 optcyc=200

0  1
 C                  -1.994525    0.774489   -0.424787
 C                  -1.693551    0.476848    1.074045
 C                  -0.187735    0.829936    1.330176
 C                  -0.564300    0.762828   -1.027731
 C                   0.297909    1.462408    0.027970
 C                  -1.326441   -1.054307    1.060740
 C                  -1.461174   -1.439084   -0.434124
 C                  -0.199420   -0.768818   -1.035219
 C                   0.899861   -1.035049    0.007005
 C                   0.173965   -0.694836    1.315043
 C                  -2.611238   -0.543749   -0.926697
 C                   2.066890   -0.116136   -0.198697
 N                   3.237963   -0.521580   -0.362607
 O                   1.301619   -2.404735   -0.023673
 O                   1.701154    1.206733   -0.184359
 O                   0.211613    2.881364    0.001881
 H                  -2.566313    1.672743   -0.617406
 H                  -2.432994    0.824470    1.778509
 H                   0.085101    1.393339    2.207485
 H                  -0.472161    1.225092   -1.999947
 H                  -1.820881   -1.709127    1.760214
 H                  -1.531893   -2.496806   -0.631342
 H                   0.075236   -1.134156   -2.013768
 H                   0.663466   -1.094963    2.187547
 H                  -2.739511   -0.568065   -2.003149
 H                  -3.556921   -0.770226   -0.446904
 H                   3.949233    0.184030   -0.490495
 H                   2.262831   -2.477793   -0.158088
 H                  -0.697465    3.208454    0.008446

 1  2 1.0  4 1.0  11 1.0  17 1.0
 2  3 1.0  6 1.0  18 1.0
 3  5 1.0  10 1.0  19 1.0
 4  5 1.0  8 1.0  20 1.0
 5  15 1.0  16 1.0
 6  7 1.0  10 1.0  21 1.0
 7  8 1.0  11 1.0  22 1.0
 8  9 1.0  23 1.0
 9  10 1.0  12 1.0  14 1.0
 10  24 1.0
 11  25 1.0  26 1.0
 12  13 2.0  15 1.0
 13  27 1.0
 14  28 1.0
 15
 16  29 1.0
 17
 18
```

```
 Entering Gaussian System, Link 0=g98
 Input=mech1s8tsF.gjf
 Output=mech1s8tsF.out
 Initial command:
 /usr/g98/l1.exe /usr/scratch/Singh/Gau-13938.inp -
scrdir=/usr/scratch/Singh/
 Default is to use a total of   2 processors:
                                2 via shared-memory
                                1 via Linda
 Entering Link 1 = /usr/g98/l1.exe PID=     13857.
```

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

Cite this work as:
Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

```
**********************************************
Gaussian 98:  DEC-AXP-OSF/1-G98RevA.7 11-Apr-1999
                  19-Mar-2002
**********************************************
%nproc=2
Will use up to    2 processors via shared memory.
%chk=mech1s8tsF
%nosave
-------------------
#N RHF/3-21+G* FREQ
-------------------
1/10=4,30=1,38=1/1,3;
2/17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
```

```
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;
-------------------------------------
Freq calc of output str of mech1s8ts
-------------------------------------
Symbolic Z-matrix:
Charge = -1 Multiplicity = 1
C                    -0.4292   -0.44597  -2.223
C                    -0.43973   1.04696  -1.80343
C                     0.79552   1.29612  -0.88421
C                     0.44568  -1.07648  -1.11844
C                     1.511    -0.05031  -0.70812
C                    -1.37974   1.06113  -0.53693
C                    -1.79206  -0.42774  -0.39119
C                    -0.4919   -1.06218   0.1494
C                     0.21571  -0.02738   1.07656
C                    -0.13472   1.3142    0.37606
C                    -1.85244  -0.91383  -1.85615
O                     2.79107  -0.1845   -1.30955
C                     0.00389  -0.15135   2.56809
N                     0.66604  -0.56874   3.48208
O                     1.63029  -0.20698   0.71501
H                    -0.09597  -0.63735  -3.23446
H                    -0.64546   1.75114  -2.59704
H                     1.45094   2.13063  -1.07262
H                     0.8626   -2.04531  -1.35061
H                    -2.19012   1.77572  -0.51423
H                    -2.67524  -0.6164    0.20305
H                    -0.60926  -2.02724   0.61843
H                    -0.11986   2.17273   1.02453
H                    -1.97984  -1.9889   -1.93786
H                    -2.62441  -0.4134   -2.43443
H                     3.44969  -0.37222  -0.62498
O                    -1.44473   0.44131   2.79939
H                    -2.01041   0.47401   2.01491

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  94 maximum allowed number of steps= 168.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

--------------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
--------------------------------------------------------------------------
  1   1  C     0  -0.429201         -0.445968         -2.222999
  2   2  C     0  -0.439735          1.046958         -1.803430
  3   3  C     0   0.795520          1.296123         -0.884210
  4   4  C     0   0.445681         -1.076475         -1.118437
```

5	5	C	0	1.510998	-0.050310	-0.708119
6	6	C	0	-1.379737	1.061130	-0.536928
7	7	C	0	-1.792060	-0.427738	-0.391191
8	8	C	0	-0.491900	-1.062177	0.149400
9	9	C	0	0.215709	-0.027381	1.076564
10	10	C	0	-0.134723	1.314200	0.376062
11	11	C	0	-1.852437	-0.913834	-1.856148
12	12	O	0	2.791070	-0.184498	-1.309548
13	13	C	0	0.003886	-0.151348	2.568091
14	14	N	0	0.666044	-0.568739	3.482078
15	15	O	0	1.630287	-0.206981	0.715014
16	16	H	0	-0.095974	-0.637350	-3.234462
17	17	H	0	-0.645455	1.751135	-2.597043
18	18	H	0	1.450939	2.130626	-1.072616
19	19	H	0	0.862604	-2.045315	-1.350607
20	20	H	0	-2.190124	1.775723	-0.514229
21	21	H	0	-2.675239	-0.616399	0.203049
22	22	H	0	-0.609259	-2.027239	0.618430
23	23	H	0	-0.119859	2.172732	1.024533
24	24	H	0	-1.979844	-1.988903	-1.937860
25	25	H	0	-2.624410	-0.413397	-2.434431
26	26	H	0	3.449687	-0.372219	-0.624977
27	27	O	0	-1.444728	0.441314	2.799386
28	28	H	0	-2.010409	0.474014	2.014912

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.429201	-0.445968	-2.222999
2	6	0	-0.439735	1.046958	-1.803430
3	6	0	0.795520	1.296123	-0.884210
4	6	0	0.445681	-1.076475	-1.118437
5	6	0	1.510998	-0.050310	-0.708119
6	6	0	-1.379737	1.061130	-0.536928
7	6	0	-1.792060	-0.427738	-0.391191
8	6	0	-0.491900	-1.062177	0.149400
9	6	0	0.215709	-0.027381	1.076564
10	6	0	-0.134723	1.314200	0.376062
11	6	0	-1.852437	-0.913834	-1.856148
12	8	0	2.791070	-0.184498	-1.309548
13	6	0	0.003886	-0.151348	2.568091
14	7	0	0.666044	-0.568739	3.482078
15	8	0	1.630287	-0.206981	0.715014
16	1	0	-0.095974	-0.637350	-3.234462
17	1	0	-0.645455	1.751135	-2.597043
18	1	0	1.450939	2.130626	-1.072616
19	1	0	0.862604	-2.045315	-1.350607
20	1	0	-2.190124	1.775723	-0.514229
21	1	0	-2.675239	-0.616399	0.203049
22	1	0	-0.609259	-2.027239	0.618430
23	1	0	-0.119859	2.172732	1.024533
24	1	0	-1.979844	-1.988903	-1.937860

25	1	0	-2.624410	-0.413397	-2.434431
26	1	0	3.449687	-0.372219	-0.624977
27	8	0	-1.444728	0.441314	2.799386
28	1	0	-2.010409	0.474014	2.014912

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.550799	0.000000			
3	C	2.515388	1.559777	0.000000		
4	C	1.543702	2.400447	2.409662	0.000000	
5	C	2.493146	2.491799	1.534861	1.535017	0.000000
6	C	2.453100	1.577286	2.215303	2.870481	3.101766
7	C	2.283252	2.449067	3.148068	2.440744	3.339624
8	C	2.451922	2.874842	2.878781	1.576919	2.402252
9	C	3.387955	3.142957	2.435668	2.443668	2.205310
10	C	3.152781	2.216898	1.566513	2.878493	2.397026
11	C	1.542426	2.417274	3.583329	2.419094	3.657368
12	O	3.357515	3.492636	2.520986	2.516544	1.420672
13	C	4.819638	4.554441	3.826257	3.826425	3.607651
14	N	5.810554	5.636472	4.749626	4.633691	4.305864
15	O	3.595904	3.492838	2.348122	2.349650	1.436692
16	H	1.082000	2.236720	3.171240	2.227955	3.051128
17	H	2.239182	1.080744	2.284128	3.372274	3.385783
18	H	3.390744	2.298494	1.077713	3.361271	2.212001
19	H	2.233325	3.385748	3.374498	1.079990	2.193912
20	H	3.310084	2.292815	3.046469	3.930340	4.131621
21	H	3.310505	3.433685	4.109263	3.420254	4.321489
22	H	3.256771	3.917248	3.908461	2.243559	3.188020
23	H	4.183270	3.060566	2.291214	3.933129	3.256331
24	H	2.206002	3.406825	4.427665	2.717931	4.178084
25	H	2.205608	2.702518	4.125720	3.405433	4.495952
26	H	4.195818	4.304697	3.145659	3.124665	1.966991
27	O	5.200280	4.750024	4.395258	4.607241	4.613090
28	H	4.615894	4.168335	4.117525	4.272502	4.482200

		6	7	8	9	10
6	C	0.000000				
7	C	1.551766	0.000000			
8	C	2.401611	1.544399	0.000000		
9	C	2.516676	2.519073	1.559213	0.000000	
10	C	1.564498	2.523845	2.413735	1.553495	0.000000
11	C	2.421625	1.544679	2.428022	3.696461	3.591300
12	O	4.420878	4.680558	3.698208	3.514356	3.694271
13	C	3.609108	3.472631	2.631631	1.511585	2.640461
14	N	4.795217	4.589594	3.562451	2.506465	3.719412
15	O	3.497958	3.603454	2.356896	1.471056	2.354600
16	H	3.436506	3.317354	3.433330	4.365106	4.104380
17	H	2.293327	3.305749	3.934622	4.171344	3.048133
18	H	3.073029	4.186479	3.932167	3.286603	2.297726
19	H	3.916653	3.253348	2.247501	3.222063	3.906711
20	H	1.080688	2.242506	3.373136	3.401447	2.286984
21	H	2.244993	1.081073	2.229028	3.076939	3.195523
22	H	3.386224	2.230864	1.079401	2.211310	3.383658
23	H	2.293711	3.400437	3.371781	2.226165	1.076017

24	H	3.409610	2.205603	2.725702	4.213641	4.434997
25	H	2.706281	2.206319	3.412433	4.532369	4.133038
26	H	5.038410	5.247252	4.075759	3.670527	4.085839
27	O	3.394022	3.325007	3.192302	2.438205	2.889730
28	H	2.693388	2.578791	2.854100	2.467285	2.628676
		11	12	13	14	15
11	C	0.000000				
12	O	4.732109	0.000000			
13	C	4.858108	4.775519	0.000000		
14	N	5.912571	5.255764	1.203346	0.000000	
15	O	4.386329	2.333832	2.466206	2.952503	0.000000
16	H	2.249746	3.499342	5.823727	6.759977	4.331692
17	H	3.017912	4.148978	5.542535	6.637587	4.470228
18	H	4.560148	2.685496	4.533885	5.352370	2.948253
19	H	2.984505	2.680169	4.436294	5.057050	2.869773
20	H	3.024648	5.411773	4.245937	5.442855	4.476348
21	H	2.237356	5.688148	3.603804	4.681717	4.355145
22	H	2.984744	4.321462	2.774183	3.457470	2.887600
23	H	4.563665	4.413386	2.792711	3.764682	2.970159
24	H	1.085672	5.139287	5.255034	6.196234	4.821414
25	H	1.086642	5.535809	5.657017	6.771728	5.297552
26	H	5.470068	0.968325	4.702979	4.965399	2.265634
27	O	4.865866	5.934388	1.582159	2.437547	3.771022
28	H	4.115359	5.877063	2.180474	3.225416	3.925322
		16	17	18	19	20
16	H	0.000000				
17	H	2.532409	0.000000			
18	H	3.837735	2.619687	0.000000		
19	H	2.539714	4.270934	4.226334	0.000000	
20	H	4.196195	2.593207	3.700688	4.961755	0.000000
21	H	4.297619	4.191152	5.118478	4.119706	2.544027
22	H	4.127957	4.961521	4.938815	2.458417	4.271366
23	H	5.102565	3.683722	2.620537	4.939478	2.609866
24	H	2.656471	4.025295	5.430418	2.903026	4.030304
25	H	2.661427	2.937329	4.993502	3.999637	2.944151
26	H	4.410376	5.016758	3.234132	3.165247	6.036008
27	O	6.276143	5.610340	5.121627	5.359995	3.649152
28	H	5.697027	4.976371	4.925254	5.091949	2.850140
		21	22	23	24	25
21	H	0.000000				
22	H	2.535998	0.000000			
23	H	3.870924	4.247845	0.000000		
24	H	2.636443	2.900792	5.436407	0.000000	
25	H	2.645769	3.998160	4.992521	1.773208	0.000000
26	H	6.185464	4.556336	4.683943	5.815250	6.338018
27	O	3.061679	3.398284	2.811261	5.351056	5.432773
28	H	2.216720	3.188989	2.727760	4.657392	4.578335
		26	27	28		
26	H	0.000000				
27	O	6.028548	0.000000			
28	H	6.123542	0.967711	0.000000		

Interatomic angles:

C1-C2-C3=107.9295 C2-C1-C4=101.7393 C1-C4-C3= 75.5033
C3-C2-C4= 71.3991 C1-C2-C5= 71.922 C1-C5-C3= 72.9468

C2-C3-C5=107.2562 C1-C4-C5=108.1525 C2-C4-C5= 74.9839
C3-C5-C4=103.4298 C1-C2-C6=103.2935 C1-C6-C3= 64.9723
C3-C2-C6= 89.8467 C4-C1-C6= 88.7815 C4-C2-C6= 89.9219
C4-C3-C6= 76.599 C5-C1-C6= 77.6676 C5-C2-C6= 96.7511
C5-C3-C6=110.2847 C5-C4-C6= 83.648 C2-C1-C7= 76.7737
C3-C1-C7= 81.8415 C3-C2-C7=101.166 C4-C1-C7= 76.5552
C2-C4-C7= 60.773 C3-C4-C7= 80.9346 C5-C1-C7= 88.6112
C5-C2-C7= 85.0464 C5-C4-C7=112.269 C1-C7-C6= 76.9213
C2-C6-C7=103.0114 C3-C6-C7=112.1733 C4-C7-C6= 89.0503
C2-C1-C8= 88.8534 C3-C1-C8= 70.824 C3-C2-C8= 74.4099
C1-C4-C8=103.5688 C2-C4-C8= 90.1203 C3-C4-C8= 89.9565
C1-C8-C5= 61.799 C2-C5-C8= 71.9212 C3-C5-C8= 91.2492
C5-C4-C8=101.0497 C1-C8-C6= 60.7087 C2-C6-C8= 90.0692
C3-C6-C8= 77.0314 C4-C8-C6= 89.8884 C5-C8-C6= 80.4336
C1-C7-C8= 76.9999 C2-C7-C8= 89.1033 C3-C8-C7= 85.0826
C4-C8-C7=102.8757 C5-C8-C7=113.8234 C6-C7-C8=101.7319
C1-C3-C9= 86.3437 C2-C3-C9=101.4843 C1-C4-C9=114.4584
C2-C4-C9= 80.9 C4-C3-C9= 60.5716 C1-C5-C9= 92.0798
C2-C5-C9= 83.7616 C3-C5-C9= 79.0431 C4-C5-C9= 79.3765
C1-C6-C9= 85.945 C2-C6-C9= 97.6488 C6-C3-C9= 65.3176
C4-C9-C6= 70.6988 C5-C9-C6= 81.837 C1-C7-C9= 89.5979
C2-C7-C9= 78.4738 C3-C9-C7= 78.8744 C7-C4-C9= 62.0934
C5-C9-C7= 89.7111 C7-C6-C9= 72.1364 C1-C8-C9=113.3879
C2-C8-C9= 84.7668 C3-C9-C8= 89.4248 C4-C8-C9=102.373
C5-C9-C8= 77.199 C6-C8-C9= 75.5785 C7-C8-C9=108.5156
C1-C2-C10=112.4018 C1-C3-C10= 98.4561 C2-C3-C10= 90.3256
C1-C4-C10= 85.2967 C4-C2-C10= 77.0172 C4-C3-C10= 90.1919
C1-C5-C10= 80.2628 C2-C10-C5= 65.2392 C5-C3-C10=101.2236
C4-C5-C10= 91.4305 C1-C6-C10=101.0766 C2-C6-C10= 89.7579
C3-C10-C6= 90.0696 C4-C6-C10= 74.4912 C5-C10-C6=100.9723
C1-C7-C10= 81.8041 C7-C2-C10= 65.2692 C3-C10-C7= 97.8983
C4-C7-C10= 70.8511 C5-C10-C7= 85.4376 C7-C6-C10=108.1705
C1-C8-C10= 80.7727 C2-C10-C8= 76.6227 C3-C10-C8= 90.0553
C4-C8-C10= 89.7963 C8-C5-C10= 60.3889 C8-C6-C10= 71.4611
C7-C8-C10= 75.7001 C2-C10-C9=111.7307 C3-C10-C9=102.6414
C4-C9-C10= 89.2519 C5-C9-C10= 77.0887 C6-C10-C9=107.6356
C7-C9-C10= 72.2255 C8-C9-C10=101.6907 C2-C1-C11=102.791
C3-C1-C11=122.192 C3-C2-C11=127.2474 C4-C1-C11=103.2308
C4-C2-C11= 60.2801 C3-C4-C11= 95.8178 C5-C1-C11=128.4403
C5-C2-C11= 96.3102 C5-C4-C11=134.0969 C1-C11-C6= 72.6666
C6-C2-C11= 71.1258 C3-C6-C11=101.1152 C4-C11-C6= 72.7384
C1-C11-C7= 95.3962 C2-C11-C7= 72.615 C4-C11-C7= 72.2304
C6-C7-C11=102.9001 C1-C11-C8= 72.4187 C2-C11-C8= 72.7865
C3-C8-C11= 84.4895 C8-C4-C11= 71.3214 C5-C8-C11= 98.4304
C8-C6-C11= 60.4488 C8-C7-C11=103.6269 C9-C4-C11= 98.9548
C9-C6-C11= 96.9074 C9-C7-C11=129.3275 C9-C8-C11=134.8232
C10-C2-C11=101.5154 C10-C4-C11= 84.8905 C10-C6-C11=127.2409
C10-C7-C11=122.085 C10-C8-C11= 95.7584 C1-C3-O12= 83.6185
C2-C3-O12=115.6982 C1-C4-O12=109.2136 C2-C4-O12= 90.4902
C3-C4-O12= 61.5156 C1-C5-O12=115.4026 C2-C5-O12=124.1174
C3-C5-O12=117.0204 C4-C5-O12=116.6809 C6-C3-O12=137.852
C6-C4-O12=110.1276 C7-C4-O12=141.526 C8-C3-O12= 86.1839
C8-C4-O12=127.7321 C8-C5-O12=149.6071 C9-C3-O12= 90.2932
C9-C4-O12= 90.2152 C9-C5-O12=150.7856 C10-C3-O12=127.7759

C10-C4-O12= 86.1567 C10-C5-O12=149.7536 C11-C4-O12=146.9706
C1-C8-C13=142.8897 C2-C8-C13=111.5293 C3-C8-C13= 87.8341
C4-C8-C13=129.055 C5-C8-C13= 91.4451 C6-C8-C13= 91.5071
C7-C8-C13=109.763 C3-C9-C13=150.7229 C4-C9-C13=149.8029
C5-C9-C13=151.6402 C6-C9-C13=125.3976 C7-C9-C13=116.7566
C8-C9-C13=117.9513 C2-C10-C13=139.1545 C3-C10-C13=129.0722
C4-C10-C13= 87.6767 C5-C10-C13= 91.3461 C6-C10-C13=115.8778
C7-C10-C13= 84.4775 C10-C8-C13= 62.9392 C10-C9-C13=118.9568
C11-C8-C13=147.5207 C3-C9-N14=147.9078 C4-C9-N14=138.8012
C5-C9-N14=131.982 C6-C9-N14=145.3476 C7-C9-N14=131.9179
C8-C9-N14=120.5894 C10-C9-N14=131.2854 C8-C13-N14=132.9763
C9-C13-N14=134.4909 C10-C13-N14=148.4243 C1-C3-O15= 95.2927
C2-C3-O15=125.4965 C1-C4-O15=133.8617 C2-C4-O15= 94.6624
C3-O15-C4= 61.7193 C1-C5-O15=130.4808 C2-C5-O15=123.26
C3-C5-O15=104.3599 C4-C5-O15=104.4483 C6-C3-O15=100.0442
C6-C4-O15= 83.5095 C7-C4-O15= 97.5488 C1-C8-O15= 96.7758
C2-C8-O15= 83.1352 C3-O15-C8= 75.447 C8-C4-O15= 70.6728
C5-O15-C8= 74.1624 C6-C8-O15= 94.626 C7-C8-O15=133.8652
C3-O15-C9= 75.3675 C4-O15-C9= 75.6499 C5-O15-C9= 98.6443
C6-C9-O15=120.321 C7-C9-O15=127.144 C8-C9-O15=102.0771
C2-C10-O15= 99.6006 C10-C3-O15= 70.766 C4-O15-C10= 75.4528
C5-O15-C10= 74.021 C6-C10-O15=125.1717 C7-C10-O15= 95.1698
C8-O15-C10= 61.6353 C10-C9-O15=102.2118 C11-C4-O15=133.7909
C11-C8-O15=132.8908 C3-O15-O12= 65.1552 C4-O15-O12= 65.0022
O12-C5-O15=109.5259 C8-O15-O12=104.0729 C9-O15-O12=133.6544
C10-O15-O12=103.9887 C3-O15-C13=105.2397 C4-O15-C13=105.1994
C5-O15-C13=133.3994 C8-O15-C13= 66.0903 C13-C9-O15=111.5464
C10-O15-C13= 66.3748 O12-O15-C13=168.4082 C3-O15-N14=126.9143
C4-O15-N14=121.4199 C5-O15-N14=156.148 C8-O15-N14= 83.4765
N14-C9-O15= 92.1053 C10-O15-N14= 88.2385 O12-O15-N14=167.5844
N14-C13-O15=101.5368 C2-C1-H16=115.1685 C3-C1-H16=118.0404
C3-C2-H16=112.0629 C4-C1-H16=114.967 C2-H16-C4= 65.0477
C3-C4-H16= 86.1899 C5-C1-H16=110.8797 C5-C2-H16= 80.1724
C5-C4-H16=106.9083 C6-C1-H16=150.5188 C6-C2-H16=127.7406
C6-C4-H16= 83.7437 C7-C1-H16=159.2634 C7-C2-H16= 90.0209
C7-C4-H16= 90.4416 C8-C1-H16=150.217 C8-C2-H16= 83.3922
C8-C4-H16=128.1169 C9-C4-H16=138.2122 C10-C2-H16=134.3168
C10-C4-H16=106.2838 C11-C1-H16=116.9271 C2-H16-C11= 65.2022
C4-H16-C11= 65.3997 C6-C11-H16= 94.6532 C7-C11-H16=120.7867
C8-C11-H16= 94.363 O12-C4-H16= 94.8528 O15-C4-H16=142.2548
C1-C2-H17=115.4596 C1-H17-C3= 67.5638 C3-C2-H17=118.6474
C4-C1-H17=125.1012 C4-C2-H17=148.8852 C4-C3-H17= 91.8143
C5-C1-H17= 91.1999 C5-C2-H17=139.3514 C5-C3-H17=123.7012
C1-H17-C6= 65.5212 C6-C2-H17=118.0561 C6-C3-H17= 61.2641
C4-C6-H17= 80.7039 C7-C1-H17= 93.9299 C7-C2-H17=135.2896
C7-C6-H17=117.266 C8-C1-H17=113.9382 C8-C2-H17=166.7505
C8-C3-H17= 98.6445 C8-C6-H17=113.851 C9-C3-H17=124.1765
C9-C6-H17=120.2039 C10-C2-H17=132.0343 C10-C3-H17=103.083
C10-C6-H17=102.7535 C11-C1-H17=104.3738 C11-C2-H17=113.6573
C11-C6-H17= 79.5435 O12-C3-H17=119.331 O15-C3-H17=149.5999
H16-C1-H17= 92.7021 H16-C2-H17= 92.8712 C3-H17-H16= 82.1824
C4-H16-H17= 89.9764 C6-H17-H16= 90.6764 C11-H16-H17= 78.0124
C1-C2-H18=122.2971 C1-C3-H18=137.6751 C2-C3-H18=120.1519
C4-C2-H18= 91.3134 C4-C3-H18=146.4825 C1-C5-H18= 92.0181

C2-H18-C5= 67.038 C5-C3-H18=114.5716 C4-C5-H18=126.6
C6-C2-H18=103.3371 C6-C3-H18=134.9676 C7-C2-H18=123.6938
C8-C2-H18= 98.328 C8-C3-H18=165.713 C8-C5-H18=116.8389
C9-C3-H18=134.9317 C9-C5-H18= 96.1513 C2-C10-H18= 61.1797
C10-C3-H18=119.5281 C4-C10-H18= 80.1314 C5-H18-C10= 64.1839
C6-C10-H18=103.8111 C7-C10-H18=120.4469 C8-C10-H18=113.1247
C9-C10-H18=115.8156 C11-C2-H18=150.4699 C2-H18-O12= 88.624
O12-C3-H18= 86.7828 C4-O12-H18= 80.4316 O12-C5-H18= 92.7417
C10-H18-O12= 95.3758 C13-C10-H18=133.1881 C2-H18-O15= 82.473
O15-C3-H18=113.4864 C4-O15-H18= 77.8547 O15-C5-H18=105.8428
C8-O15-H18= 95.0147 C9-O15-H18= 89.6404 O15-C10-H18= 78.6392
O15-O12-H18= 71.5527 C13-O15-H18=113.4276 N14-O15-H18=130.2058
H16-C2-H18=115.5965 C1-H17-H18= 88.146 H17-C2-H18= 94.7532
H17-C3-H18= 95.6424 C5-H18-H17= 88.5554 C6-H17-H18= 77.119
C10-H18-H17= 76.3001 O12-H18-H17=102.8924 O15-H18-H17=106.6579
H16-H17-H18= 96.2843 C2-C1-H19=125.9904 C3-C1-H19= 90.3688
C1-C4-H19=115.5545 C2-C4-H19=150.9985 C3-C4-H19=148.0092
C1-H19-C5= 68.5396 C2-C5-H19= 92.3115 C3-C5-H19=128.7803
C5-C4-H19=112.9078 C6-C1-H19=113.3039 C6-C4-H19=163.1545
C7-C1-H19= 92.1539 C7-C4-H19=131.0281 C1-H19-C8= 66.3498
C2-C8-H19= 81.7571 C3-C8-H19= 81.3265 C8-C4-H19=114.2363
C5-H19-C8= 65.4735 C6-C8-H19=114.7596 C7-C8-H19=116.9649
C9-C4-H19=127.9197 C9-C5-H19= 94.1784 C9-C8-H19=114.4356
C10-C4-H19=159.1486 C10-C5-H19=116.5634 C10-C8-H19=113.8383
C11-C1-H19=102.9203 C2-C11-H19= 76.8311 C11-C4-H19=111.1919
C5-H19-C11= 88.494 C6-C11-H19= 92.2545 C7-C11-H19= 85.5896
C11-C8-H19= 79.2309 C1-H19-O12= 85.6974 C3-O12-H19= 80.839
O12-C4-H19= 86.6666 O12-C5-H19= 93.2348 C8-H19-O12= 96.8753
C11-H19-O12=113.2001 C13-C8-H19=130.6372 C1-H19-O15= 88.6911
C3-O15-H19= 79.9061 O15-C4-H19=107.7633 O15-C5-H19=102.4427
O15-C8-H19= 77.0697 C9-O15-H19= 89.8784 C10-O15-H19= 96.2986
C11-H19-O15= 97.0318 O15-O12-H19= 69.4348 C13-O15-H19=112.264
N14-O15-H19=120.579 H16-C1-H19= 93.4601 C2-H16-H19= 90.0516
H16-C4-H19= 93.8126 C5-H19-H16= 79.9013 C8-H19-H16= 91.4373
C11-H16-H19= 76.8269 O12-H19-H16= 84.1479 O15-H19-H16=106.2451
H17-C1-H19=145.4655 H17-H16-H19=114.7124 H18-C5-H19=147.1703
H18-O12-H19=103.9352 H18-O15-H19= 93.1644 C1-C2-H20=117.6
C3-C2-H20=102.8528 C4-C2-H20=113.7225 C5-C2-H20=119.3709
C1-C6-H20=135.3363 C2-C6-H20=118.0153 C3-C6-H20=132.0266
C4-C6-H20=166.7903 C1-C7-H20= 94.0014 C2-H20-C7= 65.3561
C4-C7-H20=114.0519 C7-C6-H20=115.6716 C8-C2-H20= 80.6416
C8-C6-H20=148.8515 C8-C7-H20=124.91 C9-C6-H20=138.4105
C9-C7-H20= 90.9904 C2-C10-H20= 61.181 C3-C10-H20=102.8761
C4-C10-H20= 98.4361 C5-C10-H20=123.7691 C10-C6-H20=118.5242
C7-H20-C10= 67.7169 C8-C10-H20= 91.6694 C9-C10-H20=123.5419
C11-C2-H20= 79.8589 C11-C6-H20=113.8499 C11-C7-H20=104.4916
C13-C10-H20=118.8397 O15-C10-H20=149.3288 H16-C2-H20=135.7595
C1-H17-H20= 86.139 H17-C2-H20= 93.4672 C3-H17-H20= 77.0192
H17-C6-H20= 93.4407 C7-H20-H17= 85.9295 C10-H20-H17= 77.0213
H16-H17-H20=109.8984 H18-C2-H20=107.4178 H18-C10-H20=107.6425
H18-H17-H20= 90.4538 C1-C6-H21= 89.4889 C2-C6-H21=127.0032
C3-C6-H21=134.2321 C4-C6-H21= 82.9516 C1-C7-H21=158.0073
C2-C7-H21=150.8268 C4-C7-H21=150.0425 C6-C7-H21=115.8576
C1-C8-H21= 89.8897 C2-C8-H21= 83.5349 C3-C8-H21=106.4307

C4-C8-H21=127.124 C5-C8-H21=137.8186 C6-H21-C8= 64.9296
C8-C7-H21=115.0656 C9-C6-H21= 80.2887 C9-C7-H21=111.0137
C9-C8-H21=107.3066 C10-C6-H21=112.814 C10-C7-H21=119.3281
C10-C8-H21= 86.8925 C1-C11-H21=121.1925 C2-C11-H21= 94.992
C4-C11-H21= 94.4525 C6-H21-C11= 65.4022 C11-C7-H21=115.7508
C8-H21-C11= 65.8607 C13-C8-H21= 95.3475 O15-C8-H21=143.4771
H16-C11-H21=146.5796 H17-C6-H21=134.8846 H19-C8-H21=133.9367
H19-C11-H21=103.2413 C2-H20-H21= 90.3002 H20-C6-H21= 93.1211
H20-C7-H21= 93.2457 C8-H21-H20= 89.6838 C10-H20-H21= 82.6383
C11-H21-H20= 78.1928 H17-H20-H21=109.337 C1-C4-H22=117.4213
C2-C4-H22=114.9828 C3-C4-H22=114.2219 C5-C4-H22=113.7463
C6-C4-H22= 81.9365 C1-C7-H22= 92.3435 C2-C7-H22=113.5743
C4-H22-C7= 66.1153 C6-C7-H22=126.125 C1-C8-H22=130.3842
C2-C8-H22=162.3787 C3-C8-H22=159.564 C4-C8-H22=113.9473
C5-C8-H22=128.4887 C6-C8-H22=150.9798 C7-C8-H22=115.3313
C3-C9-H22=114.4217 C4-H22-C9= 66.5291 C5-C9-H22= 92.4104
C6-C9-H22= 91.2508 C7-H22-C9= 69.0922 C9-C8-H22=112.6016
C10-C4-H22= 81.6748 C10-C7-H22= 90.522 C10-C8-H22=148.817
C10-C9-H22=127.1163 C1-C11-H22= 85.7571 C2-C11-H22= 92.3549
C11-C4-H22= 79.5067 C6-C11-H22= 76.7778 C11-C7-H22=102.9621
C11-C8-H22=110.6477 C9-H22-C11= 89.4151 O12-C4-H22=130.3326
C4-H22-C13= 98.8349 C7-H22-C13= 87.1581 C13-C8-H22= 86.0182
C13-C9-H22= 94.4725 C10-C13-H22= 77.3073 C11-H22-C13=114.9911
N14-C9-H22= 94.0445 N14-C13-H22=114.8894 C3-O15-H22= 96.0283
O15-C4-H22= 77.8659 C5-O15-H22= 88.3504 C7-H22-O15= 88.5318
O15-C8-H22=108.544 O15-C9-H22=101.3856 C10-O15-H22= 79.6922
C11-H22-O15= 96.6392 O12-O15-H22=111.2726 O15-C13-H22= 66.574
N14-O15-H22= 72.5916 H16-C4-H22=134.787 H16-C11-H22=103.2143
H18-O15-H22=115.6166 C1-H19-H22= 87.7819 H19-C4-H22= 88.1538
C5-H19-H22= 86.3134 C7-H22-H19= 87.7204 H19-C8-H22= 87.9619
C9-H22-H19= 87.0898 C11-H19-H22= 65.6842 O12-H19-H22=114.4193
C13-H22-H19=115.8194 O15-H19-H22= 65.0987 H16-H19-H22=111.3494
H20-C7-H22=145.4315 C4-H22-H21= 91.1747 C6-H21-H22= 89.976
H21-C7-H22= 93.397 H21-C8-H22= 93.5459 C9-H22-H21= 80.4871
C11-H21-H22= 77.1262 C13-H22-H21= 85.3529 O15-H22-H21=106.6555
H19-H22-H21=111.1397 H20-H21-H22=114.4527 C1-C3-H23=120.9204
C2-C3-H23=103.6314 C4-C3-H23=113.5585 C5-C3-H23=115.2321
C1-C6-H23=123.5596 C2-C6-H23=102.9224 C6-C3-H23= 61.1638
C4-C6-H23= 98.5984 C7-C6-H23=123.1615 C8-C3-H23= 80.5403
C8-C6-H23= 91.7688 C3-H23-C9= 65.2367 C4-C9-H23=114.6755
C5-C9-H23= 94.5826 C6-H23-C9= 67.6508 C7-C9-H23= 91.3357
C8-C9-H23=125.0011 C2-C10-H23=133.6755 C3-C10-H23=119.068
C4-C10-H23=166.5997 C5-C10-H23=135.8315 C6-C10-H23=119.4555
C7-C10-H23=137.9851 C8-C10-H23=147.5828 C9-C10-H23=114.4673
C11-C6-H23=150.846 O12-C3-H23=132.9616 C3-H23-C13= 97.1432
C6-H23-C13= 89.8449 C8-C13-H23= 76.8027 C13-C9-H23= 94.7605
C13-C10-H23= 86.6645 N14-C9-H23=105.2464 N14-C13-H23=137.1251
O15-C3-H23= 79.6049 C4-O15-H23= 94.6305 C5-O15-H23= 88.1049
C6-H23-O15= 82.2082 C8-O15-H23= 77.5939 O15-C9-H23=105.0622
O15-C10-H23=114.7309 O12-O15-H23=112.071 O15-C13-H23= 68.4505
N14-O15-H23= 78.9343 H17-C3-H23=107.2445 H17-C6-H23=106.8489
C2-H18-H23= 76.6418 H18-C3-H23= 95.2989 C5-H18-H23= 84.275
C6-H23-H18= 77.0951 C9-H23-H18= 84.9784 H18-C10-H23= 94.9871
O12-H18-H23=112.5558 C13-H23-H18=113.7275 O15-H18-H23= 64.1491

H17-H18-H23= 89.3316
H19-O15-H23=115.5071
C2-H20-H23= 76.955
C3-H23-H20= 76.5582
H20-C6-H23= 94.4239
C7-H20-H23= 88.6427
C9-H23-H20= 89.0267
H20-C10-H23= 94.9339
C13-H23-H20=103.5581
O15-H23-H20=106.5047
H17-H20-H23= 90.1426
H18-H23-H20= 90.069
H21-C6-H23=117.0463
H21-H20-H23= 97.3577
H22-C9-H23=146.3787
H22-C13-H23= 99.468
H22-O15-H23= 92.9544
C2-C1-H24=129.3147
C3-C1-H24=139.2754
C4-C1-H24= 91.1584
C2-C4-H24= 83.2095
C3-C4-H24=119.3019
C5-C1-H24=125.414
C5-C4-H24=157.5715
C6-C1-H24= 93.9274
C6-C4-H24= 75.1411
C1-H24-C7= 62.3369
C2-C7-H24= 93.9481
C4-C7-H24= 71.3964
C6-C7-H24=129.4861
C8-C1-H24= 71.4087
C2-C8-H24= 74.8807
C3-C8-H24=104.342
C8-C4-H24= 73.4316
C5-C8-H24=108.9657
C6-C8-H24= 83.1049
C8-C7-H24= 91.5107
C9-C4-H24=109.3262
C9-C7-H24=126.0817
C9-C8-H24=158.2388
C10-C4-H24=104.7975
C10-C7-H24=139.2547
C10-C8-H24=119.1713
C1-C11-H24=113.0014
C2-C11-H24=150.8634
C4-C11-H24= 93.8911
C6-C11-H24=150.6331
C7-C11-H24=112.8042
C8-C11-H24= 93.8662
O12-C4-H24=158.0967
C13-C8-H24=157.5669
O15-C4-H24=144.0379
O15-C8-H24=143.0033
H16-C1-H24=102.3332
C2-H16-H24= 87.8139
C4-H16-H24= 66.9559
C7-H24-H16= 85.5133
C8-H24-H16= 79.2605
H16-C11-H24= 99.6255
H17-C1-H24=129.7909
H17-H16-H24=101.7203
H19-C1-H24= 81.6752
H19-C4-H24= 88.7705
C5-H19-H24=109.3262
C7-H24-H19= 77.7919
H19-C8-H24= 70.6818
C11-H24-H19= 83.6335
O12-H19-H24=133.9575
O15-H19-H24=113.2711
H19-H16-H24= 67.8867
H20-C7-H24=129.9341
C1-H24-H21= 85.7707
C4-H24-H21= 79.3855
C6-H21-H24= 88.2312
H21-C7-H24=101.0917
C8-H21-H24= 67.5416
H21-C11-H24= 99.0766
H16-H24-H21=108.5746
H19-H24-H21= 95.9757
H20-H21-H24=102.1373
C1-H24-H22= 77.9379
H22-C4-H24= 70.8231
H22-C7-H24= 81.6631
H22-C8-H24= 88.2474
C9-H22-H24=110.2972
C11-H24-H22= 83.7604
C13-H22-H24=135.6281
O15-H22-H24=112.8048
H16-H24-H22= 95.8417
H19-H22-H24= 64.986
H22-H21-H24= 68.1927
C2-C1-H25= 90.2841
C3-C1-H25=121.6945
C3-C2-H25=149.7819
C4-C1-H25=129.6945
C4-C2-H25= 83.4999
C5-C1-H25=146.1447
C5-C2-H25=119.837
C6-C1-H25= 70.8015
C6-C2-H25= 73.1761
C3-C6-H25=113.5461
C4-C6-H25= 75.2081
C1-H25-C7= 62.3318
C2-C7-H25= 70.7542
C4-C7-H25= 94.1099
C6-C7-H25= 90.4028
C8-C1-H25= 94.0721
C8-C2-H25= 75.374
C8-C6-H25= 83.6088
C8-C7-H25=130.1227
C9-C6-H25=120.3597
C9-C7-H25=147.0601
C10-C2-H25=113.9481
C10-C6-H25=149.6893
C10-C7-H25=121.6534
C1-C11-H25=112.9082
C2-C11-H25= 93.0509
C4-C11-H25=150.2437
C6-C11-H25= 93.0377
C7-C11-H25=112.8022
C8-C11-H25=149.9738
H16-C1-H25=102.6809
C2-H16-H25= 66.3156
C4-H16-H25= 87.8253
C6-H25-H16= 79.6114
C7-H25-H16= 85.3787
H16-C11-H25= 99.9051
H17-C1-H25= 82.7254
H17-C2-H25= 91.5332
C3-H17-H25=103.693
H17-C6-H25= 71.4183
C7-H25-H17= 78.5736
C11-H25-H17= 83.6964
H17-H16-H25= 68.8282
H18-C2-H25=173.6987
H18-H17-H25=127.8561
H19-C1-H25=128.588
H19-C11-H25=155.6467
H19-H16-H25=100.5009
C1-H25-H20= 78.5593
H20-C2-H25= 71.6934
H20-C6-H25= 91.726
H20-C7-H25= 82.8675
C10-H20-H25=103.6751
C11-H25-H20= 83.7163
H16-H25-H20= 96.8048
H20-H17-H25= 63.9734
C1-H25-H21= 85.5509
C2-H25-H21= 79.8769
C6-H21-H25= 66.6093
H21-C7-H25=101.6529
C8-H21-H25= 88.4261
H21-C11-H25= 99.6316
H16-H25-H21=108.147
H17-H25-H21= 97.1617
H20-H21-H25= 69.0918
H22-C7-H25=128.5941
H22-C11-H25=155.3545
H22-H21-H25=100.9712
H23-C6-H25=173.7134
H23-H20-H25=127.927
C1-H25-H24= 66.3121

C2-H25-H24= 96.9432 C4-H24-H25= 96.3469 C6-H25-H24= 96.9252
C7-H24-H25= 66.3234 C8-H24-H25= 96.361 H24-C11-H25=109.4275
H16-H24-H25= 70.6732 H17-H25-H24=115.1726 H19-H24-H25=115.4569
H20-H25-H24=115.1116 H21-H24-H25= 70.6693 H22-H24-H25=115.485
C1-C5-H26=140.0609 C2-C5-H26=149.5694 C3-C5-H26=127.4348
C4-C5-H26=125.8679 C8-C5-H26=137.5392 C9-C5-H26=123.12
C10-C5-H26=138.6538 C3-O12-H26=122.207 C4-O12-H26=120.7638
C5-O12-H26=109.3824 C3-O15-H26= 85.9493 C4-O15-H26= 85.2026
O15-C5-H26= 81.8623 C8-O15-H26=123.6882 C9-O15-H26=157.8923
C10-O15-H26=124.3286 O12-H26-O15= 81.8243 C13-O15-H26=167.326
N14-O15-H26=143.8641 H18-C5-H26=101.2496 H18-O12-H26=116.3702
H18-O15-H26= 75.4079 H19-C5-H26= 98.9081 H19-O12-H26=111.4464
H19-O15-H26= 75.0716 H22-O15-H26=123.8528 H23-O15-H26=126.3883
C3-C9-O27=128.7913 C4-C9-O27=141.3804 C5-C9-O27=166.8586
C6-C9-O27= 86.4537 C7-C9-O27= 84.2304 C8-C9-O27=103.8089
C2-C10-O27=136.5241 C3-C10-O27=160.1146 C4-C10-O27=106.0174
C5-C10-O27=121.2379 C6-C10-O27= 94.5748 C7-C10-O27= 75.4493
C8-C10-O27= 73.3979 C10-C9-O27= 89.9422 C8-C13-O27= 95.2508
C9-C13-O27=103.9948 C10-C13-O27= 82.2638 C9-O27-N14= 61.8703
C10-O27-N14= 88.1363 N14-C13-O27=121.5143 O15-C9-O27=148.4294
O15-C10-O27= 91.3724 O15-C13-O27=136.2286 O15-N14-O27= 88.255
H18-C10-O27=161.6037 H20-C10-O27= 88.8532 H22-C9-O27= 93.7944
H22-C13-O27= 98.8399 C3-H23-O27=118.5936 C6-H23-O27= 82.6721
H23-C9-O27= 73.9713 C10-H23-O27= 83.256 H23-C13-O27= 74.2463
N14-O27-H23= 91.3714 O15-H23-O27= 81.375 H18-H23-O27=141.0629
H20-H23-O27= 84.532 C1-C6-H28=127.4458 C2-C6-H28=153.9424
C3-C6-H28=113.6765 C4-C6-H28=100.2831 C1-C7-H28=143.3107
C2-C7-H28=111.9764 C4-C7-H28=116.6526 C6-C7-H28= 76.9747
C1-C8-H28=120.7146 C2-C8-H28= 93.3692 C3-C8-H28= 91.816
C4-C8-H28=147.8575 C5-C8-H28=116.7567 C8-C6-H28= 67.857
C8-C7-H28= 83.5888 C3-C9-H28=114.2375 C4-C9-H28=120.9152
C5-C9-H28=147.122 C6-C9-H28= 65.4145 C7-C9-H28= 62.2749
C8-C9-H28= 87.2231 C2-C10-H28=118.4393 C3-C10-H28=157.1624
C4-C10-H28=101.6605 C5-C10-H28=126.1528 C6-C10-H28= 75.1843
C10-C7-H28= 62.0053 C8-C10-H28= 68.7942 C10-C9-H28= 78.0223
C11-C6-H28=107.0168 C11-C7-H28=172.5737 C11-C8-H28=102.0567
C6-H28-C13= 94.9664 C7-H28-C13= 93.3366 C8-C13-H28= 72.0648
C9-C13-H28= 81.6976 C10-H28-C13= 65.8372 N14-C9-H28= 80.8512
N14-C13-H28=143.1778 O15-C8-H28= 97.2907 O15-C9-H28=170.3661
O15-C10-H28=103.8061 O15-C13-H28=115.1545 H17-C6-H28=172.5937
H18-C10-H28=177.5199 H19-C8-H28=172.8992 C2-H20-H28=107.7971
H20-C6-H28= 87.0566 H20-C7-H28= 72.0956 C8-H28-H20= 72.504
C9-H28-H20= 79.1768 H20-C10-H28= 70.4827 C13-H28-H20=114.479
H17-H20-H28=132.1313 C6-H21-H28= 74.2629 C7-H21-H28= 96.8012
C8-H21-H28= 79.8794 C9-H28-H21= 81.9395 C10-H28-H21= 82.0472
C11-H21-H28=135.0217 C13-H28-H21=110.0806 H20-H21-H28= 73.1857
H22-C7-H28= 82.7237 H22-C8-H28= 98.0108 H22-C9-H28= 85.7549
H22-C13-H28= 79.1327 H22-H21-H28= 83.9987 C3-H23-H28=109.9439
H23-C6-H28= 65.7497 C7-H28-H23= 79.6488 C8-H28-H23= 74.2838
H23-C9-H28= 70.8553 H23-C10-H28= 83.6357 C13-H28-H23= 68.3127
O15-H23-H28= 86.9776 H18-H23-H28=134.1067 H20-H23-H28= 64.5041
H21-H28-H23=102.5585 H24-C7-H28=153.4555 H24-C8-H28=113.1466
H24-H21-H28=147.2149 H25-C6-H28=115.966 H25-C7-H28=146.0838
H25-H20-H28=104.3866 H25-H21-H28=140.4705 C6-H28-O27=129.6827

```
    C7-H28-O27=134.0315     C8-H28-O27=101.5757     C9-O27-H28= 80.3158
   C10-H28-O27= 95.6869    C13-O27-H28=115.4273    N14-O27-H28=138.3514
   H20-H28-O27=140.5015    H21-H28-O27=145.2141    H23-H28-O27= 84.8494
 Stoichiometry    C12H12NO3(1-)
 Framework group  C1[X(C12H12NO3)]
 Deg. of freedom   78
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -2.204548   -0.529086   -0.429955
    2          6             0       -1.764808   -0.556954    1.056931
    3          6             0       -0.905314    0.716236    1.327413
    4          6             0       -1.153822    0.416342   -1.050564
    5          6             0       -0.783517    1.474170   -0.001684
    6          6             0       -0.452744   -1.431961    1.030764
    7          6             0       -0.306708   -1.797875   -0.470155
    8          6             0        0.159455   -0.456184   -1.076558
    9          6             0        1.063941    0.270346   -0.034825
   10          6             0        0.400092   -0.149442    1.305484
   11          6             0       -1.773249   -1.919476   -0.939735
   12          8             0       -1.450058    2.725327   -0.094620
   13          6             0        2.562390    0.137257   -0.182571
   14          7             0        3.436335    0.855198   -0.593449
   15          8             0        0.629605    1.669057   -0.172530
   16          1             0       -3.233928   -0.242452   -0.600082
   17          1             0       -2.537518   -0.820517    1.765070
   18          1             0       -1.114994    1.339582    2.181194
   19          1             0       -1.419673    0.845878   -2.005132
   20          1             0       -0.379819   -2.258333    1.723351
   21          1             0        0.328407   -2.644811   -0.689350
   22          1             0        0.620668   -0.524817   -2.050046
   23          1             0        1.058567   -0.124051    2.156118
   24          1             0       -1.863023   -2.023071   -2.016717
   25          1             0       -2.305319   -2.732272   -0.452852
   26          1             0       -0.801933    3.422242   -0.273216
   27          8             0        2.873942   -1.312656    0.368713
   28          1             0        2.119296   -1.917823    0.396032
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9283327      0.6431814      0.4884489
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,O-16,C-
12,N-14,
 O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,O-16,H-1
 Standard basis: 3-21+G* (6D, 7F)
 There are   232 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    131072 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
   232 basis functions      340 primitive gaussians
```

```
   58 alpha electrons       58 beta electrons
      nuclear repulsion energy      1206.3976134245 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   232 RedAO= T  NBF=   232
 NBsUse=   232 1.00D-04 NBFU=   232
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -736.368007717     A.U. after   19 cycles
            Convg  =    0.6421D-08             -V/T =  2.0022
            S**2   =   0.0000
 Range of M.O.s used for correlation:     1   232
 NBasis=   232 NAE=    58 NBE=    58 NFC=     0 NFV=     0
 NROrb=    232 NOA=    58 NOB=    58 NVA=   174 NVB=   174

 **** Warning!!: The largest alpha MO coefficient is  0.10698705D+03

          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   3 vectors were produced by pass 12.
   1 vectors were produced by pass 13.
 Inv2:  IOpt= 1 Iter= 1 AM= 5.75D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  40 with in-core refinement.
 PrsmSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 G2DrvN: will do   10 atoms at a time, making    3 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  44 IRICut=      44 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
          There are  87 degrees of freedom in the 1st order CPHF.
```

```
 84 vectors were produced by pass  0.
AX will form  42 AO Fock derivatives at one time.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 84 vectors were produced by pass  1.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 84 vectors were produced by pass  2.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 84 vectors were produced by pass  3.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 84 vectors were produced by pass  4.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 84 vectors were produced by pass  5.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 84 vectors were produced by pass  6.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 46 vectors were produced by pass  7.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  3 vectors were produced by pass  8.
  2 vectors were produced by pass  9.
Inv2:  IOpt= 1 Iter= 1 AM= 6.02D-15 Conv= 1.00D-12.
Inverted reduced A of dimension 639 with in-core refinement.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.

 ******************************************************************

           Population analysis using the SCF density.

 ******************************************************************

 Alpha  occ. eigenvalues --  -20.38404 -20.35738 -20.27378 -15.23354 -
11.17875
 Alpha  occ. eigenvalues --  -11.11450 -11.08296 -11.08170 -11.07903 -
11.07812
 Alpha  occ. eigenvalues --  -11.07739 -11.07266 -11.07080 -11.06826 -
11.06583
 Alpha  occ. eigenvalues --  -11.05537  -1.31659  -1.24038  -1.13605  -
1.11717
 Alpha  occ. eigenvalues --   -0.98726  -0.97529  -0.94498  -0.92251  -
0.82744
 Alpha  occ. eigenvalues --   -0.81439  -0.76392  -0.70160  -0.68405  -
0.64471
 Alpha  occ. eigenvalues --   -0.63505  -0.60863  -0.58950  -0.56587  -
0.54995
 Alpha  occ. eigenvalues --   -0.52150  -0.51748  -0.49923  -0.48919  -
0.46589
```

```
 Alpha  occ. eigenvalues --   -0.42875  -0.42496  -0.40493  -0.40242  -
0.37631
 Alpha  occ. eigenvalues --   -0.37072  -0.36472  -0.35362  -0.34140  -
0.34016
 Alpha  occ. eigenvalues --   -0.33331  -0.32142  -0.31444  -0.30159  -
0.28784
 Alpha  occ. eigenvalues --   -0.28350  -0.19147  -0.12460
 Alpha virt. eigenvalues --    0.13982   0.15822   0.16044   0.16813
0.17830
 Alpha virt. eigenvalues --    0.18015   0.18744   0.19335   0.19961
0.22014
 Alpha virt. eigenvalues --    0.22969   0.24128   0.24564   0.25357
0.25612
 Alpha virt. eigenvalues --    0.25831   0.27107   0.28032   0.28720
0.28861
 Alpha virt. eigenvalues --    0.29239   0.29333   0.30060   0.30301
0.30398
 Alpha virt. eigenvalues --    0.32482   0.33022   0.33478   0.33762
0.34612
 Alpha virt. eigenvalues --    0.35470   0.35626   0.36051   0.36186
0.36926
 Alpha virt. eigenvalues --    0.37041   0.37479   0.38290   0.38482
0.39217
 Alpha virt. eigenvalues --    0.39591   0.39738   0.40132   0.40874
0.42103
 Alpha virt. eigenvalues --    0.43377   0.44499   0.45071   0.46272
0.46315
 Alpha virt. eigenvalues --    0.47316   0.47939   0.48396   0.48472
0.49564
 Alpha virt. eigenvalues --    0.50752   0.51273   0.52492   0.53468
0.54359
 Alpha virt. eigenvalues --    0.55254   0.55742   0.56059   0.56441
0.57576
 Alpha virt. eigenvalues --    0.58012   0.59264   0.59369   0.59885
0.60044
 Alpha virt. eigenvalues --    0.61655   0.61807   0.62088   0.62753
0.63559
 Alpha virt. eigenvalues --    0.64857   0.65564   0.65617   0.66448
0.68210
 Alpha virt. eigenvalues --    0.68625   0.69078   0.70071   0.70822
0.71082
 Alpha virt. eigenvalues --    0.72561   0.73089   0.73532   0.74189
0.74587
 Alpha virt. eigenvalues --    0.76517   0.77739   0.78625   0.79881
0.82616
 Alpha virt. eigenvalues --    0.86327   0.88819   1.04815   1.21346
1.23171
 Alpha virt. eigenvalues --    1.25173   1.25953   1.26159   1.27233
1.28283
 Alpha virt. eigenvalues --    1.29040   1.29285   1.30166   1.31165
1.32578
 Alpha virt. eigenvalues --    1.32882   1.34419   1.35174   1.35741
1.36104
```

```
 Alpha virt. eigenvalues --    1.37236   1.39018   1.41692   1.43641
1.44224
 Alpha virt. eigenvalues --    1.46704   1.48170   1.50621   1.51362
1.52041
 Alpha virt. eigenvalues --    1.55630   1.55860   1.58153   1.61076
1.62349
 Alpha virt. eigenvalues --    1.63084   1.64453   1.65800   1.66701
1.69961
 Alpha virt. eigenvalues --    1.70983   1.71538   1.73419   1.74689
1.82948
 Alpha virt. eigenvalues --    1.84839   1.88509   1.91139   1.93887
1.98553
 Alpha virt. eigenvalues --    2.01846   2.03894   2.07717   2.10011
2.23376
 Alpha virt. eigenvalues --    2.26212   2.28421   2.31377   2.35366
2.39954
 Alpha virt. eigenvalues --    2.42597   2.45438   2.47891   2.49440
2.53162
 Alpha virt. eigenvalues --    2.56829   2.65260   2.67113   2.68495
2.97827
 Alpha virt. eigenvalues --    3.10694   3.29161   3.33640   3.36951
3.75643
 Alpha virt. eigenvalues --    3.80731   3.87849   4.09092   4.24841
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   12.857829  -5.383692   3.011529  -4.724627  -1.535771   3.234013
  2  C   -5.383692  18.984615 -13.508979  -1.959089   9.314727 -10.094039
  3  C    3.011529 -13.508979  46.371893  20.586784 -50.691061   9.124773
  4  C   -4.724627  -1.959089  20.586784  39.049095 -44.157883   0.349261
  5  C   -1.535771   9.314727 -50.691061 -44.157883 102.579701  -4.296946
  6  C    3.234013 -10.094039   9.124773   0.349261  -4.296946  20.332309
  7  C   -1.103392   2.375155   0.544374   3.521542  -2.668313  -6.033696
  8  C    2.461138   1.207926 -17.811080 -26.702617  39.310323   1.237185
  9  C    0.835274  -6.657080  37.560120  32.404946 -67.199787   4.750552
 10  C   -2.563873  10.889046 -32.893635 -16.139590  42.011242 -10.870599
 11  C   -2.780449   0.725394  -0.260478   0.726366   0.227696  -0.452634
 12  O    0.145382  -0.199372   0.813812   0.567879  -1.574200   0.107937
 13  C    0.934226   0.146289   2.003229   1.096239 -12.135738  -1.342541
 14  N    0.008566  -0.048401   0.152697   0.109184  -0.147386   0.071600
 15  O    0.001165  -0.061909  -0.093936  -0.045787   0.071535   0.053990
 16  H    0.552558  -0.122721   0.057395  -0.143302  -0.019617   0.053630
 17  H   -0.100499   0.594331  -0.159255   0.017352   0.027101  -0.160401
 18  H    0.030896  -0.136039   0.698441   0.061961  -0.248680   0.076391
 19  H   -0.056638  -0.006744   0.086318   0.669183  -0.256727   0.007178
 20  H    0.011342  -0.136206   0.088177   0.008490  -0.011200   0.591536
 21  H   -0.043233   0.037644  -0.017976   0.056244   0.036300  -0.052242
 22  H    0.022201   0.008783  -0.055764  -0.235857   0.168836   0.005289
 23  H   -0.003454   0.051513  -0.175403  -0.036482   0.132591  -0.087465
 24  H   -0.081762   0.027293   0.008313   0.030491  -0.031995   0.042948
 25  H   -0.052465  -0.008507   0.000100   0.005322  -0.000811   0.032068
 26  H   -0.006247   0.001030   0.059841   0.050897  -0.149739  -0.001049
 27  O    0.025724  -0.098159   0.214058   0.110083  -0.337374   0.230031
 28  H   -0.007730   0.012912   0.010684  -0.006407   0.005935  -0.064508
               7          8          9         10         11         12
```

1	C	-1.103392	2.461138	0.835274	-2.563873	-2.780449	0.145382
2	C	2.375155	1.207926	-6.657080	10.889046	0.725394	-0.199372
3	C	0.544374	-17.811080	37.560120	-32.893635	-0.260478	0.813812
4	C	3.521542	-26.702617	32.404946	-16.139590	0.726366	0.567879
5	C	-2.668313	39.310323	-67.199787	42.011242	0.227696	-1.574200
6	C	-6.033696	1.237185	4.750552	-10.870599	-0.452634	0.107937
7	C	14.302394	-8.230433	4.919659	-1.592804	-2.088119	0.033100
8	C	-8.230433	51.961904	-53.650938	28.453561	-0.832531	-0.627601
9	C	4.919659	-53.650938	120.890822	-56.224424	0.677867	1.199347
10	C	-1.592804	28.453561	-56.224424	56.111492	0.243284	-0.726600
11	C	-2.088119	-0.832531	0.677867	0.243284	11.322715	-0.023907
12	O	0.033100	-0.627601	1.199347	-0.726600	-0.023907	8.522227
13	C	1.249085	-9.644392	-16.094531	-8.764058	-0.544503	0.183782
14	N	-0.010512	0.049314	0.594344	-0.209347	-0.000747	0.004126
15	O	-0.101640	1.200859	-1.920831	1.112825	-0.036074	-0.060888
16	H	-0.034739	0.034620	0.020396	-0.034027	-0.013984	0.002452
17	H	0.015998	0.014264	-0.032199	0.124279	0.021872	0.000593
18	H	-0.008757	-0.001200	0.034443	-0.148192	0.000707	0.002273
19	H	0.023539	-0.195757	0.080902	-0.024949	0.019432	0.003087
20	H	-0.105827	0.044814	-0.014493	-0.111133	0.007022	-0.000015
21	H	0.466019	-0.081336	0.002827	0.051459	-0.017096	-0.000056
22	H	-0.116279	0.886865	-0.385520	0.165869	0.006713	-0.000723
23	H	-0.014625	0.164083	-0.340516	0.805061	-0.001666	-0.000554
24	H	-0.105086	0.040726	-0.015880	-0.000357	0.398509	0.000173
25	H	-0.107149	0.084536	-0.027018	0.006321	0.378974	0.000015
26	H	0.002722	-0.021506	0.065823	-0.025429	0.000345	0.223574
27	O	-0.039446	0.052470	-0.459324	-0.314563	-0.026320	0.002347
28	H	0.117423	-0.176965	0.288821	-0.090470	0.049673	-0.000025

		13	14	15	16	17	18
1	C	0.934226	0.008566	0.001165	0.552558	-0.100499	0.030896
2	C	0.146289	-0.048401	-0.061909	-0.122721	0.594331	-0.136039
3	C	2.003229	0.152697	-0.093936	0.057395	-0.159255	0.698441
4	C	1.096239	0.109184	-0.045787	-0.143302	0.017352	0.061961
5	C	-12.135738	-0.147386	0.071535	-0.019617	0.027101	-0.248680
6	C	-1.342541	0.071600	0.053990	0.053630	-0.160401	0.076391
7	C	1.249085	-0.010512	-0.101640	-0.034739	0.015998	-0.008757
8	C	-9.644392	0.049314	1.200859	0.034620	0.014264	-0.001200
9	C	-16.094531	0.594344	-1.920831	0.020396	-0.032199	0.034443
10	C	-8.764058	-0.209347	1.112825	-0.034027	0.124279	-0.148192
11	C	-0.544503	-0.000747	-0.036074	-0.013984	0.021872	0.000707
12	O	0.183782	0.004126	-0.060888	0.002452	0.000593	0.002273
13	C	48.242954	-0.733401	-0.696430	-0.000726	-0.000603	-0.007359
14	N	-0.733401	8.037231	0.020446	-0.000004	0.000003	-0.000079
15	O	-0.696430	0.020446	8.849993	-0.001072	0.000196	0.008545
16	H	-0.000726	-0.000004	-0.001072	0.404308	-0.000525	-0.000032
17	H	-0.000603	0.000003	0.000196	-0.000525	0.399500	-0.000337
18	H	-0.007359	-0.000079	0.008545	-0.000032	-0.000337	0.374882
19	H	-0.000500	-0.000057	0.006435	-0.000444	-0.000021	-0.000017
20	H	-0.015770	-0.000088	0.000559	-0.000018	-0.000416	-0.000087
21	H	-0.085393	0.000219	0.000019	-0.000017	-0.000014	0.000000
22	H	-0.128156	0.001277	0.013333	-0.000023	0.000001	0.000000
23	H	-0.142022	-0.001401	0.017597	0.000000	-0.000075	-0.000761
24	H	0.002345	0.000013	0.000043	-0.000127	-0.000034	0.000000
25	H	0.002386	-0.000006	0.000241	-0.000260	0.000169	0.000000

26	H	0.004718	0.000315	0.015115	0.000001	0.000000	0.000245
27	O	-0.077120	-0.063021	0.031495	-0.000011	0.000014	0.000035
28	H	-0.010113	-0.002748	-0.003504	0.000000	0.000000	-0.000001

		19	20	21	22	23	24
1	C	-0.056638	0.011342	-0.043233	0.022201	-0.003454	-0.081762
2	C	-0.006744	-0.136206	0.037644	0.008783	0.051513	0.027293
3	C	0.086318	0.088177	-0.017976	-0.055764	-0.175403	0.008313
4	C	0.669183	0.008490	0.056244	-0.235857	-0.036482	0.030491
5	C	-0.256727	-0.011200	0.036300	0.168836	0.132591	-0.031995
6	C	0.007178	0.591536	-0.052242	0.005289	-0.087465	0.042948
7	C	0.023539	-0.105827	0.466019	-0.116279	-0.014625	-0.105086
8	C	-0.195757	0.044814	-0.081336	0.886865	0.164083	0.040726
9	C	0.080902	-0.014493	0.002827	-0.385520	-0.340516	-0.015880
10	C	-0.024949	-0.111133	0.051459	0.165869	0.805061	-0.000357
11	C	0.019432	0.007022	-0.017096	0.006713	-0.001666	0.398509
12	O	0.003087	-0.000015	-0.000056	-0.000723	-0.000554	0.000173
13	C	-0.000500	-0.015770	-0.085393	-0.128156	-0.142022	0.002345
14	N	-0.000057	-0.000088	0.000219	0.001277	-0.001401	0.000013
15	O	0.006435	0.000559	0.000019	0.013333	0.017597	0.000043
16	H	-0.000444	-0.000018	-0.000017	-0.000023	0.000000	-0.000127
17	H	-0.000021	-0.000416	-0.000014	0.000001	-0.000075	-0.000034
18	H	-0.000017	-0.000087	0.000000	0.000000	-0.000761	0.000000
19	H	0.378104	0.000001	-0.000024	-0.000730	0.000001	0.000172
20	H	0.000001	0.396994	-0.000245	-0.000014	0.000082	-0.000038
21	H	-0.000024	-0.000245	0.399305	0.000188	0.000007	-0.000135
22	H	-0.000730	-0.000014	0.000188	0.363533	-0.000020	0.000065
23	H	0.000001	0.000082	0.000007	-0.000020	0.359050	0.000000
24	H	0.000172	-0.000038	-0.000135	0.000065	0.000000	0.456124
25	H	-0.000031	0.000080	-0.000132	-0.000036	0.000001	-0.019194
26	H	0.000328	0.000000	0.000000	0.000000	0.000000	0.000000
27	O	0.000071	0.001895	-0.002916	0.000387	-0.008731	0.000041
28	H	0.000000	-0.000545	-0.002864	-0.000071	-0.000320	-0.000002

		25	26	27	28
1	C	-0.052465	-0.006247	0.025724	-0.007730
2	C	-0.008507	0.001030	-0.098159	0.012912
3	C	0.000100	0.059841	0.214058	0.010684
4	C	0.005322	0.050897	0.110083	-0.006407
5	C	-0.000811	-0.149739	-0.337374	0.005935
6	C	0.032068	-0.001049	0.230031	-0.064508
7	C	-0.107149	0.002722	-0.039446	0.117423
8	C	0.084536	-0.021506	0.052470	-0.176965
9	C	-0.027018	0.065823	-0.459324	0.288821
10	C	0.006321	-0.025429	-0.314563	-0.090470
11	C	0.378974	0.000345	-0.026320	0.049673
12	O	0.000015	0.223574	0.002347	-0.000025
13	C	0.002386	0.004718	-0.077120	-0.010113
14	N	-0.000006	0.000315	-0.063021	-0.002748
15	O	0.000241	0.015115	0.031495	-0.003504
16	H	-0.000260	0.000001	-0.000011	0.000000
17	H	0.000169	0.000000	0.000014	0.000000
18	H	0.000000	0.000245	0.000035	-0.000001
19	H	-0.000031	0.000328	0.000071	0.000000
20	H	0.000080	0.000000	0.001895	-0.000545
21	H	-0.000132	0.000000	-0.002916	-0.002864

```
22  H   -0.000036   0.000000   0.000387  -0.000071
23  H    0.000001   0.000000  -0.008731  -0.000320
24  H   -0.019194   0.000000   0.000041  -0.000002
25  H    0.465488   0.000000   0.000010  -0.000002
26  H    0.000000   0.311314   0.000006   0.000000
27  O    0.000010   0.000006   9.222574   0.064192
28  H   -0.000002   0.000000   0.064192   0.449949
Total atomic charges:
             1
 1  C    0.311990
 2  C    0.044277
 3  C    0.275030
 4  C    0.730322
 5  C   -2.422758
 6  C   -0.844570
 7  C    0.789807
 8  C   -3.228232
 9  C    4.696399
10  C   -3.240388
11  C   -1.728062
12  O   -0.598165
13  C    2.558103
14  N   -0.832137
15  O   -0.382323
16  H    0.246287
17  H    0.238708
18  H    0.262721
19  H    0.267889
20  H    0.245103
21  H    0.253450
22  H    0.279852
23  H    0.283507
24  H    0.247355
25  H    0.239899
26  H    0.467697
27  O   -0.528447
28  H    0.366687
Sum of Mulliken charges=  -1.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  C    0.558277
 2  C    0.282985
 3  C    0.537751
 4  C    0.998211
 5  C   -2.422758
 6  C   -0.599467
 7  C    1.043256
 8  C   -2.948380
 9  C    4.696399
10  C   -2.956881
11  C   -1.240808
12  O   -0.130468
13  C    2.558103
14  N   -0.832137
```

```
 15  O   -0.382323
 16  H    0.000000
 17  H    0.000000
 18  H    0.000000
 19  H    0.000000
 20  H    0.000000
 21  H    0.000000
 22  H    0.000000
 23  H    0.000000
 24  H    0.000000
 25  H    0.000000
 26  H    0.000000
 27  O   -0.161761
 28  H    0.000000
 Sum of Mulliken charges=  -1.00000
 Electronic spatial extent (au):  <R**2>=  2580.5603
 Charge=    -1.0000 electrons
 Dipole moment (Debye):
    X=   -14.8667    Y=    -3.8055    Z=     1.3277  Tot=    15.4033
 Quadrupole moment (Debye-Ang):
   XX=  -167.0215   YY=  -108.4861   ZZ=   -97.9065
   XY=     0.2156   XZ=     5.0634   YZ=     3.0709
 Octapole moment (Debye-Ang**2):
  XXX=  -227.3088  YYY=    12.2152  ZZZ=     2.3702  XYY=   -14.3432
  XXY=   -21.4366  XXZ=    20.7498  XZZ=   -11.3659  YZZ=     3.5569
  YYZ=     1.1769  XYZ=    15.1100
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -2758.2306 YYYY= -1074.6744 ZZZZ=  -538.8648 XXXY=   -33.8311
 XXXZ=    79.8248 YYYX=   -13.7884 YYYZ=   -17.8984 ZZZX=    14.5482
 ZZZY=     3.2756 XXYY=  -662.2059 XXZZ=  -437.9303 YYZZ=  -287.7833
 XXYZ=    42.6109 YYXZ=     8.7625 ZZXY=   -15.4485
 N-N= 1.206397613424D+03 E-N=-4.152764916655D+03  KE= 7.347514443894D+02
  Exact polarizability: 143.602   7.642 135.283  -3.131  -3.866 112.877
 Approx polarizability: 121.870   6.806 125.367  -3.542  -5.514 109.253
 Full mass-weighted force constant matrix:
 Low frequencies --- -231.0577   -0.3502   -0.2529   -0.0004    0.0005
0.0016
 Low frequencies ---    0.2905   62.2669  155.8383
 ******    1 imaginary frequencies (negative Signs) ******
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                      1                      2                      3
                     ?A                     ?A                     ?A
 Frequencies --  -231.0577                62.2669               155.8383
 Red. masses --     1.1669                 7.2049                 6.8089
 Frc consts  --     0.0367                 0.0165                 0.0974
 IR Inten    --   124.6169                 3.5979                19.2194
 Raman Activ --     1.6063                 3.3406                 0.3295
 Depolar     --     0.7423                 0.7460                 0.4841
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.01    -0.01  -0.01   0.04     0.05  -0.06
0.04
```

2	6	0.01	0.00	0.00	0.01	0.04	0.04	0.10	-0.04	0.02
3	6	0.01	0.00	0.00	0.02	0.04	-0.01	0.03	0.02	0.00
4	6	0.00	0.00	0.00	0.00	-0.04	0.00	-0.03	0.02	0.01
5	6	0.00	0.00	0.00	0.00	-0.01	-0.05	-0.06	0.03	0.00
6	6	0.01	0.00	0.00	0.00	0.03	0.05	0.16	0.05	-0.03
7	6	-0.01	0.00	0.00	-0.02	-0.03	0.06	0.13	0.07	-0.05
8	6	-0.01	0.00	-0.01	0.00	-0.05	0.01	0.02	0.11	-0.04
9	6	0.00	0.00	0.00	0.01	0.00	-0.02	0.00	0.12	-0.05
10	6	0.01	-0.01	-0.01	0.01	0.03	0.00	0.07	0.11	-0.04
11	6	-0.01	0.00	0.00	-0.03	-0.03	0.08	0.13	-0.03	0.01
12	8	0.00	0.00	0.00	0.00	-0.01	-0.10	-0.18	-0.03	0.04
13	6	0.00	-0.01	-0.01	0.01	0.04	0.05	-0.03	-0.04	-0.01
14	7	0.00	0.00	-0.01	0.07	0.19	0.43	0.16	-0.25	0.06
15	8	0.00	0.00	-0.01	0.00	-0.01	-0.07	-0.06	0.12	-0.05
16	1	0.00	0.01	0.01	-0.01	0.00	0.04	0.02	-0.13	0.08
17	1	0.01	0.00	0.01	0.01	0.06	0.05	0.15	-0.10	0.05
18	1	0.01	0.00	0.00	0.03	0.07	-0.03	0.01	0.00	0.01
19	1	-0.01	0.00	0.00	-0.01	-0.07	-0.02	-0.10	0.01	0.02
20	1	0.02	0.00	-0.01	0.01	0.05	0.08	0.25	0.05	-0.04
21	1	-0.03	-0.02	-0.01	-0.05	-0.05	0.08	0.17	0.12	-0.09
22	1	-0.01	0.01	-0.01	-0.02	-0.09	0.01	0.00	0.15	-0.05
23	1	0.02	-0.03	-0.02	0.03	0.04	-0.01	0.11	0.14	-0.07
24	1	-0.02	0.00	0.00	-0.04	-0.06	0.09	0.10	-0.02	0.02
25	1	-0.01	0.00	0.00	-0.03	-0.01	0.12	0.21	-0.07	0.03
26	1	0.00	0.00	0.01	0.02	0.00	0.01	-0.26	0.06	0.09
27	8	-0.02	0.03	0.09	-0.06	-0.14	-0.39	-0.33	-0.16	0.05
28	1	0.19	-0.28	-0.93	-0.06	-0.15	-0.66	-0.41	-0.06	0.03

		4			5			6		
		?A			?A			?A		
Frequencies --		182.1267			189.7049			265.3599		
Red. masses --		2.5488			1.4863			5.3311		
Frc consts --		0.0498			0.0315			0.2212		
IR Inten --		21.7669			139.5665			11.7337		
Raman Activ --		1.5645			1.4819			0.9115		
Depolar --		0.7291			0.7484			0.6045		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.04	-0.01	-0.06	-0.01	0.00	0.01	0.00	-0.14	0.01
2	6	-0.05	0.01	-0.04	0.01	0.00	0.01	0.01	-0.10	0.00
3	6	-0.08	0.02	0.01	0.02	0.00	-0.01	-0.07	-0.02	-0.01
4	6	0.07	0.00	-0.01	-0.01	-0.01	-0.01	-0.09	-0.02	0.00
5	6	0.00	0.01	0.02	0.01	0.00	0.00	-0.04	0.03	0.00
6	6	-0.03	0.02	0.05	0.01	0.00	-0.02	0.06	-0.02	0.00
7	6	0.05	0.01	0.07	-0.02	-0.01	-0.02	0.08	-0.01	-0.01
8	6	0.06	0.01	0.07	-0.02	-0.01	-0.04	-0.04	0.03	-0.01
9	6	0.00	0.02	0.10	0.00	-0.01	-0.05	-0.06	0.02	-0.01
10	6	-0.05	0.03	0.08	0.02	0.00	-0.04	-0.03	0.03	0.00
11	6	0.09	-0.01	-0.02	-0.03	0.00	0.01	0.11	-0.12	0.01
12	8	-0.02	0.01	0.03	0.01	0.01	0.11	0.35	0.24	0.02
13	6	-0.01	-0.01	-0.01	0.01	0.01	0.01	-0.10	0.02	-0.01
14	7	-0.04	-0.05	-0.13	0.02	0.02	0.07	-0.11	0.04	0.01
15	8	0.00	0.02	0.09	0.00	-0.01	-0.06	-0.04	-0.04	-0.01
16	1	0.05	-0.02	-0.13	-0.01	0.01	0.03	-0.04	-0.25	0.02
17	1	-0.09	0.01	-0.08	0.03	0.00	0.02	0.04	-0.14	0.01
18	1	-0.13	0.03	-0.01	0.05	0.01	-0.01	-0.11	-0.06	0.01
19	1	0.12	-0.02	-0.03	-0.03	-0.01	0.00	-0.13	-0.06	-0.01
20	1	-0.07	0.03	0.07	0.02	0.00	-0.02	0.11	-0.02	0.00
21	1	0.07	0.01	0.11	-0.03	-0.01	-0.03	0.16	0.05	-0.02
22	1	0.12	0.00	0.10	-0.04	-0.02	-0.05	-0.04	0.07	-0.02

23	1	-0.10	0.05	0.12	0.03	0.00	-0.05	-0.02	0.08	-0.01
24	1	0.16	-0.02	-0.03	-0.06	0.00	0.01	0.10	-0.15	0.01
25	1	0.06	-0.01	-0.05	-0.03	0.01	0.02	0.17	-0.15	0.03
26	1	-0.12	-0.09	-0.74	-0.13	-0.14	-0.95	0.63	-0.03	-0.01
27	8	-0.02	-0.05	-0.13	0.00	0.02	0.05	-0.13	0.02	0.01
28	1	0.00	-0.09	-0.33	0.00	0.03	0.11	-0.13	0.03	-0.02

	7			8			9		
	?A			?A			?A		
Frequencies --	315.7142			355.0157			394.4588		
Red. masses --	4.1114			6.0265			7.1889		
Frc consts --	0.2414			0.4475			0.6590		
IR Inten --	0.9900			4.3301			15.7794		
Raman Activ --	0.8832			3.4613			9.7989		
Depolar --	0.6731			0.1883			0.5801		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	-0.02	-0.12	-0.09	-0.08	0.04	-0.06	-0.03	-0.02
2	6	-0.05	0.08	-0.09	-0.05	-0.05	0.02	-0.09	-0.05	-0.01
3	6	-0.01	0.04	-0.10	-0.12	0.03	-0.01	-0.08	-0.06	0.01
4	6	0.01	-0.02	-0.10	-0.16	0.03	0.03	-0.01	-0.05	0.01
5	6	0.00	0.00	-0.06	-0.12	0.05	0.00	-0.04	-0.04	0.03
6	6	-0.06	0.06	0.05	0.00	0.04	-0.02	-0.09	-0.04	0.00
7	6	0.01	-0.03	0.10	0.02	0.08	-0.03	-0.08	-0.05	0.02
8	6	0.02	-0.06	0.01	-0.09	0.11	-0.02	0.01	-0.04	0.02
9	6	0.00	-0.01	-0.03	-0.01	0.02	0.00	0.08	0.08	0.00
10	6	-0.03	0.05	-0.01	-0.07	0.07	-0.01	-0.04	-0.05	0.00
11	6	0.04	-0.08	0.05	0.04	-0.05	0.00	-0.11	-0.06	0.04
12	8	-0.02	0.02	0.34	-0.03	0.12	-0.03	0.08	0.02	-0.02
13	6	0.02	-0.01	-0.02	0.11	-0.14	0.02	0.22	0.14	-0.05
14	7	0.03	-0.01	0.00	0.16	-0.16	0.06	0.45	-0.10	-0.06
15	8	0.00	-0.01	-0.14	-0.07	0.04	0.00	-0.05	0.01	0.10
16	1	0.00	-0.07	-0.18	-0.12	-0.19	0.05	-0.05	0.01	-0.04

17	1	-0.10	0.15	-0.11	-0.01	-0.09	0.05	-0.11	-0.05	-0.02
18	1	-0.05	0.09	-0.14	-0.14	0.00	0.01	-0.08	-0.08	0.02
19	1	0.08	-0.04	-0.13	-0.22	0.00	0.03	0.02	-0.04	0.00
20	1	-0.11	0.11	0.11	0.07	0.02	-0.05	-0.10	-0.04	0.01
21	1	0.03	-0.03	0.18	0.11	0.15	-0.04	-0.11	-0.09	0.04
22	1	0.03	-0.15	0.02	-0.13	0.17	-0.04	-0.04	-0.09	0.00
23	1	-0.04	0.09	0.00	-0.10	0.11	0.01	-0.12	-0.08	0.07
24	1	0.08	-0.23	0.06	0.02	-0.04	0.00	-0.16	-0.15	0.06
25	1	0.02	-0.02	0.13	0.13	-0.11	0.00	-0.09	-0.01	0.14
26	1	-0.04	0.12	0.65	0.04	0.04	-0.09	0.19	-0.08	-0.02
27	8	0.03	0.00	-0.01	0.37	-0.10	-0.03	-0.13	0.26	-0.08
28	1	0.04	-0.02	-0.05	0.50	-0.27	-0.04	-0.27	0.45	-0.14

	10			11			12		
	?A			?A			?A		
Frequencies --	413.5283			495.7253			526.3839		
Red. masses --	2.1918			9.0874			4.4211		
Frc consts --	0.2208			1.3157			0.7218		
IR Inten --	1.2919			183.0839			5.9512		
Raman Activ --	0.3184			8.8479			0.3616		
Depolar --	0.6901			0.7263			0.5901		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.02	-0.02	0.05	-0.01	0.00	-0.02	0.02	0.05	0.06
2 6	-0.01	-0.01	0.06	-0.03	-0.02	0.00	0.09	-0.10	0.00
3 6	0.01	0.01	0.02	-0.02	-0.03	0.00	-0.08	-0.02	-0.04
4 6	-0.04	-0.02	0.06	0.02	-0.03	0.00	0.04	-0.06	-0.03
5 6	-0.01	-0.01	0.00	-0.07	0.01	0.01	-0.04	-0.02	-0.09
6 6	-0.03	0.00	0.07	-0.03	-0.02	0.01	0.12	-0.05	-0.06
7 6	-0.01	-0.02	0.07	-0.05	-0.06	0.04	-0.02	-0.03	-0.12
8 6	-0.01	-0.04	0.07	0.04	-0.07	0.03	0.11	-0.02	0.07
9 6	0.00	-0.01	-0.01	0.04	0.06	-0.01	0.02	0.06	0.18
10 6	0.01	0.02	0.02	0.03	-0.03	-0.02	-0.03	0.08	0.10

11	6	0.06	0.09	-0.19	-0.07	0.00	-0.01	-0.17	0.09	0.02
12	8	0.01	0.00	0.01	0.03	0.07	-0.01	0.02	0.03	0.05
13	6	0.02	0.01	-0.02	0.01	0.48	-0.16	0.03	0.04	0.22
14	7	0.04	-0.01	0.00	0.15	0.20	-0.12	-0.03	-0.04	-0.07
15	8	-0.03	-0.03	-0.13	-0.10	0.05	0.03	-0.06	0.00	-0.18
16	1	-0.02	-0.03	0.06	0.00	0.06	-0.02	0.04	0.20	0.18
17	1	0.00	0.02	0.08	-0.05	-0.02	-0.02	0.13	-0.19	0.00
18	1	0.02	0.03	0.01	0.01	-0.06	0.03	-0.21	0.03	-0.11
19	1	-0.03	-0.06	0.04	0.07	-0.06	-0.03	0.05	-0.19	-0.09
20	1	-0.01	0.02	0.10	0.00	0.01	0.04	0.18	-0.06	-0.08
21	1	-0.02	-0.03	0.09	-0.08	-0.08	0.07	-0.16	-0.11	-0.23
22	1	-0.05	-0.07	0.05	0.01	-0.13	0.02	0.26	0.13	0.13
23	1	0.01	0.03	0.02	0.01	-0.07	-0.02	-0.15	0.09	0.19
24	1	0.34	0.49	-0.26	-0.04	0.01	-0.02	-0.32	0.08	0.03
25	1	-0.07	-0.09	-0.64	-0.11	0.02	-0.04	-0.15	0.13	0.10
26	1	0.03	-0.01	0.03	0.13	-0.01	0.00	0.07	-0.01	0.08
27	8	-0.01	0.03	-0.01	0.04	-0.46	0.17	0.02	-0.02	-0.04
28	1	-0.02	0.04	0.00	0.04	-0.49	0.18	-0.02	0.03	-0.09

	13			14			15		
	?A			?A			?A		
Frequencies --	556.8021			578.1071			607.3447		
Red. masses --	4.9510			4.5999			4.3808		
Frc consts --	0.9044			0.9058			0.9521		
IR Inten --	11.2788			11.0678			0.1400		
Raman Activ --	2.8193			2.3856			5.7080		
Depolar --	0.2970			0.3055			0.0549		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.08	-0.02	0.00	-0.09	-0.06	0.13	0.08	0.13	-0.08
2 6	-0.13	0.08	0.01	-0.01	0.03	0.09	0.01	-0.06	-0.04
3 6	0.02	0.02	0.11	-0.05	0.06	-0.17	-0.13	-0.05	0.09
4 6	-0.05	0.01	0.10	-0.06	-0.10	-0.10	0.08	0.02	-0.02

```
   5   6     0.05  -0.11   0.07     0.03  -0.12  -0.14    -0.07  -0.13
0.08
   6   6    -0.12   0.08  -0.09     0.03   0.10   0.00     0.10   0.07
0.05
   7   6     0.07   0.18  -0.10    -0.02   0.08  -0.03     0.02   0.04
0.07
   8   6     0.01   0.13  -0.01     0.01   0.03  -0.09     0.00  -0.02  -
0.04
   9   6     0.04   0.01   0.06     0.03   0.02   0.01    -0.07   0.02  -
0.10
  10   6    -0.05  -0.04   0.10    -0.03   0.11  -0.04     0.00   0.12
0.00
  11   6     0.10  -0.03   0.04    -0.03   0.04  -0.03    -0.01   0.14
0.05
  12   8     0.09  -0.20  -0.01     0.10  -0.17   0.08     0.12  -0.15
0.00
  13   6     0.04   0.08   0.05     0.03   0.01   0.02    -0.10  -0.02  -
0.15
  14   7     0.02   0.04  -0.05    -0.01   0.04  -0.02     0.02  -0.06
0.07
  15   8     0.00  -0.10  -0.21     0.06   0.00   0.23    -0.14  -0.05
0.00
  16   1    -0.08  -0.11  -0.15    -0.09  -0.05   0.15     0.10   0.22  -
0.07
  17   1    -0.09   0.06   0.05     0.09   0.09   0.21    -0.07  -0.22  -
0.18
  18   1     0.01   0.09   0.06    -0.03   0.28  -0.34    -0.23  -0.06
0.07
  19   1    -0.05   0.16   0.17    -0.24  -0.22  -0.11     0.14   0.20
0.04
  20   1    -0.20  -0.04  -0.22     0.13   0.09  -0.03     0.18   0.12
0.09
  21   1     0.15   0.22  -0.02    -0.04   0.05   0.01    -0.05   0.00
0.03
  22   1     0.01   0.28  -0.02     0.05   0.02  -0.07    -0.01  -0.11  -
0.04
  23   1    -0.07  -0.21   0.12    -0.10   0.21   0.01     0.09   0.23  -
0.08
  24   1    -0.07  -0.16   0.07     0.01   0.29  -0.06     0.04   0.03
0.05
  25   1     0.32  -0.06   0.23     0.04  -0.12  -0.25    -0.12   0.25
0.10
  26   1     0.08  -0.19  -0.02     0.08  -0.16   0.07     0.26  -0.28
0.04
  27   8    -0.03  -0.05   0.01    -0.01  -0.03   0.01     0.04   0.03
0.00
  28   1    -0.09   0.03  -0.05    -0.06   0.02  -0.04     0.19  -0.15
0.10
                      16                    17                    18
                      ?A                    ?A                    ?A
 Frequencies --    636.3782              659.2061              673.6311
 Red. masses --      6.0198                4.7569                5.8295
 Frc consts  --      1.4364                1.2179                1.5586
 IR Inten    --      5.8812                1.7879                2.0026
```

Raman Activ --		3.0418			4.8589			4.5781		
Depolar --		0.6737			0.1901			0.5604		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.08	0.05	-0.11	-0.04	-0.03	-0.03	0.12	0.09	0.16
2	6	0.13	-0.03	-0.12	-0.02	-0.15	-0.06	-0.09	-0.07	0.13
3	6	0.10	-0.13	-0.15	-0.17	0.01	0.01	-0.11	-0.07	-0.10
4	6	-0.19	0.14	-0.15	0.01	0.05	0.10	0.05	0.02	-0.06
5	6	0.00	-0.04	-0.14	0.09	0.05	0.06	-0.05	0.02	-0.12
6	6	0.08	-0.13	0.12	0.09	0.03	0.02	-0.07	-0.13	0.05
7	6	-0.03	0.11	0.11	-0.03	-0.02	-0.01	0.11	0.12	0.00
8	6	-0.19	0.14	0.17	-0.06	0.01	0.04	0.12	0.03	-0.05
9	6	-0.01	-0.01	0.13	0.09	-0.04	-0.03	0.00	-0.12	-0.04
10	6	0.14	-0.08	0.20	-0.05	0.15	0.06	-0.14	-0.14	-0.03
11	6	0.00	0.05	0.02	-0.08	-0.04	-0.03	0.15	0.22	0.15
12	8	0.01	-0.05	-0.02	-0.04	-0.01	-0.01	-0.08	0.12	0.02
13	6	-0.01	0.02	-0.10	0.18	-0.16	-0.15	0.06	-0.06	-0.14
14	7	0.05	0.02	0.02	-0.01	0.19	-0.01	0.03	0.07	0.01
15	8	0.00	-0.05	-0.01	0.18	-0.01	-0.05	-0.01	-0.14	-0.03
16	1	-0.16	-0.10	0.10	-0.04	0.00	0.02	0.12	0.09	0.10
17	1	0.11	0.11	-0.09	0.00	-0.29	-0.08	-0.18	0.02	0.06
18	1	-0.08	-0.07	-0.23	-0.38	-0.08	0.02	0.01	-0.02	-0.11
19	1	-0.08	0.11	-0.20	0.05	0.12	0.12	-0.12	-0.19	-0.10
20	1	-0.09	-0.21	0.04	0.17	0.07	0.06	0.03	-0.25	-0.10
21	1	0.06	0.25	-0.13	-0.04	0.00	-0.08	0.04	0.07	-0.02
22	1	-0.11	0.08	0.21	-0.16	0.03	-0.01	0.15	0.00	-0.03
23	1	0.07	0.02	0.25	-0.13	0.28	0.12	-0.23	-0.04	0.04
24	1	0.14	-0.10	0.03	-0.05	-0.11	-0.02	-0.01	0.22	0.17
25	1	-0.04	0.11	0.07	-0.10	0.00	0.02	0.25	0.20	0.23

26	1	-0.03	-0.05	-0.15	-0.17	0.12	0.04	-0.08	0.13	0.02
27	8	-0.01	0.01	0.02	-0.05	-0.07	0.06	-0.03	0.00	0.03
28	1	0.00	-0.01	0.04	-0.30	0.25	-0.03	-0.10	0.08	-0.01

	19	20	21
	?A	?A	?A
Frequencies --	698.9438	711.6763	739.4191
Red. masses --	4.6230	8.1046	6.3066
Frc consts --	1.3306	2.4185	2.0316
IR Inten --	15.3108	6.3977	102.4851
Raman Activ --	3.1995	3.0474	1.1873
Depolar --	0.7275	0.6353	0.5321

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.05	-0.07	-0.01	-0.01	0.06	0.04	0.02	0.02
2	6	-0.01	-0.03	-0.01	-0.16	-0.20	0.06	0.05	-0.04	-0.03
3	6	0.02	-0.09	-0.01	-0.03	-0.18	-0.13	-0.11	0.08	0.00
4	6	-0.07	0.10	-0.04	0.07	0.05	0.06	-0.05	0.12	0.01
5	6	-0.06	-0.03	0.04	0.17	0.03	-0.04	0.12	0.07	0.02
6	6	0.03	0.01	0.07	-0.06	-0.18	0.09	0.09	0.02	0.03
7	6	-0.02	0.03	0.13	-0.03	0.02	0.13	0.02	-0.04	-0.01
8	6	-0.04	0.00	-0.09	-0.04	0.09	0.04	-0.12	-0.07	-0.13
9	6	0.05	-0.01	-0.09	0.00	0.18	-0.08	-0.10	-0.15	-0.02
10	6	0.04	-0.01	-0.15	-0.13	-0.04	-0.16	-0.10	0.05	0.03
11	6	0.06	0.06	0.04	0.00	0.02	0.05	0.06	0.00	0.01
12	8	0.00	0.00	-0.02	0.10	-0.14	0.00	-0.06	0.00	0.00
13	6	0.21	-0.04	0.35	-0.14	0.10	0.07	-0.14	0.32	0.16
14	7	-0.05	0.07	-0.12	-0.04	-0.10	0.02	0.08	-0.12	-0.04
15	8	-0.08	-0.03	0.02	0.20	0.34	-0.13	0.19	-0.25	0.02
16	1	-0.03	-0.04	-0.04	0.00	0.02	0.01	0.00	-0.08	0.12
17	1	-0.08	-0.01	-0.08	-0.25	-0.05	0.03	0.05	-0.13	-0.06
18	1	0.14	-0.18	0.08	0.09	-0.24	-0.06	-0.25	0.04	-0.01
19	1	-0.06	0.24	0.02	0.01	0.03	0.07	-0.14	0.24	0.09

20	1	0.12	0.06	0.13	0.19	-0.16	0.09	0.15	0.05	0.06
21	1	-0.04	0.02	0.12	0.01	0.07	0.06	0.05	0.01	-0.06
22	1	-0.19	-0.21	-0.15	-0.13	-0.07	0.01	-0.18	-0.10	-0.16
23	1	0.09	0.09	-0.20	-0.19	0.08	-0.12	-0.04	0.16	-0.03
24	1	0.23	-0.01	0.04	0.05	-0.03	0.05	0.11	0.02	0.01
25	1	-0.04	0.11	0.01	-0.02	0.04	0.07	-0.02	0.02	-0.03
26	1	0.09	-0.08	-0.04	-0.04	-0.02	-0.01	-0.32	0.24	0.02
27	8	-0.01	-0.08	-0.01	0.04	0.02	-0.03	0.01	0.04	-0.05
28	1	-0.33	0.32	-0.21	0.24	-0.24	0.05	0.17	-0.18	-0.02

	22			23			24		
	?A			?A			?A		
Frequencies --	818.7595			828.2500			844.3427		
Red. masses --	5.5231			4.8798			2.7651		
Frc consts --	2.1814			1.9723			1.1615		
IR Inten --	0.2121			2.6486			7.3803		
Raman Activ --	9.2645			6.9330			1.1317		
Depolar --	0.0221			0.0198			0.5976		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.25	-0.03	0.02	-0.13	-0.07	-0.09	0.05	-0.02	-0.08
2 6	0.07	0.03	0.13	-0.11	-0.15	0.16	-0.08	0.03	0.12
3 6	-0.02	0.08	0.13	0.02	-0.09	0.15	0.06	0.03	-0.10
4 6	0.02	0.07	-0.18	0.07	-0.04	-0.19	0.08	0.04	0.09
5 6	0.02	0.00	-0.02	0.01	0.00	-0.02	-0.04	-0.01	0.01
6 6	-0.09	-0.14	0.20	0.04	0.11	0.07	0.06	-0.07	0.12
7 6	-0.05	-0.06	-0.08	-0.10	0.23	0.06	-0.03	0.02	-0.08
8 6	-0.08	0.07	-0.24	0.12	0.02	-0.10	-0.01	0.09	0.09
9 6	-0.06	0.03	-0.03	0.04	0.00	0.00	0.00	-0.05	0.02
10 6	-0.07	-0.01	0.20	0.13	0.00	0.07	-0.02	0.07	-0.10
11 6	-0.04	-0.13	-0.08	-0.10	-0.05	-0.06	-0.05	-0.07	-0.09
12 8	0.04	-0.05	0.00	-0.06	0.10	-0.01	-0.01	0.00	0.00
13 6	0.06	-0.03	0.01	-0.05	0.02	0.00	-0.01	0.02	0.00

14	7	0.02	0.03	-0.02	-0.02	-0.03	0.01	0.01	0.00	0.00
15	8	-0.04	0.11	-0.04	0.08	-0.05	-0.02	-0.04	-0.10	0.01
16	1	0.24	0.05	0.16	-0.08	0.07	-0.14	0.09	0.09	-0.18
17	1	-0.17	0.17	-0.06	-0.10	-0.26	0.14	-0.19	0.31	0.10
18	1	-0.14	0.22	0.01	0.09	-0.05	0.15	0.35	0.07	-0.06
19	1	-0.28	0.21	-0.03	0.05	-0.01	-0.18	0.21	0.06	0.07
20	1	-0.14	-0.23	0.11	0.27	-0.03	-0.11	0.36	-0.05	0.12
21	1	0.07	0.04	-0.11	-0.08	0.20	0.22	0.06	0.11	-0.21
22	1	0.06	0.00	-0.18	0.32	-0.18	0.00	-0.03	0.23	0.08
23	1	0.04	0.04	0.13	0.24	-0.06	-0.02	-0.09	0.33	-0.05
24	1	-0.11	-0.04	-0.08	0.03	-0.13	-0.06	-0.16	-0.23	-0.07
25	1	-0.13	-0.07	-0.09	0.03	-0.14	-0.06	-0.01	0.00	0.09
26	1	0.03	-0.05	0.01	-0.07	0.11	-0.01	0.03	-0.03	0.01
27	8	0.02	-0.03	0.01	-0.01	0.02	-0.01	0.00	0.00	0.00
28	1	-0.12	0.14	-0.08	0.08	-0.09	0.07	0.01	-0.01	0.00

	25	26	27
	?A	?A	?A
Frequencies --	883.0757	907.9514	925.6983
Red. masses --	3.7233	2.5463	2.6197
Frc consts --	1.7107	1.2368	1.3226
IR Inten --	0.5712	0.2861	8.3563
Raman Activ --	19.9048	0.6436	1.4861
Depolar --	0.0184	0.5618	0.7194

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.18	-0.03	0.09	-0.02	-0.06	0.05	-0.01	-0.03	0.04
2	6	0.17	-0.09	-0.05	0.00	0.06	-0.12	0.05	-0.03	0.01
3	6	-0.04	0.00	-0.08	-0.03	-0.12	-0.08	0.02	-0.02	-0.06
4	6	0.11	-0.02	0.06	-0.01	-0.05	0.08	-0.07	0.21	-0.04
5	6	-0.02	0.00	-0.01	0.00	0.00	0.06	-0.02	0.00	0.05
6	6	-0.15	0.11	-0.05	-0.07	-0.02	0.13	-0.04	0.06	0.00
7	6	-0.10	0.17	0.10	0.05	0.03	-0.04	-0.02	-0.09	0.05

```
   8   6    -0.06   0.10   0.07     0.11   0.04  -0.08     0.19   0.05  -
0.04
   9   6     0.00  -0.02  -0.02     0.03  -0.01  -0.07     0.03   0.01
0.08
  10   6     0.00  -0.04  -0.08     0.12   0.06   0.05    -0.06  -0.01  -
0.07
  11   6    -0.07  -0.11  -0.06    -0.06   0.03   0.00    -0.04  -0.05
0.00
  12   8     0.00   0.00   0.01    -0.02   0.03  -0.01     0.01  -0.03  -
0.01
  13   6     0.00   0.01   0.03    -0.02   0.02   0.03    -0.02  -0.02  -
0.06
  14   7     0.00   0.00  -0.01    -0.02  -0.02   0.00     0.00   0.00
0.02
  15   8    -0.03  -0.06  -0.01     0.01  -0.02   0.00    -0.02  -0.04  -
0.02
  16   1     0.24   0.29   0.34    -0.01  -0.01   0.06    -0.09  -0.18
0.23
  17   1     0.18  -0.20  -0.10    -0.04   0.37  -0.05     0.10  -0.02
0.06
  18   1    -0.12  -0.06  -0.06    -0.32  -0.36   0.02     0.15  -0.09
0.02
  19   1     0.06  -0.12   0.03    -0.11  -0.03   0.12    -0.15   0.47
0.10
  20   1    -0.26   0.07  -0.11    -0.37  -0.08   0.09     0.01   0.19
0.15
  21   1     0.16   0.32   0.31    -0.01  -0.03  -0.01    -0.09  -0.20
0.24
  22   1    -0.14  -0.02   0.05     0.07   0.13  -0.11     0.43   0.13
0.07
  23   1    -0.02  -0.13  -0.07     0.23   0.39  -0.04    -0.23  -0.04
0.06
  24   1    -0.04  -0.10  -0.05    -0.21   0.12   0.00     0.00   0.00  -
0.01
  25   1    -0.05  -0.11  -0.03     0.03  -0.03   0.00    -0.11  -0.05  -
0.06
  26   1     0.01  -0.01   0.02     0.02   0.00  -0.01     0.00  -0.03  -
0.03
  27   8     0.00   0.00   0.00     0.00   0.01  -0.01    -0.01   0.01
0.00
  28   1     0.00   0.00  -0.01     0.05  -0.07   0.00     0.06  -0.08
0.06
                     28                    29                    30
                     ?A                    ?A                    ?A
 Frequencies --    943.3077              976.8009              996.5969
 Red. masses --      2.0992                2.1961                2.0455
 Frc consts  --      1.1005                1.2346                1.1970
 IR Inten    --      6.4181                6.9103                1.8767
 Raman Activ --      4.0920                3.8130                7.3899
 Depolar     --      0.7211                0.0755                0.5582
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.12  -0.01  -0.01    -0.03   0.00  -0.04     0.02   0.00  -
0.01
```

2	6	-0.10	-0.04	-0.06	0.02	-0.11	0.07	0.04	-0.08	-0.02
3	6	0.05	-0.01	0.06	-0.06	0.13	-0.01	0.15	-0.03	0.02
4	6	-0.10	-0.08	0.00	-0.04	0.06	0.05	-0.05	-0.03	-0.01
5	6	-0.01	0.00	-0.05	-0.02	-0.02	-0.06	0.00	0.01	0.01
6	6	0.00	0.10	0.05	-0.10	-0.02	0.05	-0.10	0.00	-0.01
7	6	0.05	-0.08	0.00	0.02	-0.05	-0.03	-0.02	0.04	-0.03
8	6	-0.02	0.10	0.01	0.06	0.00	0.04	0.00	-0.08	0.00
9	6	0.00	0.02	0.04	0.02	-0.01	-0.06	-0.02	-0.01	0.01
10	6	0.02	-0.03	-0.04	0.12	-0.02	-0.01	-0.08	0.15	0.03
11	6	-0.05	0.04	0.00	0.04	0.06	-0.06	0.04	0.05	-0.04
12	8	0.00	0.00	0.00	0.00	-0.01	0.01	0.00	0.00	0.00
13	6	0.00	0.00	0.00	-0.01	0.01	0.03	0.00	0.01	-0.01
14	7	0.00	0.00	0.00	-0.01	-0.01	0.00	0.01	0.00	0.00
15	8	0.05	-0.03	0.00	0.01	0.01	0.02	0.01	0.01	0.02
16	1	0.13	0.00	-0.05	-0.06	-0.11	-0.03	0.00	-0.05	0.07
17	1	-0.28	-0.20	-0.33	0.09	-0.33	0.07	0.03	-0.24	-0.08
18	1	0.21	0.02	0.07	-0.16	0.41	-0.23	0.51	-0.09	0.15
19	1	-0.31	-0.28	-0.04	0.03	0.04	0.02	-0.11	-0.07	-0.01
20	1	0.07	0.29	0.27	-0.28	-0.01	0.09	-0.28	-0.08	-0.08
21	1	0.08	-0.06	0.01	-0.05	-0.11	0.00	-0.06	-0.01	0.03
22	1	0.02	0.33	0.01	-0.03	0.06	0.00	0.01	-0.17	0.01
23	1	0.06	-0.18	-0.06	0.33	-0.07	-0.16	-0.18	0.48	0.10
24	1	-0.13	0.10	0.00	-0.18	-0.28	-0.01	-0.12	-0.15	0.00
25	1	-0.23	0.16	0.00	0.09	0.22	0.28	0.15	0.12	0.20
26	1	-0.04	0.03	-0.01	0.01	-0.02	0.01	0.00	0.00	-0.01
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
28	1	-0.01	0.01	0.01	0.03	-0.04	0.02	-0.03	0.03	-0.05

	31			32			33		
	?A			?A			?A		
Frequencies --	997.9804			1006.9106			1016.8614		
Red. masses --	2.8829			2.7036			5.3347		
Frc consts --	1.6917			1.6150			3.2500		
IR Inten --	3.2664			35.6357			3.9407		
Raman Activ --	9.6796			1.3563			1.4609		
Depolar --	0.0314			0.7461			0.6821		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.14	0.21	0.05	-0.02	0.02	0.06	-0.11	-0.18	-0.10
2 6	-0.02	-0.01	0.00	0.03	0.06	0.03	0.16	-0.01	-0.13
3 6	0.02	-0.01	0.02	-0.08	-0.05	0.13	0.05	0.22	0.07
4 6	-0.02	0.00	-0.01	0.00	0.03	-0.17	0.01	-0.12	-0.03
5 6	0.01	0.00	-0.03	-0.02	0.03	-0.01	0.00	0.04	0.09
6 6	0.00	-0.03	0.02	-0.06	-0.04	0.00	0.05	-0.12	0.12
7 6	0.24	-0.03	0.05	-0.03	-0.04	-0.07	0.10	0.13	0.08
8 6	0.02	-0.01	-0.01	-0.01	0.03	0.16	0.10	0.09	0.02
9 6	-0.01	0.01	-0.05	-0.08	0.03	-0.01	-0.09	-0.01	-0.10
10 6	-0.05	0.00	0.01	0.03	0.07	-0.14	-0.22	-0.11	-0.06
11 6	-0.08	-0.12	-0.09	0.05	-0.03	0.01	-0.15	0.12	0.03
12 8	0.00	0.00	0.00	0.02	-0.05	0.00	0.02	-0.03	0.00
13 6	0.01	-0.01	0.01	0.01	0.00	0.00	0.01	0.00	0.00
14 7	0.00	0.00	0.00	0.02	0.01	-0.01	0.02	0.01	-0.01
15 8	-0.01	-0.01	0.01	0.06	-0.05	0.00	0.01	0.00	0.00
16 1	-0.07	0.60	0.25	-0.07	-0.09	0.19	-0.18	-0.31	0.06
17 1	0.05	-0.13	0.02	-0.03	0.06	-0.03	0.21	-0.06	-0.10
18 1	0.10	0.03	0.01	-0.14	-0.25	0.26	0.15	0.14	0.16
19 1	0.02	-0.06	-0.05	0.17	-0.10	-0.27	0.24	-0.03	-0.06
20 1	-0.12	0.01	0.09	-0.13	0.07	0.13	0.00	-0.08	0.17
21 1	0.47	0.11	0.13	0.00	0.03	-0.22	0.06	0.17	-0.15
22 1	-0.03	0.02	-0.04	0.21	0.02	0.27	0.15	-0.05	0.05

23	1	-0.01	0.07	-0.02	0.27	0.12	-0.33	-0.10	-0.10	-0.16
24	1	-0.08	-0.20	-0.09	-0.09	0.08	0.01	-0.18	0.21	0.02
25	1	-0.03	-0.14	-0.05	0.21	-0.15	-0.02	-0.11	0.06	-0.03
26	1	-0.03	0.03	0.00	-0.09	0.05	0.01	-0.03	0.02	0.02
27	8	0.00	0.00	0.00	0.02	-0.01	0.01	0.02	-0.01	0.01
28	1	0.00	0.00	-0.03	-0.11	0.14	-0.08	-0.11	0.14	-0.07

	34			35			36		
	?A			?A			?A		
Frequencies --	1041.4363			1043.0623			1052.6172		
Red. masses --	2.1043			2.2255			1.8775		
Frc consts --	1.3447			1.4266			1.2256		
IR Inten --	1.7933			13.9333			11.3121		
Raman Activ --	4.6697			1.5102			7.8629		
Depolar --	0.7297			0.5784			0.4864		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.08	-0.02	0.03	-0.01	-0.02	0.08	-0.03	0.02	-0.07
2	6	-0.03	-0.08	-0.02	-0.03	-0.02	-0.07	0.11	0.02	0.09
3	6	0.05	-0.02	-0.04	0.01	-0.01	-0.03	-0.01	-0.10	-0.01
4	6	0.16	0.03	-0.01	0.02	0.05	-0.01	0.00	-0.07	0.01
5	6	0.03	0.01	-0.02	0.05	0.02	0.00	0.01	0.01	0.00
6	6	-0.04	0.06	0.03	0.03	0.12	0.11	-0.02	0.09	0.05
7	6	0.01	-0.07	-0.05	0.00	0.06	-0.10	0.00	-0.04	-0.02
8	6	-0.06	0.08	-0.05	-0.02	-0.12	0.03	-0.02	0.03	-0.04
9	6	-0.04	-0.06	0.00	0.00	-0.08	0.02	-0.05	-0.02	0.01
10	6	0.02	0.01	0.04	-0.01	-0.08	0.01	-0.07	-0.04	0.00
11	6	0.01	-0.01	0.11	0.02	0.01	-0.07	0.04	0.05	-0.07
12	8	0.00	0.01	0.00	0.01	-0.01	0.00	0.00	0.01	0.00
13	6	0.00	0.01	0.00	0.01	0.00	0.00	-0.01	0.01	-0.01
14	7	0.01	-0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.00
15	8	-0.06	0.01	0.00	-0.07	0.07	0.00	0.02	0.02	-0.01
16	1	-0.07	-0.03	-0.09	-0.06	-0.08	0.30	0.00	0.07	-0.16

17	1	0.13	-0.36	0.06	-0.16	0.04	-0.19	0.34	0.17	0.40
18	1	0.19	0.07	-0.07	-0.03	-0.06	-0.01	-0.18	-0.27	0.07
19	1	0.39	0.10	-0.05	0.10	0.08	-0.02	0.01	-0.16	-0.03
20	1	-0.30	0.14	0.16	0.22	0.30	0.31	0.05	0.24	0.21
21	1	-0.04	-0.07	-0.16	0.04	0.12	-0.22	-0.08	-0.12	0.08
22	1	-0.04	0.32	-0.05	-0.01	-0.31	0.05	-0.03	0.23	-0.05
23	1	0.05	0.12	0.01	-0.01	-0.26	0.02	-0.11	-0.16	0.03
24	1	0.16	0.30	0.07	-0.32	-0.04	-0.03	-0.01	-0.28	-0.03
25	1	-0.01	-0.19	-0.22	0.34	-0.07	0.14	0.04	0.20	0.19
26	1	-0.01	0.02	0.00	-0.04	0.03	-0.01	-0.01	0.01	0.00
27	8	0.02	-0.01	0.00	-0.01	0.01	0.00	0.02	-0.01	0.01
28	1	-0.11	0.15	-0.08	0.02	-0.02	0.02	-0.14	0.19	-0.08

	37			38			39		
	?A			?A			?A		
Frequencies --	1065.6172			1078.3566			1104.3488		
Red. masses --	1.7916			1.8625			1.8170		
Frc consts --	1.1986			1.2761			1.3056		
IR Inten --	22.9099			88.8302			38.7236		
Raman Activ --	4.5865			6.0198			8.8700		
Depolar --	0.7378			0.7489			0.7499		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	-0.06	-0.01	-0.04	0.05	0.00	-0.01	-0.01	-0.02
2 6	0.01	0.02	0.07	0.06	0.01	-0.03	0.01	-0.01	0.02
3 6	-0.01	-0.05	0.00	-0.01	0.03	0.03	-0.01	0.00	0.03
4 6	0.04	0.05	-0.06	0.01	-0.05	-0.02	0.00	-0.02	0.00
5 6	-0.04	-0.05	0.01	-0.09	-0.08	0.03	0.12	0.10	-0.03
6 6	-0.04	0.04	-0.03	-0.01	-0.02	0.07	-0.01	-0.02	0.00
7 6	0.12	-0.03	-0.01	-0.06	-0.01	-0.04	-0.01	-0.01	0.01
8 6	-0.08	-0.03	0.03	-0.01	0.03	-0.02	0.00	0.03	-0.01
9 6	0.06	0.04	-0.01	0.10	0.05	0.00	0.03	0.00	0.00
10 6	-0.01	0.01	0.01	-0.04	-0.02	-0.02	-0.01	0.02	-0.02

```
  11   6    -0.06   0.04   0.00     0.06  -0.02   0.02     0.00   0.01
0.00
  12   8    -0.03   0.03   0.00    -0.04   0.04   0.00     0.05  -0.04
0.00
  13   6     0.01  -0.01   0.02     0.02  -0.01   0.01     0.07  -0.04
0.03
  14   7    -0.01   0.01  -0.01    -0.01   0.02  -0.01     0.01   0.04  -
0.02
  15   8     0.04  -0.01  -0.01     0.08  -0.01  -0.01    -0.11  -0.03
0.01
  16   1    -0.03  -0.35  -0.12    -0.02   0.22   0.16    -0.01  -0.05  -
0.11
  17   1     0.11   0.02   0.18     0.01  -0.06  -0.11     0.09  -0.03
0.10
  18   1     0.02  -0.04   0.00     0.07   0.04   0.03    -0.04  -0.14
0.12
  19   1     0.23   0.15  -0.07     0.07   0.00  -0.01    -0.06  -0.18  -
0.06
  20   1    -0.11   0.07   0.01    -0.08   0.14   0.27    -0.05  -0.01
0.02
  21   1     0.39   0.17   0.03    -0.19  -0.04  -0.29    -0.02  -0.01  -
0.01
  22   1    -0.22  -0.18  -0.02    -0.14   0.04  -0.09    -0.03   0.06  -
0.03
  23   1    -0.13  -0.03   0.10    -0.19  -0.04   0.09     0.01   0.04  -
0.04
  24   1    -0.35   0.21   0.00     0.19  -0.06   0.01     0.05  -0.03
0.00
  25   1    -0.22   0.16   0.01     0.22  -0.14  -0.03    -0.05   0.05
0.01
  26   1     0.12  -0.10  -0.01     0.23  -0.20   0.01    -0.37   0.33
0.00
  27   8    -0.03   0.01  -0.01    -0.05   0.02  -0.01    -0.07   0.02  -
0.02
  28   1     0.18  -0.24   0.08     0.31  -0.42   0.20     0.41  -0.57
0.26
                     40                    41                    42
                     ?A                    ?A                    ?A
 Frequencies --  1123.9392             1155.6212             1184.5924
 Red. masses --     3.5030                1.3631                3.8395
 Frc consts  --     2.6072                1.0725                3.1744
 IR Inten    --   117.6498               10.7117               19.5033
 Raman Activ --     1.8179                1.7197                3.2618
 Depolar     --     0.6374                0.7445                0.6096
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.03  -0.03   0.04    -0.02  -0.02   0.04    -0.07  -0.01
0.00
   2   6    -0.02  -0.02  -0.03     0.00   0.01  -0.02     0.02  -0.05  -
0.01
   3   6     0.05  -0.01   0.00     0.03  -0.02   0.04    -0.08   0.12  -
0.03
   4   6     0.06   0.00   0.01     0.02   0.02  -0.01     0.06  -0.11  -
0.05
```

```
    5    6      0.06    0.02   -0.02     -0.02   -0.01   -0.04      0.01    0.02
0.09
    6    6     -0.02   -0.02    0.01      0.01    0.01   -0.03     -0.07   -0.07
0.02
    7    6     -0.02   -0.03    0.01     -0.02   -0.04    0.04      0.05   -0.01
0.03
    8    6     -0.02    0.00   -0.03      0.01    0.05    0.01     -0.14   -0.03  -
0.16
    9    6      0.08    0.36   -0.06      0.00   -0.05   -0.08      0.04    0.00
0.30
   10    6     -0.01    0.00    0.04     -0.03    0.02    0.06      0.14    0.01  -
0.14
   11    6      0.02    0.02   -0.04      0.01    0.02   -0.05      0.03    0.08  -
0.03
   12    8      0.01    0.01    0.00     -0.01    0.00    0.00      0.01   -0.01
0.00
   13    6     -0.05   -0.02   -0.03      0.01    0.01    0.02     -0.01   -0.01  -
0.05
   14    7     -0.05   -0.03    0.03      0.00    0.00   -0.01      0.00    0.00
0.01
   15    8     -0.05   -0.18    0.03      0.00    0.01    0.01     -0.01    0.00  -
0.04
   16    1     -0.05   -0.08    0.13     -0.11   -0.19    0.35     -0.14   -0.02
0.38
   17    1     -0.06    0.07   -0.04     -0.19    0.16   -0.17     -0.21    0.17  -
0.17
   18    1     -0.05    0.07   -0.09     -0.03    0.00    0.01      0.14   -0.12
0.20
   19    1      0.12    0.06    0.01      0.38   -0.12   -0.18      0.18    0.15
0.03
   20    1      0.04    0.10    0.16      0.22   -0.11   -0.19      0.18   -0.14  -
0.08
   21    1     -0.13   -0.10   -0.07     -0.14   -0.21    0.36      0.15   -0.02
0.38
   22    1     -0.27   -0.20   -0.14     -0.20    0.33   -0.11     -0.02    0.17  -
0.12
   23    1     -0.16   -0.24    0.16     -0.01   -0.01    0.04      0.01    0.08  -
0.04
   24    1     -0.12   -0.08   -0.01     -0.07   -0.12   -0.02     -0.06   -0.09
0.00
   25    1      0.17    0.01    0.11      0.05    0.07    0.09      0.05    0.17
0.14
   26    1     -0.31    0.30    0.00      0.06   -0.06    0.00     -0.03    0.03
0.03
   27    8      0.06   -0.03    0.02     -0.01    0.00    0.00      0.00    0.00
0.00
   28    1     -0.22    0.31   -0.14      0.06   -0.08    0.04     -0.05    0.08
0.00
                      43                     44                     45
                      ?A                     ?A                     ?A
 Frequencies --   1199.5003              1227.7212              1234.3327
 Red. masses --      2.1000                 2.5705                 3.1249
 Frc consts  --      1.7802                 2.2828                 2.8051
 IR Inten    --     71.8850                 6.4452                17.8515
```

Raman Activ --		2.8048			0.3849			0.9038		
Depolar --		0.5246			0.1058			0.6087		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	0.02	-0.03	0.00	0.04	-0.10	0.02	0.04	-0.07
2	6	0.03	0.04	0.04	0.11	-0.05	0.04	0.02	-0.14	0.04
3	6	-0.10	0.04	0.01	0.04	-0.05	0.07	0.05	0.06	-0.12
4	6	-0.06	0.03	-0.01	-0.08	0.00	0.09	-0.07	-0.02	-0.06
5	6	-0.05	0.07	-0.01	0.05	-0.06	-0.12	-0.07	0.09	0.18
6	6	0.01	0.01	0.02	-0.13	-0.01	0.04	-0.08	0.10	0.05
7	6	0.00	0.01	-0.03	0.03	0.06	-0.08	0.05	-0.01	-0.10
8	6	0.05	0.00	0.01	0.06	-0.08	-0.01	-0.03	-0.08	0.06
9	6	0.17	-0.07	-0.04	0.04	-0.01	0.06	-0.08	0.08	-0.10
10	6	0.06	-0.05	0.00	-0.06	0.08	-0.05	0.04	-0.05	0.05
11	6	-0.02	-0.03	0.02	-0.03	-0.04	0.10	-0.01	-0.01	0.09
12	8	0.04	-0.06	0.00	0.00	0.03	0.01	0.03	-0.04	-0.01
13	6	-0.07	0.04	-0.01	-0.02	0.00	-0.03	0.03	-0.02	0.03
14	7	-0.04	-0.05	0.03	-0.01	-0.01	0.01	0.01	0.02	-0.01
15	8	-0.02	0.02	0.00	-0.02	0.02	0.02	0.04	-0.02	0.00
16	1	-0.01	-0.05	-0.01	-0.06	-0.09	0.09	0.08	0.28	0.00
17	1	-0.01	-0.15	-0.07	-0.22	0.24	-0.21	-0.14	0.28	0.03
18	1	0.26	-0.22	0.29	-0.27	0.06	-0.09	-0.07	-0.05	-0.07
19	1	0.13	-0.28	-0.20	0.26	0.09	0.03	0.12	-0.08	-0.15
20	1	-0.09	-0.04	-0.02	0.29	0.00	0.00	0.27	-0.16	-0.30
21	1	-0.01	0.02	-0.08	0.12	0.13	-0.09	-0.05	-0.17	0.22
22	1	-0.30	0.02	-0.16	-0.21	0.12	-0.15	0.17	0.20	0.13
23	1	-0.37	0.11	0.33	0.16	-0.20	-0.21	-0.09	-0.08	0.16
24	1	0.06	0.05	0.01	0.24	0.19	0.05	0.03	0.26	0.05
25	1	-0.07	-0.06	-0.09	-0.22	-0.08	-0.20	0.10	-0.20	-0.14

```
  26   1    -0.16   0.12   0.01    -0.07   0.08  -0.02    -0.08   0.05
0.00
  27   8     0.02   0.00   0.00     0.01   0.00   0.00    -0.01   0.00
0.00
  28   1    -0.17   0.23  -0.12    -0.05   0.07  -0.03     0.09  -0.12
0.05
                     46                     47                     48
                     ?A                     ?A                     ?A
 Frequencies --  1240.5528              1256.5643              1267.1108
 Red. masses --     3.8419                 1.0996                 2.0581
 Frc consts  --     3.4836                 1.0230                 1.9469
 IR Inten    --    41.1195                 0.4118                 8.2317
 Raman Activ --     4.4347                15.6694                 2.1224
 Depolar     --     0.6525                 0.7449                 0.7497
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.01  -0.01     0.00  -0.01   0.02    -0.03  -0.01
0.05
   2   6     0.01  -0.02   0.03    -0.03  -0.01   0.01    -0.04  -0.10  -
0.06
   3   6     0.00  -0.01   0.00     0.00   0.00  -0.02     0.11   0.08
0.01
   4   6    -0.05  -0.12  -0.13     0.02  -0.01   0.00     0.05   0.06  -
0.02
   5   6     0.22  -0.12   0.18    -0.01   0.01   0.02    -0.09   0.08
0.00
   6   6    -0.07  -0.03  -0.06     0.00   0.04  -0.01    -0.06  -0.06  -
0.04
   7   6    -0.01  -0.06   0.02     0.01   0.00  -0.02    -0.01  -0.03
0.03
   8   6    -0.03   0.11   0.08     0.01  -0.02  -0.01     0.02   0.05  -
0.03
   9   6     0.15  -0.12  -0.12    -0.02   0.02  -0.02     0.06  -0.07
0.01
  10   6     0.02   0.08  -0.02     0.01  -0.01   0.02     0.00   0.10
0.02
  11   6     0.02   0.03   0.00     0.00   0.01   0.00     0.01   0.01
0.01
  12   8    -0.04   0.08  -0.02     0.00  -0.01   0.00     0.00  -0.04
0.00
  13   6    -0.04   0.05   0.02     0.00   0.00   0.00    -0.01   0.01  -
0.01
  14   7    -0.03  -0.04   0.01     0.00   0.00   0.00    -0.01  -0.01
0.01
  15   8    -0.09   0.03   0.00     0.01   0.00   0.00     0.00  -0.01
0.01
  16   1    -0.02   0.07   0.18    -0.09  -0.12   0.38     0.03   0.08  -
0.18
  17   1    -0.07   0.07  -0.02    -0.07   0.13   0.03     0.09   0.26
0.22
  18   1    -0.21   0.28  -0.26     0.05  -0.03   0.02    -0.35  -0.22
0.12
  19   1    -0.17   0.15   0.03     0.07  -0.07  -0.04    -0.21  -0.31  -
0.11
```

20	1	0.25	0.14	0.11	-0.16	0.00	-0.05	0.26	0.14	0.17
21	1	0.13	0.09	-0.12	0.07	0.13	-0.35	0.13	0.12	-0.13
22	1	0.26	0.02	0.23	0.14	-0.04	0.05	-0.09	-0.24	-0.07
23	1	-0.32	-0.04	0.25	0.02	0.00	0.00	0.03	-0.30	0.02
24	1	0.03	-0.03	0.01	0.47	-0.32	-0.01	0.01	-0.01	0.01
25	1	0.00	0.07	0.05	-0.43	0.29	0.02	-0.05	0.05	0.03
26	1	-0.03	0.09	0.00	0.01	-0.01	0.00	0.17	-0.19	0.00
27	8	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	-0.08	0.11	-0.08	0.01	-0.01	0.00	-0.03	0.04	-0.02

	49			50			51		
	?A			?A			?A		
Frequencies --	1295.3557			1314.0119			1337.2646		
Red. masses --	1.6966			1.6809			2.0102		
Frc consts --	1.6773			1.7100			2.1180		
IR Inten --	0.5246			7.9274			33.9386		
Raman Activ --	0.6428			2.7512			0.6065		
Depolar --	0.6909			0.7458			0.5996		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.03	0.13	0.05	0.06	0.01	0.01	0.01	-0.01	0.03
2	6	0.01	0.00	-0.04	-0.05	0.01	0.00	-0.04	-0.06	-0.06
3	6	0.02	0.01	-0.01	0.03	-0.03	-0.02	0.01	0.09	0.03
4	6	0.00	-0.03	0.02	-0.06	0.04	-0.05	0.00	0.02	-0.05
5	6	0.01	0.00	0.04	0.04	0.01	0.15	0.09	-0.07	-0.06
6	6	0.02	-0.01	0.06	0.03	0.00	0.00	0.03	0.08	0.08
7	6	-0.11	0.00	-0.05	0.02	0.04	0.01	0.01	-0.02	-0.05
8	6	0.02	-0.01	-0.02	0.03	-0.01	-0.01	-0.03	-0.01	0.07
9	6	0.00	0.04	-0.01	0.03	0.00	0.09	0.11	0.03	0.00
10	6	-0.01	-0.05	-0.01	-0.06	-0.02	-0.02	-0.08	-0.06	-0.03
11	6	0.08	-0.07	-0.01	-0.03	-0.02	-0.01	0.01	0.00	0.01
12	8	-0.01	0.00	0.00	-0.01	0.00	-0.02	-0.04	0.03	0.01
13	6	0.00	-0.01	0.00	-0.01	0.00	-0.02	-0.02	0.01	-0.01

14	7	0.00	0.00	0.00	0.00	0.00	0.01	-0.02	-0.02
0.01									
15	8	0.00	-0.01	0.00	-0.01	0.00	-0.02	-0.04	0.00
0.01									
16	1	-0.15	-0.47	-0.22	0.03	-0.05	0.05	0.06	0.13	-
0.07									
17	1	0.07	-0.19	-0.05	0.13	-0.08	0.16	0.17	0.18
0.25									
18	1	-0.15	0.03	-0.06	-0.14	0.27	-0.29	-0.06	-0.31
0.31									
19	1	0.06	-0.22	-0.08	0.16	-0.40	-0.31	-0.18	0.16
0.06									
20	1	0.13	-0.05	-0.01	-0.17	0.03	0.06	-0.09	-0.31	-
0.37									
21	1	0.31	0.25	0.23	-0.20	-0.12	-0.01	-0.08	-0.13
0.09									
22	1	0.19	0.07	0.04	-0.38	-0.03	-0.20	-0.11	0.11
0.03									
23	1	-0.07	0.18	0.02	0.24	0.14	-0.26	0.19	0.18	-
0.24									
24	1	-0.20	0.12	0.00	0.04	-0.04	-0.01	0.05	-0.02
0.00									
25	1	-0.31	0.19	-0.01	0.01	-0.05	-0.03	-0.11	0.07	-
0.01									
26	1	0.07	-0.07	0.01	0.03	-0.03	0.00	0.18	-0.16
0.00									
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
0.00									
28	1	0.00	0.00	-0.01	-0.02	0.03	0.01	-0.03	0.05	-
0.01									

	52	53	54
	?A	?A	?A
Frequencies --	1353.8454	1358.8044	1372.5137
Red. masses --	1.3874	1.5210	1.7451
Frc consts --	1.4983	1.6546	1.9368
IR Inten --	2.5291	2.3071	16.4605
Raman Activ --	0.6019	1.2374	1.9418
Depolar --	0.6167	0.6128	0.7314

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	0.03	-0.01	-0.02	0.00	-0.03	-0.03	-0.05	-
0.02										
2	6	0.04	-0.07	-0.04	0.02	0.00	-0.01	0.04	0.03	-
0.05										
3	6	-0.11	-0.03	0.00	-0.04	0.00	-0.02	-0.05	-0.04
0.08										
4	6	0.01	0.02	0.01	0.01	-0.04	-0.01	0.08	0.12
0.03										
5	6	0.02	-0.01	0.03	-0.02	-0.01	0.00	0.04	0.00	-
0.01										
6	6	0.05	0.00	0.01	-0.06	0.03	-0.05	-0.08	0.00
0.02										
7	6	-0.03	0.00	0.00	-0.03	-0.06	-0.03	0.05	0.01	-
0.03										

```
    8   6     0.01   0.00   0.00     0.06   0.09   0.03    -0.05  -0.06
0.00
    9   6     0.01  -0.01  -0.01    -0.02   0.00   0.02    -0.01   0.03  -
0.02
   10   6    -0.02   0.07   0.03    -0.01  -0.08   0.08     0.04  -0.05  -
0.02
   11   6     0.02  -0.02   0.01     0.04   0.00   0.02    -0.05   0.03
0.02
   12   8    -0.01   0.01   0.00     0.01   0.00   0.00    -0.02   0.00
0.00
   13   6     0.00   0.00   0.00     0.00  -0.01   0.00     0.00   0.00
0.00
   14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   15   8     0.00   0.00   0.00     0.01   0.00  -0.01    -0.01  -0.01
0.00
   16   1    -0.04  -0.07  -0.06    -0.02   0.10   0.14    -0.03  -0.01  -
0.01
   17   1    -0.02   0.47   0.08     0.04   0.06   0.03     0.10   0.02
0.01
   18   1     0.59   0.21   0.00     0.25   0.03   0.03     0.14   0.29  -
0.11
   19   1    -0.10  -0.17  -0.05    -0.08   0.10   0.08    -0.39  -0.47  -
0.10
   20   1    -0.24  -0.02   0.01     0.42   0.14   0.03     0.38   0.03
0.01
   21   1     0.07   0.05   0.08     0.12   0.04   0.01     0.00  -0.05
0.07
   22   1     0.01   0.00   0.00    -0.30  -0.43  -0.11     0.12   0.13
0.07
   23   1     0.17  -0.41  -0.10     0.30   0.42  -0.16    -0.14   0.29
0.11
   24   1    -0.12   0.09   0.01    -0.06   0.07   0.02     0.21  -0.11
0.01
   25   1    -0.01   0.00  -0.01    -0.08   0.06  -0.01     0.06  -0.07  -
0.02
   26   1     0.01   0.00   0.01    -0.08   0.08   0.00     0.17  -0.16
0.01
   27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   28   1     0.00   0.01   0.00     0.01  -0.01   0.00     0.01  -0.01
0.00
                     55                     56                     57
                     ?A                     ?A                     ?A
 Frequencies --  1376.6560              1391.3972              1399.0028
 Red. masses --     1.4688                 1.6702                 1.7224
 Frc consts  --     1.6401                 1.9051                 1.9862
 IR Inten    --    26.0364                60.5307                 7.2258
 Raman Activ --     1.7650                 3.2321                 1.9656
 Depolar     --     0.7207                 0.6218                 0.5148
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.03   0.02   0.00     0.01   0.07   0.00     0.07   0.00
0.04
```

2	6	-0.02	0.08	-0.01	0.04	-0.05	0.08	-0.06	-0.05	-0.09
3	6	-0.04	0.01	-0.09	-0.02	0.06	-0.04	-0.03	0.05	0.05
4	6	-0.01	-0.02	-0.01	-0.02	0.00	0.02	-0.08	0.00	0.00
5	6	0.05	0.01	0.02	0.12	0.01	-0.02	0.02	-0.07	-0.04
6	6	-0.07	-0.04	0.03	0.00	0.00	-0.07	-0.03	-0.06	-0.05
7	6	0.02	0.03	0.02	0.04	0.02	0.02	-0.01	0.07	0.02
8	6	0.01	-0.03	0.00	0.01	0.04	-0.01	0.01	-0.05	-0.02
9	6	-0.01	0.02	-0.02	-0.06	0.03	0.00	-0.06	0.01	-0.01
10	6	0.01	0.07	0.05	0.03	-0.03	0.02	0.07	-0.03	0.00
11	6	-0.01	-0.02	-0.01	-0.05	-0.01	-0.01	0.00	-0.03	0.00
12	8	-0.02	0.00	0.00	-0.05	0.01	0.01	0.00	0.02	0.00
13	6	0.00	0.00	0.00	0.01	-0.01	0.00	0.01	-0.01	0.01
14	7	0.00	0.00	0.00	0.01	0.01	0.00	0.01	0.01	0.00
15	8	0.00	-0.01	0.00	-0.02	-0.02	0.00	0.01	0.01	0.01
16	1	-0.02	-0.10	0.08	-0.06	-0.33	-0.21	0.11	0.08	-0.04
17	1	0.25	-0.47	0.08	-0.30	0.15	-0.22	0.29	0.26	0.42
18	1	0.27	-0.24	0.16	0.00	-0.28	0.21	0.13	0.01	0.12
19	1	0.00	0.03	0.00	0.05	-0.11	-0.05	0.41	0.12	-0.08
20	1	0.40	-0.08	-0.05	-0.12	0.20	0.17	0.14	0.26	0.31
21	1	-0.11	-0.03	-0.15	-0.18	-0.13	-0.05	-0.10	0.02	-0.02
22	1	-0.06	0.17	-0.05	-0.02	-0.21	0.00	0.04	0.22	-0.02
23	1	0.21	-0.40	-0.08	-0.02	0.15	0.05	-0.15	0.21	0.17
24	1	0.01	-0.01	-0.01	0.06	-0.07	-0.02	-0.01	0.06	-0.01
25	1	-0.04	0.00	-0.01	0.13	-0.16	-0.05	-0.08	0.05	0.04
26	1	0.16	-0.16	0.00	0.35	-0.34	0.01	-0.08	0.09	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.01	-0.01	0.02	0.01	-0.01	0.01	0.01	-0.02	0.01

		58			59			60		
		?A			?A			?A		
Frequencies --		1408.2266			1419.0405			1426.5539		
Red. masses --		1.4582			1.5004			1.5552		
Frc consts --		1.7038			1.7801			1.8647		
IR Inten --		19.2419			9.0987			5.4182		
Raman Activ --		1.9456			9.1951			2.0989		
Depolar --		0.6759			0.7203			0.7463		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	0.07	0.05	0.00	-0.07	-0.02	-0.02	-0.01	0.11
2	6	0.01	-0.03	-0.01	-0.01	0.02	0.04	0.05	0.02	-0.01
3	6	0.01	0.01	0.00	0.00	0.02	-0.04	-0.01	-0.01	-0.02
4	6	0.08	-0.05	-0.08	-0.02	0.02	-0.01	-0.02	0.00	0.00
5	6	-0.06	-0.01	0.02	0.02	0.01	0.01	-0.05	-0.01	0.02
6	6	-0.01	-0.01	-0.02	0.04	-0.06	-0.05	-0.02	-0.03	0.00
7	6	0.01	0.03	0.00	-0.08	-0.02	-0.05	0.06	0.05	-0.08
8	6	0.03	-0.06	0.06	0.01	-0.06	0.00	-0.07	0.02	0.00
9	6	-0.01	-0.02	-0.01	0.04	0.03	-0.02	0.08	-0.01	-0.01
10	6	0.00	-0.01	0.01	-0.04	-0.01	0.05	-0.04	0.01	0.03
11	6	-0.06	0.01	-0.01	-0.02	0.07	0.03	-0.02	-0.01	-0.01
12	8	0.03	0.00	0.00	-0.01	0.00	0.00	0.02	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.01	0.00
14	7	0.00	0.00	0.00	-0.01	0.00	0.00	-0.01	-0.01	0.00
15	8	0.01	0.01	0.00	-0.01	-0.01	0.01	0.01	0.01	0.00
16	1	-0.09	-0.40	-0.15	0.07	0.23	0.08	0.08	0.01	-0.44
17	1	-0.03	0.09	-0.01	-0.06	-0.10	-0.06	-0.06	-0.05	-0.17
18	1	-0.01	0.03	-0.02	0.01	-0.15	0.09	0.11	0.03	-0.03
19	1	-0.41	0.27	0.20	0.04	-0.02	-0.05	0.21	0.08	-0.03
20	1	0.01	0.10	0.10	-0.11	0.22	0.30	0.11	0.11	0.16
21	1	0.00	0.03	0.01	0.46	0.28	0.39	-0.23	-0.26	0.30
22	1	-0.37	0.37	-0.15	0.03	0.28	-0.01	0.25	-0.21	0.17

23	1	0.01	0.04	0.00	0.21	0.05	-0.13	0.20	-0.03	-0.14
24	1	0.21	-0.17	-0.02	0.22	-0.06	0.02	0.26	-0.20	-0.02
25	1	0.10	-0.10	-0.01	0.18	-0.05	0.04	-0.20	0.12	0.00
26	1	-0.17	0.17	0.00	0.08	-0.08	0.00	-0.13	0.13	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	-0.01	0.01	-0.02	0.00	0.01	0.00

	61			62			63		
	?A			?A			?A		
Frequencies --	1435.4794			1441.3583			1460.8589		
Red. masses --	1.7640			1.5177			1.5849		
Frc consts --	2.1416			1.8577			1.9928		
IR Inten --	13.6861			2.0652			8.5150		
Raman Activ --	3.1045			1.0254			2.9146		
Depolar --	0.7396			0.7477			0.7307		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.06	0.08	-0.07	-0.01	-0.02	0.09	-0.05	-0.04	-0.01
2	6	-0.03	-0.02	0.00	0.05	-0.01	-0.01	0.04	-0.01	0.05
3	6	0.01	0.00	0.00	-0.01	0.00	-0.01	0.00	0.00	-0.02
4	6	0.01	-0.03	0.05	-0.05	0.03	-0.01	0.03	0.02	-0.03
5	6	-0.06	0.02	-0.02	0.00	-0.04	0.03	-0.01	0.03	0.02
6	6	-0.01	0.01	-0.04	-0.04	0.06	0.00	-0.01	-0.01	-0.07
7	6	0.01	-0.02	0.07	-0.03	-0.07	0.10	0.02	0.07	0.07
8	6	-0.09	0.00	-0.05	0.02	-0.02	-0.04	-0.02	-0.08	0.01
9	6	0.13	0.00	-0.02	0.00	0.01	0.01	0.05	0.01	-0.02
10	6	-0.06	-0.04	0.04	-0.01	-0.02	0.01	-0.03	-0.03	0.03
11	6	-0.04	0.00	-0.01	-0.03	0.04	-0.03	0.09	-0.06	-0.02
12	8	0.02	-0.01	0.00	0.01	0.01	0.00	0.00	-0.01	0.00
13	6	-0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	-0.02	-0.01	0.01	0.00	0.00	0.00	-0.01	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00
16	1	-0.12	-0.37	0.27	0.12	0.10	-0.47	0.02	0.23	-0.02

17	1	0.11	0.08	0.19	-0.10	0.04	-0.17	-0.20	0.05	-0.19
18	1	0.01	0.00	0.00	0.08	0.00	0.00	-0.01	-0.02	-0.01
19	1	0.03	-0.05	0.04	0.25	-0.04	-0.12	-0.18	0.00	0.02
20	1	0.08	0.06	0.00	0.15	-0.13	-0.25	-0.02	0.18	0.14
21	1	-0.04	0.01	-0.18	0.21	0.25	-0.47	-0.25	-0.04	-0.27
22	1	0.47	0.08	0.20	0.03	0.18	-0.05	0.02	0.40	0.00
23	1	0.28	0.19	-0.21	0.08	0.08	-0.07	0.14	0.17	-0.10
24	1	-0.07	0.07	-0.01	0.05	-0.15	-0.02	-0.38	0.22	0.00
25	1	0.33	-0.24	-0.01	0.21	-0.07	0.06	-0.34	0.24	0.03
26	1	-0.07	0.07	0.00	-0.08	0.08	0.00	0.04	-0.05	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	-0.01	0.02	-0.01	0.00	0.00	0.00	-0.01	0.01	0.00

	64			65			66		
	?A			?A			?A		
Frequencies --	1506.8219			1636.2265			1961.2946		
Red. masses --	2.2515			1.1026			12.6684		
Frc consts --	3.0119			1.7392			28.7117		
IR Inten --	42.2923			3.0111			220.8395		
Raman Activ --	2.1538			9.2839			101.7898		
Depolar --	0.5567			0.6796			0.1988		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.02	0.00	0.04	-0.01	0.00	0.00	0.00	0.00	0.00
2 6	0.00	-0.01	-0.03	0.00	0.00	0.00	0.00	0.00	0.00
3 6	-0.03	-0.09	0.06	0.00	0.00	0.00	0.00	0.00	0.00
4 6	-0.05	-0.10	-0.03	0.00	0.00	0.00	0.00	0.00	0.00
5 6	0.02	0.26	-0.04	0.00	0.00	0.00	0.00	-0.01	0.00
6 6	-0.01	0.02	0.01	0.00	0.00	0.00	0.00	0.00	0.00
7 6	-0.01	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
8 6	0.01	-0.01	0.01	0.00	0.01	0.00	-0.01	0.00	0.00
9 6	0.05	0.00	0.00	0.00	0.00	0.00	-0.11	0.02	0.01
10 6	0.00	-0.01	-0.02	0.00	0.00	0.00	0.00	0.00	0.00

11	6	-0.01	0.01	-0.01	-0.04	-0.07	-0.04	0.00	0.00	0.00
12	8	-0.03	-0.05	0.01	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.65	0.36	-0.23
14	7	-0.01	-0.01	0.00	0.00	0.00	0.00	-0.45	-0.35	0.20
15	8	-0.01	-0.03	0.01	0.00	0.00	0.00	0.01	0.00	0.00
16	1	0.05	0.03	-0.11	-0.02	-0.01	-0.01	0.00	0.00	0.00
17	1	0.07	0.10	0.07	-0.01	-0.01	-0.02	0.00	0.00	0.00
18	1	0.07	0.37	-0.23	0.00	-0.01	0.00	0.01	-0.01	0.00
19	1	0.19	0.46	0.14	-0.02	-0.02	-0.01	0.01	-0.01	0.00
20	1	0.03	-0.02	-0.04	-0.01	-0.02	-0.02	0.00	0.00	0.00
21	1	0.05	0.05	-0.03	0.00	-0.02	-0.01	-0.01	0.00	0.00
22	1	-0.04	0.07	-0.02	-0.01	-0.02	-0.01	0.03	0.01	0.01
23	1	-0.04	0.08	0.01	0.00	-0.01	0.00	0.00	0.01	0.00
24	1	0.08	-0.03	-0.01	0.38	0.58	-0.12	0.00	0.00	0.00
25	1	0.02	0.03	0.05	0.16	0.23	0.64	0.00	0.00	0.00
26	1	0.41	-0.43	0.01	0.00	0.01	0.00	-0.01	0.00	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	-0.03	0.04	-0.01
28	1	-0.01	0.01	-0.01	0.00	0.00	0.00	0.05	-0.06	0.01

	67	68	69
	?A	?A	?A
Frequencies --	3184.9021	3227.5006	3242.9700
Red. masses --	1.0586	1.1049	1.0868
Frc consts --	6.3266	6.7813	6.7342
IR Inten --	71.5250	40.7311	10.7185
Raman Activ --	141.8856	99.0737	55.9945
Depolar --	0.2372	0.7450	0.6212

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	0.00	0.00	-0.01	0.00	0.00	-0.06	0.02	-0.01
2	6	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.01	-0.03
3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01

```
    5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
    6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.02
0.02
    7   6     0.00   0.01   0.00     0.00   0.00   0.00    -0.01   0.01
0.00
    8   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
    9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   10   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   11   6    -0.04  -0.05  -0.02    -0.02  -0.03   0.09     0.00   0.00  -
0.01
   12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   16   1    -0.12   0.03  -0.02     0.06  -0.01   0.01     0.67  -0.19
0.11
   17   1    -0.01   0.00   0.01    -0.02  -0.01   0.01    -0.41  -0.14
0.37
   18   1     0.00   0.00   0.00     0.00   0.00   0.00     0.02  -0.04  -
0.06
   19   1     0.00   0.00  -0.01     0.00   0.00   0.01    -0.04   0.05  -
0.13
   20   1     0.00  -0.01   0.01     0.00  -0.01   0.01    -0.02   0.24  -
0.20
   21   1     0.05  -0.08  -0.02    -0.02   0.03   0.01     0.12  -0.16  -
0.04
   22   1     0.00   0.00  -0.01     0.00   0.00   0.01    -0.02   0.00
0.04
   23   1     0.00   0.00   0.00     0.00   0.00   0.00     0.02   0.00
0.02
   24   1     0.04   0.04   0.57    -0.07  -0.08  -0.80     0.00   0.01
0.07
   25   1     0.39   0.59  -0.37     0.29   0.44  -0.25     0.01   0.02  -
0.01
   26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                      70                     71                     72
                      ?A                     ?A                     ?A
 Frequencies --   3253.8652              3260.2791              3273.9647
 Red. masses --      1.0880                 1.0872                 1.0896
 Frc consts  --      6.7871                 6.8088                 6.8811
 IR Inten    --     27.5260                69.8150                90.0418
```

Raman Activ --		117.2521			97.2002			153.4163		
Depolar --		0.6233			0.7155			0.1494		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.04	-0.01	0.01	0.02	-0.01	0.00	-0.02	0.00	0.00
2	6	0.01	0.00	-0.01	0.04	0.01	-0.03	-0.03	-0.01	0.02
3	6	0.00	0.00	0.00	0.00	0.01	0.01	0.00	-0.01	-0.01
4	6	0.00	0.00	-0.01	0.00	0.01	-0.01	0.00	-0.01	0.02
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	-0.05	0.04	0.00	0.00	0.00	0.00	-0.04	0.04
7	6	-0.02	0.03	0.01	0.03	-0.05	-0.01	0.03	-0.03	-0.01
8	6	0.00	0.00	0.00	-0.01	0.00	0.01	-0.01	0.00	0.01
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01
11	6	0.00	0.00	0.01	0.00	0.00	0.00	0.00	-0.01	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	-0.51	0.14	-0.09	-0.25	0.07	-0.04	0.19	-0.05	0.03
17	1	-0.13	-0.05	0.13	-0.44	-0.15	0.41	0.31	0.10	-0.28
18	1	0.01	-0.02	-0.03	0.03	-0.07	-0.10	-0.03	0.07	0.11
19	1	0.04	-0.06	0.14	0.04	-0.06	0.15	-0.05	0.08	-0.19
20	1	-0.05	0.53	-0.44	0.00	-0.02	0.01	-0.04	0.48	-0.41
21	1	0.23	-0.30	-0.07	-0.40	0.53	0.14	-0.30	0.40	0.10
22	1	-0.02	0.00	0.04	0.08	-0.01	-0.17	0.08	-0.01	-0.16
23	1	0.04	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.07
24	1	-0.01	-0.01	-0.09	0.00	0.00	0.03	0.01	0.01	0.06
25	1	-0.02	-0.04	0.02	0.01	0.00	0.00	0.03	0.05	-0.03

26	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	73	74	75
	?A	?A	?A
Frequencies --	3278.6992	3297.4150	3303.4519
Red. masses --	1.0886	1.0893	1.0898
Frc consts --	6.8948	6.9780	7.0071
IR Inten --	39.3645	47.4779	26.5358
Raman Activ --	92.1043	128.8407	198.3775
Depolar --	0.4098	0.1093	0.1809

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	0.00	0.00	-0.01	0.00	0.00	0.01	0.00	0.00
2	6	-0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.01	-0.01
3	6	0.00	0.00	-0.01	0.00	-0.01	-0.02	0.01	-0.04	-0.06
4	6	-0.02	0.03	-0.06	-0.01	0.01	-0.03	0.00	-0.01	0.01
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	-0.01	0.01	0.00	0.00	0.00
7	6	0.00	0.01	0.00	0.01	-0.02	0.00	0.00	0.00	0.00
8	6	-0.02	0.00	0.04	0.03	0.00	-0.06	-0.01	0.00	0.01
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.02
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	0.25	-0.06	0.04	0.10	-0.03	0.02	-0.08	0.02	-0.01
17	1	0.09	0.03	-0.08	0.01	0.00	-0.01	-0.14	-0.05	0.13
18	1	-0.02	0.06	0.08	-0.05	0.16	0.22	-0.17	0.51	0.71
19	1	0.20	-0.32	0.72	0.11	-0.17	0.38	-0.04	0.06	-0.14

```
  20   1     0.00   0.03  -0.02    -0.01   0.06  -0.05     0.00  -0.03
0.03
  21   1     0.06  -0.08  -0.02    -0.13   0.18   0.04     0.03  -0.05  -
0.01
  22   1     0.20  -0.03  -0.43    -0.35   0.05   0.74     0.08  -0.01  -
0.16
  23   1     0.00   0.00  -0.01     0.01   0.00   0.01    -0.17  -0.01  -
0.22
  24   1     0.00   0.00   0.02     0.01   0.01   0.05     0.00   0.00  -
0.02
  25   1     0.01   0.01  -0.01     0.01   0.02  -0.01    -0.01  -0.01
0.01
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                      76                     77                     78
                      ?A                     ?A                     ?A
 Frequencies --  3331.3027              3849.8062              3870.3420
 Red. masses --     1.0909                 1.0665                 1.0655
 Frc consts  --     7.1328                 9.3130                 9.4040
 IR Inten    --    22.0824                 7.4389                97.3724
 Raman Activ --   169.4697               142.8453                90.4358
 Depolar     --     0.1150                 0.1961                 0.2133
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   2   6     0.01   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   3   6     0.01  -0.01  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
   4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.01  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
   7   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   8   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6    -0.05   0.00  -0.07     0.00   0.00   0.00     0.00   0.00
0.00
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.04   0.05  -
0.01
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

```
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1    -0.02   0.01   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  17   1    -0.05  -0.02   0.04     0.00   0.00   0.00     0.00   0.00
0.00
  18   1    -0.05   0.15   0.20     0.00   0.00   0.00     0.00   0.00
0.00
  19   1    -0.01   0.01  -0.03     0.00   0.00   0.00     0.00   0.00
0.00
  20   1     0.01  -0.10   0.08     0.00   0.00   0.00     0.00   0.00
0.00
  21   1     0.02  -0.03  -0.01     0.01   0.00   0.00     0.00   0.00
0.00
  22   1     0.02   0.00  -0.05     0.00   0.00   0.00     0.00   0.00
0.00
  23   1     0.58   0.02   0.75     0.00   0.00   0.00     0.00   0.00
0.00
  24   1     0.00   0.00  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
  25   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  26   1     0.00   0.00   0.00    -0.01  -0.01   0.00    -0.65  -0.74
0.18
  27   8     0.00   0.00   0.00     0.05   0.04   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00    -0.78  -0.62   0.03     0.01   0.01
0.00

 --------------------
 - Thermochemistry -
 --------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Atom  1 has atomic number  6 and mass  12.00000
 Atom  2 has atomic number  6 and mass  12.00000
 Atom  3 has atomic number  6 and mass  12.00000
 Atom  4 has atomic number  6 and mass  12.00000
 Atom  5 has atomic number  6 and mass  12.00000
 Atom  6 has atomic number  6 and mass  12.00000
 Atom  7 has atomic number  6 and mass  12.00000
 Atom  8 has atomic number  6 and mass  12.00000
 Atom  9 has atomic number  6 and mass  12.00000
 Atom 10 has atomic number  6 and mass  12.00000
 Atom 11 has atomic number  6 and mass  12.00000
 Atom 12 has atomic number  8 and mass  15.99491
 Atom 13 has atomic number  6 and mass  12.00000
 Atom 14 has atomic number  7 and mass  14.00307
 Atom 15 has atomic number  8 and mass  15.99491
 Atom 16 has atomic number  1 and mass   1.00783
 Atom 17 has atomic number  1 and mass   1.00783
 Atom 18 has atomic number  1 and mass   1.00783
 Atom 19 has atomic number  1 and mass   1.00783
```

```
 Atom 20 has atomic number  1 and mass   1.00783
 Atom 21 has atomic number  1 and mass   1.00783
 Atom 22 has atomic number  1 and mass   1.00783
 Atom 23 has atomic number  1 and mass   1.00783
 Atom 24 has atomic number  1 and mass   1.00783
 Atom 25 has atomic number  1 and mass   1.00783
 Atom 26 has atomic number  1 and mass   1.00783
 Atom 27 has atomic number  8 and mass  15.99491
 Atom 28 has atomic number  1 and mass   1.00783
 Molecular mass:   218.08172 amu.
 Principal axes and moments of inertia in atomic units:
                           1         2         3
     EIGENVALUES --  1944.06718 2805.95980 3694.84104
           X            0.99988   0.01322   0.00789
           Y           -0.01329   0.99987   0.00918
           Z           -0.00777  -0.00928   0.99993
 THIS MOLECULE IS AN ASYMMETRIC TOP.
 ROTATIONAL SYMMETRY NUMBER  1.
 WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
           MAY CAUSE SIGNIFICANT ERROR
 ROTATIONAL TEMPERATURES (KELVIN)      0.04455     0.03087     0.02344
 ROTATIONAL CONSTANTS (GHZ)            0.92833     0.64318     0.48845
    1 IMAGINARY FREQUENCIES IGNORED.
 Zero-point vibrational energy     621512.4 (Joules/Mol)
                                  148.54504 (Kcal/Mol)
 WARNING-- EXPLICIT CONSIDERATION OF  14 DEGREES OF FREEDOM AS
           VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
 VIBRATIONAL TEMPERATURES:     89.59   224.22   262.04   272.94   381.79
          (KELVIN)            454.24   510.79   567.54   594.97   713.23
                              757.34   801.11   831.76   873.83   915.60
                              948.45   969.20  1005.62  1023.94  1063.85
                             1178.01  1191.66  1214.81  1270.54  1306.33
                             1331.87  1357.20  1405.39  1433.87  1435.86
                             1448.71  1463.03  1498.39  1500.73  1514.47
                             1533.18  1551.51  1588.90  1617.09  1662.67
                             1704.35  1725.80  1766.41  1775.92  1784.87
                             1807.91  1823.08  1863.72  1890.56  1924.01
                             1947.87  1955.01  1974.73  1980.69  2001.90
                             2012.84  2026.11  2041.67  2052.48  2065.32
                             2073.78  2101.84  2167.97  2354.15  2821.85
                             4582.34  4643.63  4665.88  4681.56  4690.79
                             4710.48  4717.29  4744.22  4752.90  4792.97
                             5538.98  5568.53

 Zero-point correction=                           0.236722
(Hartree/Particle)
 Thermal correction to Energy=                    0.246705
 Thermal correction to Enthalpy=                  0.247649
 Thermal correction to Gibbs Free Energy=         0.200957
 Sum of electronic and zero-point Energies=          -736.131286
 Sum of electronic and thermal Energies=             -736.121302
 Sum of electronic and thermal Enthalpies=           -736.120358
 Sum of electronic and thermal Free Energies=        -736.167051
```

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	154.810	43.344	98.272
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	42.042
ROTATIONAL	0.889	2.981	31.378
VIBRATIONAL	153.032	37.382	24.852
VIBRATION 1	0.597	1.972	4.384
VIBRATION 2	0.620	1.896	2.600
VIBRATION 3	0.630	1.864	2.307
VIBRATION 4	0.633	1.854	2.231
VIBRATION 5	0.671	1.737	1.626
VIBRATION 6	0.703	1.644	1.332
VIBRATION 7	0.731	1.565	1.144
VIBRATION 8	0.761	1.482	0.983
VIBRATION 9	0.777	1.441	0.914
VIBRATION 10	0.851	1.260	0.669
VIBRATION 11	0.881	1.192	0.595
VIBRATION 12	0.912	1.125	0.530
VIBRATION 13	0.935	1.079	0.489
VIBRATION 14	0.966	1.016	0.437

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.368751D-92	-92.433266	-212.835461
TOTAL V=0	0.282075D+17	16.450365	37.878365
VIB (BOT)	0.181259-106	-106.741699	-245.781846
VIB (BOT) 1	0.331554D+01	0.520554	1.198620
VIB (BOT) 2	0.129892D+01	0.113584	0.261536
VIB (BOT) 3	0.110200D+01	0.042182	0.097127
VIB (BOT) 4	0.105513D+01	0.023305	0.053661
VIB (BOT) 5	0.730014D+00	-0.136669	-0.314692
VIB (BOT) 6	0.596941D+00	-0.224069	-0.515938
VIB (BOT) 7	0.517997D+00	-0.285673	-0.657785
VIB (BOT) 8	0.453678D+00	-0.343252	-0.790367
VIB (BOT) 9	0.426706D+00	-0.369871	-0.851660
VIB (BOT) 10	0.332799D+00	-0.477818	-1.100218
VIB (BOT) 11	0.304850D+00	-0.515914	-1.187936
VIB (BOT) 12	0.280005D+00	-0.552835	-1.272949
VIB (BOT) 13	0.264090D+00	-0.578249	-1.331467
VIB (BOT) 14	0.244000D+00	-0.612611	-1.410589
VIB (V=0)	0.138654D+03	2.141932	4.931980
VIB (V=0) 1	0.385303D+01	0.585802	1.348859
VIB (V=0) 2	0.189183D+01	0.276883	0.637547
VIB (V=0) 3	0.171013D+01	0.233028	0.536567
VIB (V=0) 4	0.166760D+01	0.222092	0.511386
VIB (V=0) 5	0.138483D+01	0.141396	0.325576
VIB (V=0) 6	0.127868D+01	0.106761	0.245826
VIB (V=0) 7	0.121995D+01	0.086340	0.198806
VIB (V=0) 8	0.117515D+01	0.070092	0.161393
VIB (V=0) 9	0.115733D+01	0.063456	0.146113
VIB (V=0) 10	0.110063D+01	0.041641	0.095882
VIB (V=0) 11	0.108561D+01	0.035672	0.082138
VIB (V=0) 12	0.107306D+01	0.030626	0.070518
VIB (V=0) 13	0.106546D+01	0.027537	0.063405
VIB (V=0) 14	0.105636D+01	0.023812	0.054828

```
ELECTRONIC      0.100000D+01          0.000000          0.000000
TRANSLATIONAL   0.126587D+09          8.102389         18.656441
ROTATIONAL      0.160710D+07          6.206044         14.289943
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6           0.000000754    0.000000457    0.000000593
   2          6          -0.000001163    0.000000221   -0.000000835
   3          6           0.000000592   -0.000000377   -0.000000778
   4          6          -0.000000096    0.000000191   -0.000000885
   5          6           0.000000186    0.000000502    0.000000868
   6          6           0.000000528   -0.000000275    0.000000305
   7          6           0.000000594    0.000000108    0.000000146
   8          6          -0.000000462    0.000000344    0.000001857
   9          6           0.000000068   -0.000000813   -0.000002776
  10          6          -0.000000836    0.000000257    0.000000579
  11          6           0.000000028   -0.000000286    0.000000180
  12          8           0.000000151    0.000000016   -0.000000876
  13          6          -0.000002145    0.000002114    0.000000672
  14          7           0.000000301   -0.000000516    0.000001229
  15          8           0.000000365   -0.000000820    0.000000407
  16          1           0.000000114    0.000000060   -0.000000535
  17          1           0.000000022   -0.000000181    0.000000068
  18          1          -0.000000268   -0.000000346    0.000000025
  19          1           0.000000177   -0.000000140    0.000000181
  20          1          -0.000000252    0.000000025    0.000000031
  21          1          -0.000000169    0.000000049   -0.000000115
  22          1           0.000000062    0.000000249   -0.000000406
  23          1           0.000000145    0.000000119   -0.000000010
  24          1           0.000000077    0.000000235    0.000000001
  25          1          -0.000000200    0.000000164   -0.000000243
  26          1           0.000000009   -0.000000133    0.000000220
  27          8           0.000001202   -0.000001299   -0.000000180
  28          1           0.000000217    0.000000076    0.000000276
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000002776 RMS     0.000000673
-------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------
  1  C         0.000001(   1)      0.000000(  29)      0.000001(  57)
  2  C        -0.000001(   2)      0.000000(  30)     -0.000001(  58)
  3  C         0.000001(   3)      0.000000(  31)     -0.000001(  59)
  4  C         0.000000(   4)      0.000000(  32)     -0.000001(  60)
  5  C         0.000000(   5)      0.000001(  33)      0.000001(  61)
  6  C         0.000001(   6)      0.000000(  34)      0.000000(  62)
  7  C         0.000001(   7)      0.000000(  35)      0.000000(  63)
  8  C         0.000000(   8)      0.000000(  36)      0.000002(  64)
  9  C         0.000000(   9)     -0.000001(  37)     -0.000003(  65)
 10  C        -0.000001(  10)      0.000000(  38)      0.000001(  66)
 11  C         0.000000(  11)      0.000000(  39)      0.000000(  67)
 12  O         0.000000(  12)      0.000000(  40)     -0.000001(  68)
```

```
 13  C        -0.000002(  13)      0.000002(  41)      0.000001(  69)
 14  N         0.000000(  14)     -0.000001(  42)      0.000001(  70)
 15  O         0.000000(  15)     -0.000001(  43)      0.000000(  71)
 16  H         0.000000(  16)      0.000000(  44)     -0.000001(  72)
 17  H         0.000000(  17)      0.000000(  45)      0.000000(  73)
 18  H         0.000000(  18)      0.000000(  46)      0.000000(  74)
 19  H         0.000000(  19)      0.000000(  47)      0.000000(  75)
 20  H         0.000000(  20)      0.000000(  48)      0.000000(  76)
 21  H         0.000000(  21)      0.000000(  49)      0.000000(  77)
 22  H         0.000000(  22)      0.000000(  50)      0.000000(  78)
 23  H         0.000000(  23)      0.000000(  51)      0.000000(  79)
 24  H         0.000000(  24)      0.000000(  52)      0.000000(  80)
 25  H         0.000000(  25)      0.000000(  53)      0.000000(  81)
 26  H         0.000000(  26)      0.000000(  54)      0.000000(  82)
 27  O         0.000001(  27)     -0.000001(  55)      0.000000(  83)
 28  H         0.000000(  28)      0.000000(  56)      0.000000(  84)
---------------------------------------------------------------------
Internal  Forces:  Max     0.000002776 RMS     0.000000673

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   1 out of a maximum of  94
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
    Eigenvalues ---   -0.00406   0.00123   0.00168   0.00651   0.00817
    Eigenvalues ---    0.01222   0.01306   0.02079   0.02645   0.03232
    Eigenvalues ---    0.03757   0.04226   0.04335   0.04518   0.04596
    Eigenvalues ---    0.04765   0.04880   0.05040   0.05076   0.05142
    Eigenvalues ---    0.05269   0.05272   0.05400   0.05838   0.06538
    Eigenvalues ---    0.07142   0.07755   0.08979   0.10563   0.10960
    Eigenvalues ---    0.11751   0.12157   0.14990   0.15366   0.15883
    Eigenvalues ---    0.17858   0.18735   0.19639   0.20169   0.21506
    Eigenvalues ---    0.24735   0.26432   0.28774   0.29322   0.34382
    Eigenvalues ---    0.35033   0.36213   0.36805   0.39664   0.40083
    Eigenvalues ---    0.47412   0.48341   0.49892   0.51579   0.52514
    Eigenvalues ---    0.56757   0.58831   0.61632   0.62665   0.65468
    Eigenvalues ---    0.66929   0.71718   0.73751   0.77022   0.84507
    Eigenvalues ---    0.85921   0.94307   0.94363   0.95188   0.97611
    Eigenvalues ---    0.98456   1.02143   1.04220   1.05692   1.07285
    Eigenvalues ---    1.09424   1.14135   1.86851
Eigenvalue   1 out of range, new value =    0.004062 Eigenvector:
                           1
          X1          -0.00561
          Y1          -0.00380
          Z1           0.00593
          X2           0.00724
          Y2          -0.00037
          Z2          -0.00551
          X3           0.00566
          Y3          -0.00424
          Z3          -0.00441
          X4          -0.01198
          Y4          -0.00354
```

Z4	0.01182
X5	-0.00487
Y5	-0.00960
Z5	0.00534
X6	0.00204
Y6	0.01585
Z6	-0.01171
X7	-0.00885
Y7	0.01856
Z7	0.00616
X8	-0.01543
Y8	0.01316
Z8	0.01029
X9	-0.00344
Y9	0.00279
Z9	0.00577
X10	0.00553
Y10	0.01178
Z10	-0.00574
X11	-0.01049
Y11	0.01232
Z11	0.00906
X12	-0.00633
Y12	-0.01915
Z12	0.00652
X13	0.02694
Y13	0.00135
Z13	0.00930
X14	0.11392
Y14	0.18612
Z14	0.02497
X15	-0.00732
Y15	0.00580
Z15	0.00517
X16	-0.00623
Y16	-0.01199
Z16	0.00723
X17	0.01491
Y17	-0.00346
Z17	-0.00995
X18	0.01267
Y18	-0.01016
Z18	-0.00542
X19	-0.01891
Y19	-0.00778
Z19	0.01736
X20	0.00721
Y20	0.02432
Z20	-0.03014
X21	0.00441
Y21	0.02866
Z21	0.02420
X22	-0.03375
Y22	0.02037

Z22	0.01765
X23	0.03264
Y23	0.02883
Z23	-0.02118
X24	-0.01925
Y24	0.01313
Z24	0.01577
X25	-0.00546
Y25	0.01384
Z25	0.00344
X26	-0.00599
Y26	-0.02073
Z26	0.00595
X27	-0.17268
Y27	-0.49063
Z27	0.01475
X28	0.27582
Y28	0.72509
Z28	-0.25467

Angle between quadratic step and forces= 81.34 degrees.
Linear search not attempted -- first point.
TrRot= 0.000000 0.000001 0.000002 0.000001 0.000000 0.000001

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
X1	-0.81107	0.00000	0.00000	0.00000	0.00000	-0.81107
Y1	-0.84276	0.00000	0.00000	0.00001	0.00001	-0.84275
Z1	-4.20086	0.00000	0.00000	0.00000	0.00000	-4.20086
X2	-0.83098	0.00000	0.00000	0.00000	0.00000	-0.83098
Y2	1.97846	0.00000	0.00000	0.00001	0.00001	1.97847
Z2	-3.40799	0.00000	0.00000	0.00000	0.00000	-3.40799
X3	1.50331	0.00000	0.00000	0.00001	0.00000	1.50332
Y3	2.44932	0.00000	0.00000	0.00000	0.00000	2.44932
Z3	-1.67091	0.00000	0.00000	0.00000	0.00000	-1.67092
X4	0.84221	0.00000	0.00000	-0.00001	0.00000	0.84221
Y4	-2.03424	0.00000	0.00000	0.00000	0.00000	-2.03424
Z4	-2.11354	0.00000	0.00000	0.00000	0.00000	-2.11354
X5	2.85537	0.00000	0.00000	0.00000	0.00000	2.85537
Y5	-0.09507	0.00000	0.00000	-0.00001	0.00000	-0.09507
Z5	-1.33815	0.00000	0.00000	0.00000	0.00000	-1.33815
X6	-2.60732	0.00000	0.00000	0.00001	0.00000	-2.60732
Y6	2.00525	0.00000	0.00000	0.00001	0.00001	2.00525
Z6	-1.01465	0.00000	0.00000	0.00000	0.00000	-1.01465
X7	-3.38650	0.00000	0.00000	0.00000	0.00000	-3.38651
Y7	-0.80831	0.00000	0.00000	0.00002	0.00001	-0.80830
Z7	-0.73924	0.00000	0.00000	0.00000	0.00000	-0.73924
X8	-0.92956	0.00000	0.00000	-0.00001	-0.00001	-0.92956
Y8	-2.00722	0.00000	0.00000	0.00001	0.00001	-2.00721
Z8	0.28233	0.00000	0.00000	0.00001	0.00001	0.28233
X9	0.40763	0.00000	0.00000	0.00000	0.00000	0.40763
Y9	-0.05174	0.00000	0.00000	0.00000	0.00000	-0.05174
Z9	2.03441	0.00000	0.00000	0.00000	0.00000	2.03441
X10	-0.25459	0.00000	0.00000	0.00000	0.00000	-0.25459
Y10	2.48348	0.00000	0.00000	0.00001	0.00001	2.48348
Z10	0.71065	0.00000	0.00000	0.00000	0.00000	0.71065

X11	-3.50060	0.00000	0.00000	0.00000	0.00000	-3.50060
Y11	-1.72690	0.00000	0.00000	0.00001	0.00001	-1.72689
Z11	-3.50761	0.00000	0.00000	0.00000	0.00000	-3.50761
X12	5.27436	0.00000	0.00000	0.00000	0.00000	5.27435
Y12	-0.34865	0.00000	0.00000	-0.00001	0.00000	-0.34865
Z12	-2.47469	0.00000	0.00000	0.00000	0.00000	-2.47469
X13	0.00734	0.00000	0.00000	0.00000	0.00000	0.00735
Y13	-0.28601	0.00000	0.00000	0.00003	0.00003	-0.28598
Z13	4.85299	0.00000	0.00000	0.00001	0.00002	4.85300
X14	1.25864	0.00000	0.00000	0.00006	0.00006	1.25870
Y14	-1.07476	0.00000	0.00000	0.00013	0.00013	-1.07463
Z14	6.58017	0.00000	0.00000	0.00003	0.00003	6.58020
X15	3.08080	0.00000	0.00000	0.00000	0.00000	3.08079
Y15	-0.39114	0.00000	0.00000	-0.00001	0.00000	-0.39114
Z15	1.35118	0.00000	0.00000	0.00000	0.00000	1.35118
X16	-0.18136	0.00000	0.00000	0.00000	0.00000	-0.18136
Y16	-1.20442	0.00000	0.00000	0.00000	0.00001	-1.20441
Z16	-6.11225	0.00000	0.00000	0.00000	0.00000	-6.11225
X17	-1.21973	0.00000	0.00000	0.00001	0.00000	-1.21973
Y17	3.30917	0.00000	0.00000	0.00000	0.00000	3.30917
Z17	-4.90770	0.00000	0.00000	-0.00001	0.00000	-4.90770
X18	2.74188	0.00000	0.00000	0.00001	0.00001	2.74188
Y18	4.02630	0.00000	0.00000	-0.00001	0.00000	4.02630
Z18	-2.02695	0.00000	0.00000	0.00000	0.00000	-2.02695
X19	1.63009	0.00000	0.00000	-0.00001	-0.00001	1.63008
Y19	-3.86508	0.00000	0.00000	0.00000	0.00000	-3.86508
Z19	-2.55228	0.00000	0.00000	0.00001	0.00001	-2.55227
X20	-4.13873	0.00000	0.00000	0.00001	0.00000	-4.13873
Y20	3.35563	0.00000	0.00000	0.00002	0.00001	3.35564
Z20	-0.97175	0.00000	0.00000	-0.00001	0.00000	-0.97175
X21	-5.05547	0.00000	0.00000	-0.00001	-0.00001	-5.05548
Y21	-1.16483	0.00000	0.00000	0.00002	0.00002	-1.16481
Z21	0.38371	0.00000	0.00000	-0.00001	-0.00001	0.38370
X22	-1.15133	0.00000	0.00000	-0.00002	-0.00001	-1.15135
Y22	-3.83093	0.00000	0.00000	0.00001	0.00001	-3.83092
Z22	1.16866	0.00000	0.00000	0.00000	0.00000	1.16867
X23	-0.22650	0.00000	0.00000	0.00001	0.00001	-0.22649
Y23	4.10587	0.00000	0.00000	0.00001	0.00001	4.10588
Z23	1.93609	0.00000	0.00000	-0.00001	0.00000	1.93608
X24	-3.74136	0.00000	0.00000	-0.00001	0.00000	-3.74136
Y24	-3.75848	0.00000	0.00000	0.00002	0.00001	-3.75847
Z24	-3.66202	0.00000	0.00000	0.00000	0.00000	-3.66202
X25	-4.95942	0.00000	0.00000	0.00000	0.00000	-4.95941
Y25	-0.78121	0.00000	0.00000	0.00002	0.00001	-0.78120
Z25	-4.60041	0.00000	0.00000	-0.00001	0.00000	-4.60041
X26	6.51896	0.00000	0.00000	-0.00001	-0.00001	6.51895
Y26	-0.70339	0.00000	0.00000	-0.00007	-0.00006	-0.70345
Z26	-1.18104	0.00000	0.00000	-0.00001	-0.00001	-1.18104
X27	-2.73014	0.00000	0.00000	-0.00004	-0.00004	-2.73018
Y27	0.83396	0.00000	0.00000	-0.00016	-0.00016	0.83380
Z27	5.29007	0.00000	0.00000	0.00000	0.00000	5.29007
X28	-3.79912	0.00000	0.00000	0.00001	0.00001	-3.79911
Y28	0.89576	0.00000	0.00000	-0.00006	-0.00007	0.89569
Z28	3.80763	0.00000	0.00000	-0.00003	-0.00003	3.80760

```
         Item               Value     Threshold  Converged?
Maximum Force            0.000003     0.000450     YES
RMS     Force            0.000001     0.000300     YES
Maximum Displacement     0.000162     0.001800     YES
RMS     Displacement     0.000027     0.001200     YES
Predicted change in Energy=-8.323169D-11
Optimization completed.
   -- Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1\1\GINC-PELICAN\Freq\RHF\3-21+G*\C12H12N1O3(1-)\SINGH\19-Mar-2002\0\\
#N RHF/3-21+G* FREQ\\Freq calc of output str of mech1s8ts\\-1,1\C,-0.4
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000120,0.00000130,0.00000018,-0.00000022,-0.00000008,-0.00000028\\\@

IN SO FAR AS QUANTUM MECHANICS IS CORRECT, CHEMICAL
QUESTIONS ARE PROBLEMS IN APPLIED MATHEMATICS.

-- EYRING, WALTER, & KIMBALL, 1944

Job cpu time: 0 days 3 hours 19 minutes 12.8 seconds.

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 File lengths (MBytes):  RWF=  309 Int=    0 D2E=    0 Chk=    7 Scr=
1
 Normal termination of Gaussian 98.
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Entering Link 1 = C:\G98W\l1.exe PID=   156.

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Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

****
Gaussian 98: x86-Win32-G98RevA.7 11-Apr-1999
04-Mar-2002
****
%chk=mech1s10ts2F
Default route: MaxDisk=2000MB

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3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
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8/6=4,11=11,27=262144000/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Freq calc of output of mech1s10ts2

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C -1.99452 0.77449 -0.42479

C	-1.69355	0.47685	1.07404
C	-0.18774	0.82994	1.33018
C	-0.5643	0.76283	-1.02773
C	0.29791	1.46241	0.02797
C	-1.32644	-1.05431	1.06074
C	-1.46117	-1.43908	-0.43412
C	-0.19942	-0.76882	-1.03522
C	0.89986	-1.03505	0.00701
C	0.17397	-0.69484	1.31504
C	-2.61124	-0.54375	-0.9267
C	2.06689	-0.11614	-0.1987
N	3.23796	-0.52158	-0.36261
O	1.30162	-2.40474	-0.02367
O	1.70115	1.20673	-0.18436
O	0.21161	2.88136	0.00188
H	-2.56631	1.67274	-0.61741
H	-2.43299	0.82447	1.77851
H	0.0851	1.39334	2.20749
H	-0.47216	1.22509	-1.99995
H	-1.82088	-1.70913	1.76021
H	-1.53189	-2.49681	-0.63134
H	0.07524	-1.13416	-2.01377
H	0.66347	-1.09496	2.18755
H	-2.73951	-0.56807	-2.00315
H	-3.55692	-0.77023	-0.4469
H	3.94923	0.18403	-0.4905
H	2.26283	-2.47779	-0.15809
H	-0.69747	3.20845	0.00845

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 97 maximum allowed number of steps= 174.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C	0	-1.994525		0.774489		-0.424787	
2	2	C	0	-1.693551		0.476848		1.074045	
3	3	C	0	-0.187735		0.829936		1.330176	
4	4	C	0	-0.564300		0.762828		-1.027731	
5	5	C	0	0.297909		1.462408		0.027970	
6	6	C	0	-1.326441		-1.054307		1.060740	
7	7	C	0	-1.461174		-1.439084		-0.434124	
8	8	C	0	-0.199420		-0.768818		-1.035219	
9	9	C	0	0.899861		-1.035049		0.007005	
10	10	C	0	0.173965		-0.694836		1.315043	
11	11	C	0	-2.611238		-0.543749		-0.926697	
12	12	C	0	2.066890		-0.116136		-0.198697	
13	13	N	0	3.237963		-0.521580		-0.362607	
14	14	O	0	1.301619		-2.404735		-0.023673	

15	15	O	0	1.701154	1.206733	-0.184359
16	16	O	0	0.211613	2.881364	0.001881
17	17	H	0	-2.566313	1.672743	-0.617406
18	18	H	0	-2.432994	0.824470	1.778509
19	19	H	0	0.085101	1.393339	2.207485
20	20	H	0	-0.472161	1.225092	-1.999947
21	21	H	0	-1.820881	-1.709127	1.760214
22	22	H	0	-1.531893	-2.496806	-0.631342
23	23	H	0	0.075236	-1.134156	-2.013768
24	24	H	0	0.663466	-1.094963	2.187547
25	25	H	0	-2.739511	-0.568065	-2.003149
26	26	H	0	-3.556921	-0.770226	-0.446904
27	27	H	0	3.949233	0.184030	-0.490495
28	28	H	0	2.262831	-2.477793	-0.158088
29	29	H	0	-0.697465	3.208454	0.008446

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.994525	0.774489	-0.424787
2	6	0	-1.693551	0.476848	1.074045
3	6	0	-0.187735	0.829936	1.330176
4	6	0	-0.564300	0.762828	-1.027731
5	6	0	0.297909	1.462408	0.027970
6	6	0	-1.326441	-1.054307	1.060740
7	6	0	-1.461174	-1.439084	-0.434124
8	6	0	-0.199420	-0.768818	-1.035219
9	6	0	0.899861	-1.035049	0.007005
10	6	0	0.173965	-0.694836	1.315043
11	6	0	-2.611238	-0.543749	-0.926697
12	6	0	2.066890	-0.116136	-0.198697
13	7	0	3.237963	-0.521580	-0.362607
14	8	0	1.301619	-2.404735	-0.023673
15	8	0	1.701154	1.206733	-0.184359
16	8	0	0.211613	2.881364	0.001881
17	1	0	-2.566313	1.672743	-0.617406
18	1	0	-2.432994	0.824470	1.778509
19	1	0	0.085101	1.393339	2.207485
20	1	0	-0.472161	1.225092	-1.999947
21	1	0	-1.820881	-1.709127	1.760214
22	1	0	-1.531893	-2.496806	-0.631342
23	1	0	0.075236	-1.134156	-2.013768
24	1	0	0.663466	-1.094963	2.187547
25	1	0	-2.739511	-0.568065	-2.003149
26	1	0	-3.556921	-0.770226	-0.446904
27	1	0	3.949233	0.184030	-0.490495
28	1	0	2.262831	-2.477793	-0.158088
29	1	0	-0.697465	3.208454	0.008446

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				

2	C	1.557457	0.000000			
3	C	2.519417	1.567723	0.000000		
4	C	1.552167	2.403010	2.388730	0.000000	
5	C	2.435873	2.455914	1.526961	1.532097	0.000000
6	C	2.449004	1.574605	2.218021	2.871332	3.168435
7	C	2.276940	2.449361	3.143701	2.450545	3.424406
8	C	2.444755	2.869339	2.855038	1.574526	2.521126
9	C	3.440689	3.185937	2.532156	2.539056	2.569062
10	C	3.144562	2.217778	1.567158	2.856293	2.515079
11	C	1.539480	2.426260	3.585227	2.430495	3.660491
12	C	4.164063	4.014028	2.883720	2.895347	2.381695
13	N	5.390973	5.232653	4.053087	4.068083	3.568288
14	O	4.597056	4.298785	3.809748	3.810937	3.995610
15	O	3.728630	3.693282	2.450244	2.457765	1.442064
16	O	3.080262	3.249751	2.476329	2.479987	1.421817
17	H	1.082083	2.247862	3.187637	2.237044	2.943555
18	H	2.247057	1.078836	2.289590	3.372062	3.305931
19	H	3.411257	2.299618	1.077745	3.359448	2.190969
20	H	2.236462	3.391326	3.365526	1.080454	2.182149
21	H	3.312511	2.294674	3.049416	3.932200	4.189102
22	H	3.310297	3.431777	4.089196	3.423240	4.411150
23	H	3.232908	3.906217	3.887000	2.231552	3.310653
24	H	4.169419	3.044011	2.272634	3.911114	3.367128
25	H	2.201972	3.413942	4.424593	2.730249	4.180214
26	H	2.197206	2.709359	4.131579	3.412242	4.479941
27	H	5.973376	5.862980	4.565801	4.582097	3.903232
28	H	5.364098	5.089304	4.377359	4.387548	4.406895
29	H	2.791817	3.096669	2.768419	2.659414	2.009932

		6	7	8	9	10
6	C	0.000000				
7	C	1.549459	0.000000			
8	C	2.396815	1.550031	0.000000		
9	C	2.463158	2.435637	1.538027	0.000000	
10	C	1.563684	2.507423	2.380887	1.534156	0.000000
11	C	2.421008	1.538473	2.424727	3.666196	3.578489
12	C	3.739123	3.775295	2.502384	1.499557	2.491880
13	N	4.810769	4.788404	3.511287	2.422186	3.497515
14	O	3.147429	2.955330	2.439788	1.427722	2.446941
15	O	3.978556	4.130744	2.870356	2.388363	2.862949
16	O	4.356179	4.653449	3.816851	3.976431	3.809858
17	H	3.433695	3.307324	3.426072	4.442566	4.104743
18	H	2.295529	3.311171	3.929947	4.207607	3.052757
19	H	3.049335	4.170334	3.907813	3.376835	2.272625
20	H	3.910660	3.244654	2.231763	3.319418	3.884940
21	H	1.078204	2.239962	3.365674	3.306140	2.281748
22	H	2.232970	1.078273	2.219131	2.908204	3.153643
23	H	3.379893	2.224593	1.080031	2.184800	3.359127
24	H	2.287155	3.392001	3.352188	2.194137	1.077486
25	H	3.408902	2.203329	2.725666	4.183757	4.417557
26	H	2.707163	2.199930	3.408655	4.487658	4.126700
27	H	5.636714	5.648910	4.291383	3.321495	4.276099
28	H	4.049040	3.875993	3.122921	1.991596	3.116474
29	H	4.435546	4.730616	4.141978	4.534178	4.207405

		11	12	13	14	15

11	C	0.000000				
12	C	4.753706	0.000000			
13	N	5.876380	1.250065	0.000000		
14	O	4.425966	2.419496	2.722238	0.000000	
15	O	4.712958	1.372571	2.319616	3.637052	0.000000
16	O	4.534550	3.530905	4.568553	5.397371	2.248957
17	H	2.238418	4.984172	6.210442	5.651482	4.314623
18	H	3.036764	5.004302	6.209346	5.255755	4.592402
19	H	4.565704	3.463483	4.495868	4.569830	2.892640
20	H	2.975956	3.389716	4.415514	4.497510	2.831960
21	H	3.033523	4.635700	5.613247	3.662804	4.968736
22	H	2.250922	4.336590	5.169648	2.899401	4.936455
23	H	2.957608	2.880544	3.620003	2.660614	3.386755
24	H	4.552586	2.936301	3.668799	2.648063	3.464179
25	H	1.084340	5.153812	6.198688	4.860289	5.116386
26	H	1.084347	5.667159	6.799954	5.143555	5.623580
27	H	6.615113	1.928331	1.010023	3.732223	2.488674
28	H	5.299796	2.370119	2.195331	0.973311	3.727184
29	H	4.314632	4.328679	5.434927	5.958629	3.130085

		16	17	18	19	20
16	O	0.000000				
17	H	3.092112	0.000000			
18	H	3.792251	2.545142	0.000000		
19	H	2.663628	3.884337	2.616951	0.000000	
20	H	2.686652	2.548977	4.275757	4.247509	0.000000
21	H	5.319340	4.200689	2.606555	3.668530	4.956561
22	H	5.689068	4.295970	4.201219	5.080043	4.104709
23	H	4.495091	4.099548	4.950636	4.920092	2.421959
24	H	4.559878	5.095040	3.666006	2.554711	4.920103
25	H	4.962644	2.640360	4.041540	5.436449	2.890726
26	H	5.266628	2.641680	2.959515	4.999112	3.988606
27	H	4.635499	6.684662	6.803776	4.865495	4.786542
28	H	5.740527	6.384243	6.058558	5.032306	4.958224
29	H	0.966154	2.498538	3.439268	2.956827	2.831630

		21	22	23	24	25
21	H	0.000000				
22	H	2.534461	0.000000			
23	H	4.262487	2.520075	0.000000		
24	H	2.594570	3.838085	4.242475	0.000000	
25	H	4.038416	2.657111	2.871127	5.424003	0.000000
26	H	2.960868	2.667552	3.972414	4.985725	1.769442
27	H	6.476415	6.103234	4.366443	4.427640	6.898773
28	H	4.576837	3.824168	3.167725	3.157878	5.663456
29	H	5.339790	5.801344	4.852286	5.011987	4.741156

		26	27	28	29
26	H	0.000000			
27	H	7.566694	0.000000		
28	H	6.071961	3.168556	0.000000	
29	H	4.920745	5.566676	6.412838	0.000000

Interatomic angles:

C1-C2-C3=107.4457	C2-C1-C4=101.2056	C1-C4-C3= 76.2082
C2-C3-C4= 71.3967	C2-C1-C5= 72.1353	C1-C5-C3= 75.0615
C2-C3-C5=105.0371	C1-C4-C5=104.327	C2-C4-C5= 73.5083
C3-C5-C4=102.6806	C1-C2-C6=102.871	C1-C6-C3= 65.125

C3-C2-C6= 89.7967 C4-C1-C6= 88.7768 C4-C2-C6= 89.9297
C4-C3-C6= 77.0144 C5-C1-C6= 80.875 C5-C2-C6=101.3952
C5-C3-C6=114.3027 C5-C4-C6= 86.3971 C2-C1-C7= 76.8731
C3-C1-C7= 81.7361 C3-C2-C7=100.6988 C4-C1-C7= 77.0127
C4-C2-C7= 60.6564 C3-C4-C7= 81.0153 C5-C1-C7= 93.1453
C5-C2-C7= 88.5505 C5-C4-C7=116.7014 C1-C7-C6= 76.9967
C2-C6-C7=103.2592 C3-C6-C7=111.8882 C4-C7-C6= 88.7818
C2-C1-C8= 88.7254 C3-C1-C8= 70.1989 C2-C3-C8= 74.6087
C1-C4-C8=102.867 C2-C4-C8= 89.8449 C3-C4-C8= 89.7416
C5-C1-C8= 62.203 C2-C5-C8= 70.3977 C3-C5-C8= 86.0047
C5-C4-C8=108.4842 C1-C8-C6= 60.7631 C2-C6-C8= 90.0683
C3-C6-C8= 76.328 C4-C8-C6= 90.1571 C5-C8-C6= 80.177
C1-C7-C8= 76.8135 C2-C7-C8= 88.7257 C3-C8-C7= 85.6522
C4-C8-C7=103.3065 C5-C8-C7=112.3174 C6-C7-C8=101.3011
C1-C3-C9= 85.8609 C2-C3-C9= 99.2823 C1-C4-C9=112.2325
C2-C4-C9= 80.2284 C4-C3-C9= 62.0445 C1-C5-C9= 86.8158
C2-C5-C9= 78.6593 C5-C3-C9= 73.9087 C5-C4-C9= 73.62
C1-C6-C9= 88.9246 C2-C6-C9=101.9312 C3-C6-C9= 65.2477
C4-C9-C6= 70.0422 C5-C9-C6= 78.0143 C1-C7-C9= 93.73
C2-C7-C9= 81.413 C3-C9-C7= 78.49 C4-C7-C9= 62.6154
C5-C9-C7= 86.308 C6-C7-C9= 72.5293 C1-C8-C9=117.7024
C2-C8-C9= 87.0877 C3-C9-C8= 85.3895 C4-C8-C9=109.317
C5-C8-C9= 74.1235 C6-C8-C9= 73.9118 C7-C8-C9=104.1328
C1-C2-C10=111.6088 C1-C3-C10= 97.8962 C2-C3-C10= 90.0559
C1-C4-C10= 85.6058 C4-C2-C10= 76.2435 C4-C3-C10= 89.9724
C1-C5-C10= 78.8434 C5-C2-C10= 64.8798 C5-C3-C10=108.7452
C4-C5-C10= 86.1718 C1-C6-C10=100.8792 C2-C6-C10= 89.9308
C3-C10-C6= 90.2166 C4-C10-C6= 74.6875 C5-C10-C6= 99.2789
C1-C7-C10= 82.0294 C7-C2-C10= 64.7711 C3-C10-C7= 98.3383
C4-C7-C10= 70.3429 C5-C10-C7= 85.9708 C7-C6-C10=107.303
C1-C8-C10= 81.3185 C2-C10-C8= 77.12 C3-C10-C8= 90.2045
C4-C8-C10= 90.0814 C5-C10-C8= 61.9151 C6-C10-C8= 71.4482
C7-C8-C10= 76.0124 C2-C10-C9=115.0202 C3-C10-C9=109.4631
C4-C9-C10= 85.2728 C5-C10-C9= 74.3699 C6-C10-C9=105.3295
C7-C9-C10= 74.487 C8-C9-C10=101.6067 C2-C1-C11=103.1514
C3-C1-C11=122.2242 C3-C2-C11=126.3531 C4-C1-C11=103.6534
C4-C2-C11= 60.4328 C3-C4-C11= 96.1329 C5-C1-C11=132.7993
C5-C2-C11= 97.1385 C5-C4-C11=133.6916 C1-C11-C6= 72.5633
C2-C6-C11= 71.2247 C3-C6-C11=101.129 C4-C11-C6= 72.5756
C1-C11-C7= 95.4216 C2-C11-C7= 72.4247 C4-C11-C7= 72.3376
C6-C7-C11=103.2601 C1-C11-C8= 72.2785 C2-C11-C8= 72.5265
C3-C8-C11= 85.1247 C4-C8-C11= 71.2758 C5-C8-C11= 95.4623
C8-C6-C11= 60.4323 C8-C7-C11=103.4558 C9-C4-C11= 95.0521
C9-C6-C11= 97.286 C9-C7-C11=133.3212 C9-C8-C11=134.1603
C10-C2-C11=100.7119 C10-C4-C11= 84.7927 C10-C6-C11=126.4583
C10-C7-C11=122.554 C10-C8-C11= 96.2534 C1-C3-C12=100.6128
C2-C3-C12=126.1899 C1-C4-C12=136.7544 C2-C4-C12= 98.0762
C4-C3-C12= 65.8393 C1-C5-C12=119.6128 C2-C5-C12=112.138
C3-C5-C12= 92.4565 C4-C5-C12= 92.853 C6-C3-C12= 93.3413
C6-C4-C12= 80.8412 C7-C4-C12= 89.4535 C1-C8-C12=114.6376
C2-C8-C12= 96.4669 C3-C8-C12= 64.7404 C4-C8-C12= 87.396
C5-C12-C8= 62.0963 C6-C8-C12= 99.4737 C7-C8-C12=136.0854
C3-C9-C12= 87.3989 C4-C9-C12= 87.6485 C5-C12-C9= 79.342
C6-C9-C12=140.0752 C7-C9-C12=146.2243 C8-C9-C12=110.9291

C2-C10-C12=116.8053 C3-C10-C12= 87.4344 C4-C10-C12= 65.1383
C5-C12-C10= 62.0886 C6-C10-C12=133.1171 C7-C10-C12= 98.079
C8-C10-C12= 61.7508 C10-C9-C12=110.4445 C11-C4-C12=126.175
C11-C8-C12=149.5043 C3-C9-N13=109.7678 C4-C9-N13=110.1419
C5-C9-N13= 91.2229 C6-C9-N13=159.9513 C7-C9-N13=160.6044
C8-C9-N13=123.355 C10-C9-N13=122.6718 C3-C12-N13=155.2803
C4-C12-N13=155.8192 C5-C12-N13=157.406 C8-C12-N13=136.0548
C9-C12-N13=123.2509 C10-C12-N13=135.7223 C1-C7-O14=122.4162
C2-C7-O14=104.9967 C4-C7-O14= 89.1459 C6-C7-O14= 82.2911
C1-C8-O14=140.4889 C2-C8-O14=107.8593 C3-C8-O14= 91.688
C4-C8-O14=142.4533 C5-C8-O14=107.2899 C6-C8-O14= 81.1913
C7-C8-O14= 92.8708 C3-C9-O14=147.0003 C4-C9-O14=146.3893
C5-C9-O14=177.1017 C6-C9-O14=104.8347 C7-C9-O14= 96.3007
C8-C9-O14=110.6481 C2-C10-O14=134.2499 C3-C10-O14=142.3293
C4-C10-O14= 91.5468 C5-C10-O14=107.2587 C6-C10-O14=101.1031
C7-C10-O14= 73.2293 C10-C8-O14= 60.9927 C10-C9-O14=111.359
C11-C7-O14=158.9803 C11-C8-O14=130.9682 C3-C12-O14= 91.4142
C4-C12-O14= 91.1707 C5-C12-O14=112.651 C7-O14-C12= 88.6574
C8-O14-C12= 61.9892 C12-C9-O14=111.4651 C10-O14-C12= 61.5985
C7-O14-N13=114.9381 C8-O14-N13= 85.5354 N13-C9-O14= 85.8976
C10-O14-N13= 84.9811 N13-C12-O14= 89.9427 C1-C3-O15= 97.2193
C2-C3-O15=132.3847 C1-C4-O15=135.6174 C2-C4-O15= 98.8893
C4-C3-O15= 61.0338 C1-C5-O15=146.9654 C2-C5-O15=141.3174
C3-C5-O15=111.1994 C4-C5-O15=111.42 C6-C3-O15=116.8285
C6-C4-O15= 96.2793 C7-C4-O15=114.615 C1-C8-O15= 88.7217
C2-C8-O15= 80.1011 C8-C3-O15= 64.986 C8-C4-O15= 87.9208
C8-C5-O15= 88.45 C6-C8-O15= 97.707 C7-C8-O15=136.1915
C3-O15-C9= 63.0956 C4-O15-C9= 63.1741 C5-O15-C9= 80.1047
C6-C9-O15=110.1728 C7-C9-O15=117.8019 C8-C9-O15= 91.3192
C2-C10-O15= 92.3709 C10-C3-O15= 88.036 C10-C4-O15= 64.6894
C10-C5-O15= 88.3514 C6-C10-O15=125.4057 C7-C10-O15=100.3499
C8-C10-O15= 65.6258 C10-C9-O15= 91.0834 C11-C4-O15=149.218
C11-C8-O15=125.5533 C3-O15-C12= 93.6499 C4-O15-C12= 93.8964
C5-O15-C12=115.5757 C8-C12-O15= 90.7763 C9-C12-O15=112.4449
C10-C12-O15= 90.8632 C3-O15-N13=116.3377 C4-O15-N13=116.7274
C5-O15-N13=142.0091 C8-O15-N13= 84.4389 C9-O15-N13= 61.9057
C10-O15-N13= 84.1902 N13-C12-O15=124.3042 O14-C8-O15= 86.056
O14-C9-O15=143.5468 O14-C10-O15= 86.0882 O14-C12-O15=145.7523
O14-N13-O15= 91.9828 C1-C3-O16= 76.1278 C2-C3-O16=104.7049
C1-C4-O16= 96.9267 C2-C4-O16= 83.4291 C4-C3-O16= 61.2636
C1-C5-O16=102.7861 C2-C5-O16=111.0445 C3-C5-O16=114.1869
C4-C5-O16=114.1356 C6-C3-O16=136.1689 C6-C4-O16=108.7651
C7-C4-O16=141.3999 C8-C3-O16= 91.1545 C8-C4-O16=139.5046
C8-C5-O16=149.7141 C9-C3-O16=105.1048 C9-C4-O16=104.7899
C9-C5-O16=169.8155 C10-C3-O16=139.7834 C10-C4-O16= 90.8342
C10-C5-O16=149.5868 C11-C4-O16=134.867 C12-C3-O16= 82.0281
C12-C4-O16= 81.7282 C12-C5-O16=134.8119 C3-O15-O16= 63.4317
C4-O15-O16= 63.4105 O15-C5-O16=103.4914 C8-O15-O16= 95.6524
C9-O15-O16=118.0396 C10-O15-O16= 95.6185 C12-O15-O16=153.5098
N13-O15-O16=179.6568 C2-C1-H17=115.5985 C3-C1-H17=118.9913
C3-C2-H17=112.089 C4-C1-H17=115.0867 C2-H17-C4= 64.7957
C3-C4-H17= 87.0535 C5-C1-H17=107.2145 C5-C2-H17= 77.3397
C3-C5-H17= 84.6696 C5-C4-H17=101.0416 C6-C1-H17=150.6938
C6-C2-H17=126.9772 C6-C4-H17= 83.4803 C7-C1-H17=158.4441

C7-C2-H17= 89.4075 C7-C4-H17= 89.6282 C8-C1-H17=150.1786
C8-C2-H17= 83.1077 C8-C4-H17=127.1523 C8-C5-H17= 77.2223
C9-C4-H17=136.8306 C9-C5-H17=107.1976 C10-C2-H17=133.6129
C10-C4-H17=106.7649 C10-C5-H17= 97.2118 C11-C1-H17=116.1741
C2-H17-C11= 65.4782 C4-H17-C11= 65.7859 C5-H17-C11= 88.8006
C6-C11-H17= 94.8611 C7-C11-H17=121.1326 C8-C11-H17= 94.4813
C12-C4-H17=152.159 C12-C5-H17=138.5225 O15-C4-H17=133.512
O15-C5-H17=158.0088 O16-C4-H17= 81.7427 O16-C5-H17= 82.2764
C1-C2-H18=115.7455 C1-H18-C3= 67.4618 C3-C2-H18=118.6258
C4-C1-H18=124.115 C4-C2-H18=148.7462 C4-C3-H18= 92.2139
C5-C1-H18= 89.7197 C5-C2-H18=134.7983 C5-C3-H18=118.6768
C1-H18-C6= 65.2375 C6-C2-H18=118.5969 C6-C3-H18= 61.2042
C4-C6-H18= 80.6433 C7-C1-H18= 94.0916 C7-C2-H18=135.9836
C7-C6-H18=117.5804 C8-C1-H18=113.7125 C8-C2-H18=167.6356
C8-C3-H18= 99.0259 C8-C6-H18=113.7415 C9-C3-H18=121.4505
C9-C6-H18=124.2676 C10-C2-H18=132.5657 C10-C3-H18=103.0558
C10-C6-H18=102.9169 C11-C1-H18=105.1029 C11-C2-H18=114.5044
C11-C6-H18= 80.1115 C12-C3-H18=150.4285 O15-C3-H18=151.3273
O16-C3-H18=105.3762 H17-C1-H18= 93.0362 H17-C2-H18= 93.0845
C3-H18-H17= 82.313 C4-H17-H18= 89.4399 C5-H17-H18= 73.6693
C6-H18-H17= 90.2111 C11-H17-H18= 78.5272 C1-C2-H19=123.2048
C1-C3-H19=139.4714 C2-C3-H19=119.5965 C4-C2-H19= 91.1571
C4-C3-H19=149.1054 C1-C5-H19= 94.8522 C2-H19-C5= 66.2582
C5-C3-H19=113.4009 C4-C5-H19=128.0536 C6-C2-H19=102.2033
C6-C3-H19=132.2947 C7-C2-H19=122.8098 C8-C2-H19= 97.6188
C8-C3-H19=165.509 C8-C5-H19=111.8667 C9-C3-H19=134.56
C9-C5-H19= 90.0132 C2-C10-H19= 61.5958 C10-C3-H19=117.2616
C4-C10-H19= 80.9713 C5-H19-C10= 68.5634 C6-C10-H19=103.7434
C7-C10-H19=121.4107 C8-C10-H19=114.2086 C9-C10-H19=123.8538
C11-C2-H19=150.0693 C12-C3-H19=113.9005 C12-C5-H19= 98.3906
C12-C10-H19= 93.1452 O14-C10-H19=151.0375 C2-H19-O15= 89.9342
O15-C3-H19=103.1567 C4-O15-H19= 77.316 O15-C5-H19=103.6149
C8-O15-H19= 85.3877 C9-O15-H19= 78.8641 O15-C10-H19= 67.4326
C12-O15-H19=102.6901 N13-O15-H19=118.7994 C2-H19-O16= 81.4456
O16-C3-H19= 87.8653 C4-O16-H19= 81.4712 O16-C5-H19= 92.5114
C10-H19-O16=100.7358 O15-O16-H19= 71.5817 H17-C2-H19=117.3325
H17-C5-H19= 97.2296 C1-H18-H19= 88.7282 H18-C2-H19= 94.5811
H18-C3-H19= 95.1696 C5-H19-H18= 86.4022 C6-H18-H19= 76.4279
C10-H19-H18= 76.91 O15-H19-H18=112.8306 O16-H19-H18= 91.7997
H17-H18-H19= 97.6004 C2-C1-H20=125.7859 C3-C1-H20= 89.8858
C1-C4-H20=115.1445 C2-C4-H20=151.4038 C3-C4-H20=149.6265
C1-H20-C5= 66.896 C2-C5-H20= 93.7864 C3-C5-H20=129.4385
C5-C4-H20=112.128 C6-C1-H20=113.078 C6-C4-H20=161.4209
C7-C1-H20= 91.9219 C7-C4-H20=129.3171 C1-H20-C8= 66.3423
C2-C8-H20= 82.3146 C3-C8-H20= 81.8561 C8-C4-H20=113.0883
C5-H20-C8= 69.6543 C6-C8-H20=115.2751 C7-C8-H20=117.032
C9-C4-H20=128.3509 C9-C5-H20= 88.2453 C9-C8-H20=122.3385
C10-C4-H20=159.123 C10-C5-H20=111.4016 C10-C8-H20=114.7157
C11-C1-H20=102.4502 C2-C11-H20= 77.0266 C11-C4-H20=109.8296
C5-H20-C11= 89.0343 C6-C11-H20= 92.2896 C7-C11-H20= 85.6444
C11-C8-H20= 79.3306 C12-C4-H20=108.0613 C12-C5-H20= 95.8305
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C3-O15-H20= 78.7944 O15-C4-H20= 98.7945 O15-C5-H20=100.7941
C8-H20-O15= 67.8699 C9-O15-H20= 78.462 C10-O15-H20= 86.0263

C11-H20-O15=108.4545 C12-O15-H20=101.7733 N13-O15-H20=117.6458
C1-H20-O16= 76.8602 C3-O16-H20= 81.2527 O16-C4-H20= 88.9349
O16-C5-H20= 94.0176 C8-H20-O16=101.3961 C11-H20-O16=106.2988
O15-O16-H20= 69.379 H17-C1-H20= 93.8456 C2-H17-H20= 89.7546
H17-C4-H20= 93.8613 C5-H20-H17= 76.5128 C8-H20-H17= 91.3091
C11-H17-H20= 76.5642 O15-H20-H17=106.493 O16-H20-H17= 72.3436
H18-C1-H20=144.9785 H18-H17-H20=114.1434 H19-C5-H20=152.4686
H19-O15-H20= 95.794 H19-O16-H20=105.0994 C1-C2-H21=117.3292
C3-C2-H21=102.6502 C4-C2-H21=113.6401 C5-C2-H21=123.6869
C1-C6-H21=136.2146 C2-C6-H21=118.5659 C3-C6-H21=132.2645
C4-C6-H21=167.9406 C1-C7-H21= 94.3339 C2-H21-C7= 65.374
C4-C7-H21=113.8535 C7-C6-H21=115.7973 C8-C2-H21= 80.5112
C8-C6-H21=148.7904 C8-C7-H21=124.2461 C9-C6-H21=134.1675
C9-C7-H21= 89.8992 C2-C10-H21= 61.3056 C3-C10-H21=103.2286
C4-C10-H21= 99.2597 C5-C10-H21=121.6147 C10-C6-H21=118.3028
C7-H21-C10= 67.3493 C8-C10-H21= 92.3883 C9-C10-H21=118.7789
C11-C2-H21= 79.9141 C11-C6-H21=114.6626 C11-C7-H21=105.2935
C12-C10-H21=152.3592 O14-C7-H21= 88.5489 O14-C10-H21=101.4789
O15-C10-H21=149.745 H17-C2-H21=135.2575 C1-H18-H21= 85.7375
H18-C2-H21= 94.2244 C3-H18-H21= 76.7416 H18-C6-H21= 94.1955
C7-H21-H18= 85.8369 C10-H21-H18= 76.9734 H17-H18-H21=109.2479
H19-C2-H21=105.9737 H19-C10-H21=107.3162 H19-H18-H21= 89.2253
C1-C6-H22= 89.8653 C2-C6-H22=127.8159 C3-C6-H22=133.4778
C4-C6-H22= 83.2278 C1-C7-H22=159.8891 C2-C7-H22=150.8923
C4-C7-H22=149.4418 C6-C7-H22=115.1986 C1-C8-H22= 90.2994
C2-C8-H22= 83.7765 C3-C8-H22=106.7211 C4-C8-H22=128.1308
C5-C8-H22=136.9565 C6-H22-C8= 65.1427 C8-C7-H22=113.9939
C3-C9-H22= 97.2241 C4-C9-H22= 77.5419 C5-C9-H22=107.1271
C9-C6-H22= 76.3517 C9-C7-H22=105.036 C9-C8-H22= 99.8485
C10-C6-H22=111.102 C10-C7-H22=117.4854 C10-C8-H22= 86.4859
C10-C9-H22= 84.4319 C1-C11-H22=120.5376 C2-C11-H22= 94.3249
C4-C11-H22= 93.9022 C6-H22-C11= 65.3569 C11-C7-H22=117.5993
C8-H22-C11= 65.695 C9-H22-C11= 89.6354 C12-C8-H22=133.319
C12-C9-H22=158.2249 N13-C9-H22=151.6665 C6-H22-O14= 74.3805
C7-H22-O14= 82.3236 O14-C8-H22= 76.8114 C9-O14-H22= 76.1114
C10-O14-H22= 71.7287 C11-H22-O14=117.9411 C12-O14-H22=108.9039
N13-O14-H22=133.7104 O15-C8-H22=151.5897 O15-C9-H22=137.2845
H17-C11-H22=146.2445 H18-C6-H22=136.1626 H20-C8-H22=134.5058
H20-C11-H22=102.6138 C2-H21-H22= 90.4339 H21-C6-H22= 93.2718
H21-C7-H22= 92.8881 C8-H22-H21= 89.8967 C9-H22-H21= 74.4552
C10-H21-H22= 81.626 C11-H22-H21= 78.4326 O14-H22-H21= 84.4794
H18-H21-H22=109.6022 C1-C4-H23=116.2381 C2-C4-H23=114.8334
C3-C4-H23=114.5107 C5-C4-H23=122.0963 C6-C4-H23= 81.9224
C1-C7-H23= 91.8013 C2-C7-H23=113.299 C4-H23-C7= 66.7235
C6-C7-H23=126.2258 C1-C8-H23=128.792 C2-C8-H23=160.9627
C3-C8-H23=159.8896 C4-C8-H23=113.0974 C5-C8-H23=129.1455
C6-C8-H23=150.6446 C7-C8-H23=114.3363 C3-C9-H23=110.7696
C4-H23-C9= 70.1792 C5-C9-H23= 87.8916 C6-C9-H23= 93.106
C7-H23-C9= 67.0531 C9-C8-H23=111.941 C10-C4-H23= 81.6352
C10-C7-H23= 90.2452 C10-C8-H23=149.8843 C10-C9-H23=128.3214
C1-C11-H23= 85.8075 C2-C11-H23= 92.4933 C11-C4-H23= 78.6238
C6-C11-H23= 77.1495 C11-C7-H23=102.0735 C11-C8-H23=108.9595
C9-H23-C11= 89.6462 C3-C12-H23= 84.8039 C4-H23-C12= 67.6231
C5-C12-H23= 77.3298 C7-H23-C12= 94.5044 C12-C8-H23= 99.253

C12-C9-H23=101.2249 C10-C12-H23= 77.025 C11-H23-C12=109.0191
N13-C9-H23=103.4627 N13-C12-H23=116.7744 C4-H23-O14=101.9787
C7-H23-O14= 73.8447 O14-C8-H23= 89.5633 O14-C9-H23= 92.454
C10-O14-H23= 82.131 C11-H23-O14=103.833 C12-O14-H23= 68.8979
N13-O14-H23= 84.5134 O15-C4-H23= 92.3494 O15-C8-H23=109.4514
O15-C9-H23= 95.4571 O15-C12-H23= 99.3789 O16-C4-H23=145.0808
H17-C4-H23=133.1014 H17-C11-H23=103.3102 C1-H20-H23= 87.7995
H20-C4-H23= 86.6555 C5-H20-H23= 91.804 C7-H23-H20= 88.4743
H20-C8-H23= 86.6542 C9-H23-H20= 92.054 C11-H23-H20= 66.3063
C12-H23-H20= 78.9546 O14-H23-H20=124.409 O15-H20-H23= 79.857
O16-H20-H23=123.1785 H17-H20-H23=111.0912 H21-C7-H23=145.3915
C4-H23-H22= 91.9768 C6-H22-H23= 90.4416 H22-C7-H23= 92.8591
H22-C8-H23= 93.1065 C9-H23-H22= 75.9866 C11-H22-H23= 76.388
C12-H23-H22=106.641 O14-H23-H22= 68.0015 H20-H23-H22=112.2997
H21-H22-H23=114.98 C1-C3-H24=120.8473 C2-C3-H24=103.334
C4-C3-H24=114.0567 C5-C3-H24=123.6029 C1-C6-H24=123.3302
C2-C6-H24=102.4722 C6-C3-H24= 61.222 C4-C6-H24= 97.9702
C7-C6-H24=123.1305 C8-C3-H24= 80.7813 C8-C6-H24= 91.366
C3-H24-C9= 69.0412 C4-C9-H24=111.236 C5-C9-H24= 89.6099
C6-H24-C9= 66.649 C7-C9-H24= 94.0728 C8-C9-H24=126.953
C2-C10-H24=131.8155 C3-C10-H24=117.2801 C4-C10-H24=166.1948
C5-C10-H24=135.2771 C6-C10-H24=118.8316 C7-C10-H24=138.6699
C8-C10-H24=149.2101 C9-C10-H24=113.1478 C11-C6-H24=150.4473
C12-C3-H24= 68.2413 C4-C12-H24= 84.2345 C5-C12-H24= 77.7957
C6-H24-C12= 90.5465 C8-C12-H24= 75.6322 C12-C9-H24=103.704
C12-C10-H24=103.4762 N13-C9-H24=105.1553 N13-C12-H24=116.4997
C3-H24-O14=101.1963 C6-H24-O14= 78.876 C7-O14-H24= 74.2804
C8-O14-H24= 82.3163 O14-C9-H24= 91.4598 O14-C10-H24= 88.5193
C12-O14-H24= 70.6567 N13-O14-H24= 86.1712 O15-C3-H24= 94.2842
O15-C9-H24= 98.1291 O15-C10-H24=115.3665 O15-C12-H24=100.6866
O16-C3-H24=147.5243 H18-C3-H24=106.9416 H18-C6-H24=106.2542
C2-H19-H24= 77.4716 H19-C3-H24= 92.3417 C5-H19-H24= 90.0545
C6-H24-H19= 77.852 C9-H24-H19= 90.318 H19-C10-H24= 92.3493
C12-H24-H19= 77.8694 O14-H24-H19=122.8767 O15-H19-H24= 78.7105
O16-H19-H24=121.7968 H18-H19-H24= 90.2769 C2-H21-H24= 76.7394
C3-H24-H21= 77.2748 H21-C6-H24= 93.9319 C7-H21-H24= 88.7994
C9-H24-H21= 86.9013 H21-C10-H24= 94.2505 C12-H24-H21=113.7478
O14-H24-H21= 88.6327 H18-H21-H24= 89.6343 H19-H24-H21= 90.8635
H22-C6-H24=116.225 H22-C9-H24= 96.5647 H22-O14-H24= 87.4325
H22-H21-H24= 96.8808 H23-C9-H24=151.3171 H23-C12-H24= 93.6578
H23-O14-H24=106.0995 C2-C1-H25=129.6931 C3-C1-H25=139.0559
C4-C1-H25= 91.6461 C2-C4-H25= 83.1118 C3-C4-H25=119.4684
C5-C1-H25=128.5958 C5-C4-H25=156.5081 C6-C1-H25= 94.117
C6-C4-H25= 74.9236 C1-H25-C7= 62.2442 C2-C7-H25= 94.2558
C4-C7-H25= 71.617 C6-C7-H25=129.74 C8-C1-H25= 71.6123
C2-C8-H25= 75.1555 C3-C8-H25=104.8793 C4-C8-H25= 73.3862
C5-C8-H25=105.5695 C6-C8-H25= 83.1721 C8-C7-H25= 91.4429
C9-C4-H25=105.0614 C9-C7-H25=128.7417 C9-C8-H25=156.8475
C10-C4-H25=104.4887 C10-C7-H25=139.2689 C10-C8-H25=119.6308
C1-C11-H25=112.9697 C2-C11-H25=150.7853 C4-C11-H25= 94.0379
C6-C11-H25=150.808 C7-C11-H25=113.1551 C8-C11-H25= 94.0803
C12-C4-H25=132.7136 C12-C8-H25=160.6481 O14-C7-H25=140.3951
O14-C8-H25=140.3507 O15-C4-H25=160.9097 O15-C8-H25=132.1932
O16-C4-H25=144.4892 H17-C1-H25=101.5226 C2-H17-H25= 88.2167

C4-H17-H25= 67.4953 C5-H17-H25= 96.7914 C7-H25-H17= 85.624
C8-H25-H17= 79.3389 H17-C11-H25= 99.3084 H18-C1-H25=130.5702
H18-H17-H25=102.3944 H20-C1-H25= 81.2745 H20-C4-H25= 87.4223
C5-H20-H25=110.1992 C7-H25-H20= 77.8404 H20-C8-H25= 70.537
C11-H25-H20= 83.8117 O15-H20-H25=126.7712 O16-H20-H25=125.6521
H20-H17-H25= 67.6777 H21-C7-H25=130.7001 C1-H25-H22= 85.3392
C4-H25-H22= 78.8896 C6-H22-H25= 87.9437 H22-C7-H25=102.6789
C8-H22-H25= 67.276 C9-H22-H25= 97.3829 H22-C11-H25= 99.6441
O14-H22-H25=121.9589 H17-H25-H22=108.3768 H20-H25-H22= 95.3491
H21-H22-H25=102.1078 C1-H25-H23= 77.9469 H23-C4-H25= 69.8846
H23-C7-H25= 80.8427 H23-C8-H25= 86.5691 C9-H23-H25=110.9566
C11-H25-H23= 83.8069 C12-H23-H25=127.2884 O14-H23-H25=122.9071
H17-H25-H23= 96.0251 H20-H23-H25= 65.5651 H23-H22-H25= 67.3023
C2-C1-H26= 90.7303 C3-C1-H26=122.1701 C3-C2-H26=148.8678
C4-C1-H26=130.2427 C4-C2-H26= 83.5104 C5-C1-H26=150.4153
C5-C2-H26=120.2179 C6-C1-H26= 71.0402 C2-C6-H26= 73.1763
C3-C6-H26=113.6717 C4-C6-H26= 75.3576 C1-H26-C7= 62.3727
C2-C7-H26= 71.0572 C4-C7-H26= 94.2473 C6-C7-H26= 90.7414
C8-C1-H26= 94.3475 C8-C2-H26= 75.2644 C8-C6-H26= 83.5645
C8-C7-H26=129.922 C9-C6-H26=120.3728 C9-C7-H26=150.9364
C10-C2-H26=113.3883 C10-C6-H26=148.9839 C10-C7-H26=122.347
C1-C11-H26=112.579 C2-C11-H26= 93.0294 C4-C11-H26=149.9014
C6-C11-H26= 93.1842 C7-C11-H26=112.8753 C8-C11-H26=150.215
O14-C7-H26=172.1921 H17-C1-H26=101.8917 C2-H17-H26= 66.7361
C4-H17-H26= 88.3542 C5-H17-H26=106.5381 C6-H26-H17= 79.8646
C7-H26-H17= 85.659 H17-C11-H26= 99.3915 H18-C1-H26= 83.4975
H18-C2-H26= 92.4924 C3-H18-H26=103.0886 H18-C6-H26= 72.006
C7-H26-H18= 78.327 C11-H26-H18= 83.6255 H18-H17-H26= 69.5533
H19-C2-H26=172.7824 H19-H18-H26=127.2875 H20-C1-H26=128.2135
H20-C11-H26=155.5862 H20-H17-H26=100.4093 C1-H26-H21= 78.3755
H21-C2-H26= 72.0143 H21-C6-H26= 92.7048 H21-C7-H26= 83.648
C10-H21-H26=103.0741 C11-H26-H21= 83.3798 H17-H26-H21= 96.9784
H21-H18-H26= 63.9057 C1-H26-H22= 85.1775 C2-H26-H22= 79.3177
C6-H22-H26= 66.3798 H22-C7-H26=103.5739 C8-H22-H26= 87.96
C9-H22-H26=107.1131 H22-C11-H26=100.3064 O14-H22-H26=134.9782
H17-H26-H22=108.0251 H18-H26-H22= 96.4572 H21-H22-H26= 69.3315
H23-C7-H26=127.7445 H23-C11-H26=155.9386 H23-H22-H26= 99.9082
H24-C6-H26=173.253 H24-H21-H26=127.5268 C1-H26-H25= 66.4243
C2-H26-H25= 97.09 C4-H25-H26= 96.2878 C6-H26-H25= 96.9603
C7-H26-H25= 66.4071 C8-H25-H26= 96.3016 H25-C11-H26=109.3538
H17-H25-H26= 70.4682 H18-H26-H25=115.1096 H20-H25-H26=115.6096
H21-H26-H25=114.8967 H22-H25-H26= 70.9101 H23-H25-H26=115.6971
C3-C12-H27=142.4065 C4-C12-H27=142.798 C5-C12-H27=129.5134
C8-C12-H27=150.9359 C9-C12-H27=151.1438 C10-C12-H27=150.4115
C9-N13-H27=147.9065 C12-N13-H27=116.7263 O14-C12-H27=117.8356
O14-N13-H27=179.4225 C3-O15-H27=135.1708 C4-O15-H27=135.7424
C5-O15-H27=165.9251 C8-O15-H27=106.1901 C9-O15-H27= 85.8251
C10-O15-H27=105.863 O15-C12-H27= 96.4111 O15-N13-H27= 87.4648
O16-O15-H27=156.1319 H19-O15-H27=129.2638 H20-O15-H27=128.0998
H23-C12-H27=129.3895 H24-C12-H27=129.898 C3-C9-H28=150.5525
C4-C9-H28=150.9044 C5-C9-H28=149.9116 C6-C9-H28=130.4174
C7-C9-H28=121.885 C8-C9-H28=123.9424 C10-C9-H28=123.7199
C3-C12-H28=112.4858 C4-C12-H28=112.4904 C5-C12-H28=136.07
C8-C12-H28= 79.6714 C12-C9-H28= 84.2574 C10-C12-H28= 79.6877

```
    C9-H28-N13= 70.5       C12-N13-H28= 81.9915     C7-O14-H28=158.214
    C8-O14-H28=126.9171     C9-O14-H28=110.6634    C10-O14-H28=125.6703
   C12-H28-O14= 81.1371    N13-H28-O14=112.6216     O15-C9-H28=116.341
   O15-C12-H28=169.1727    O15-N13-H28=111.253      H22-C9-H28=100.9488
   H22-O14-H28=159.0351     H23-C9-H28= 98.5557    H23-C12-H28= 73.4893
   H23-O14-H28=112.8151     H24-C9-H28= 97.8357    H24-C12-H28= 72.1471
   H24-O14-H28=112.9818    H27-C12-H28= 94.416     H27-N13-H28=161.2822
     C2-C1-H29= 85.8419      C1-C3-H29= 63.5318      C2-C3-H29= 86.4826
     C1-C4-H29= 78.2057      C2-C4-H29= 75.234       C3-C4-H29= 66.2629
     C1-C5-H29= 77.1419      C2-C5-H29= 87.2017      C3-C5-H29=102.1576
     C4-C5-H29= 96.3889      C6-C1-H29=115.4779      C6-C3-H29=125.2642
     C6-C4-H29=106.5764      C7-C1-H29=137.6776      C7-C4-H29=135.5286
     C8-C1-H29=104.3573      C8-C3-H29= 94.8648      C8-C4-H29=155.2336
     C8-C5-H29=131.8383      C9-C3-H29=117.5416      C9-C4-H29=121.4166
     C9-C5-H29=163.8327     C10-C3-H29=150.9043     C10-C4-H29= 99.3621
    C10-C5-H29=136.5253     C11-C1-H29=169.4945     C11-C4-H29=115.8485
    C12-C3-H29= 99.945      C12-C4-H29=102.305      C12-C5-H29=160.5041
    O15-C3-H29= 73.4239     O15-C4-H29= 75.3071     O15-C5-H29=129.3819
    C1-H29-O16= 98.1022     C3-O16-H29= 97.1851     C4-O16-H29= 89.8648
    C5-O16-H29=113.2567    O15-O16-H29=151.146      C1-H17-H29= 94.0367
    C2-H17-H29= 81.2631     C3-H29-H17= 74.29       C4-H17-H29= 68.072
    C5-H29-H17= 80.7296    C11-H17-H29=131.1662    O16-H29-H17=119.6039
    H18-C1-H29= 85.3601     H18-C3-H29= 85.1229    H18-H17-H29= 85.9788
    C1-H29-H19= 72.7335     C2-H19-H29= 70.9364     H19-C3-H29= 89.2045
    C4-H29-H19= 73.2614     H19-C5-H29= 89.3667    C10-H19-H29=106.4003
   O15-H19-H29= 64.6913    H19-O16-H29= 97.9791    H17-H29-H19= 90.3977
   H18-H19-H29= 75.9284     H20-C1-H29= 67.5046     C3-H29-H20= 73.8707
    H20-C4-H29= 87.7887     H20-C5-H29= 84.8758     C8-H20-H29=109.2025
   C11-H20-H29= 95.9314    O15-H20-H29= 67.1005    H20-O16-H29= 88.5273
   H20-H17-H29= 68.2408    H19-H29-H20= 94.3852     H23-C4-H29=165.5231
   H23-H20-H29=134.7751     H24-C3-H29=167.6284    H24-H19-H29=130.6947
    H25-C1-H29=143.1273     H25-C4-H29=123.2012    H25-H17-H29=134.6006
   H25-H20-H29=111.8924     H26-C1-H29=160.8824    H26-H17-H29=146.3799
Stoichiometry    C12H13NO3
Framework group  C1[X(C12H13NO3)]
Deg. of freedom   81
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0       -2.070510    0.503996   -0.466246
   2          6             0       -1.754155    0.288512    1.043443
   3          6             0       -0.308394    0.836132    1.303527
   4          6             0       -0.642422    0.656537   -1.054905
   5          6             0        0.110705    1.488547   -0.011890
   6          6             0       -1.196732   -1.183712    1.078350
   7          6             0       -1.262176   -1.623774   -0.405863
   8          6             0       -0.087226   -0.816294   -1.014191
   9          6             0        1.023041   -0.912368    0.045813
  10          6             0        0.242882   -0.630497    1.336369
```

11	6	0	-2.509389	-0.895057	-0.935325
12	6	0	2.067468	0.140663	-0.175472
13	7	0	3.282379	-0.117848	-0.316284
14	8	0	1.594697	-2.220582	0.058972
15	8	0	1.537662	1.406556	-0.203253
16	8	0	-0.153503	2.883929	-0.080215
17	1	0	-2.748430	1.317050	-0.690458
18	1	0	-2.540742	0.559265	1.730364
19	1	0	-0.120361	1.453640	2.166580
20	1	0	-0.596530	1.099579	-2.039277
21	1	0	-1.613804	-1.876126	1.791888
22	1	0	-1.196334	-2.687012	-0.572785
23	1	0	0.244167	-1.170989	-1.978989
24	1	0	0.767410	-0.941150	2.224817
25	1	0	-2.619392	-0.965262	-2.011785
26	1	0	-3.425192	-1.225884	-0.458179
27	1	0	3.900603	0.668208	-0.457917
28	1	0	2.559134	-2.175221	-0.064066
29	1	0	-1.096580	3.093505	-0.091885

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9248457      0.7185732      0.5229206
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,N-
14,O-16,
 O-16,O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1
 Standard basis: 3-21+G* (6D, 7F)
 There are   234 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    262144 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
   234 basis functions      343 primitive gaussians
    58 alpha electrons       58 beta electrons
       nuclear repulsion energy      1246.1499143811 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   234 RedAO= T  NBF=   234
 NBsUse=   234 1.00D-04 NBFU=   234
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -736.994836223     A.U. after   16 cycles
             Convg  =    0.6818D-08             -V/T =  2.0021
             S**2   =   0.0000
 Range of M.O.s used for correlation:     1   234
 NBasis=   234 NAE=    58 NBE=    58 NFC=     0 NFV=     0
 NROrb=    234 NOA=    58 NOB=    58 NVA=   176 NVB=   176

 **** Warning!!: The largest alpha MO coefficient is  0.12960626D+03

          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
```

```
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   2 vectors were produced by pass 12.
 Inv2:  IOpt= 1 Iter= 1 AM= 7.61D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  38 with in-core refinement.
 G2DrvN: will do   29 atoms at a time, making    1 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  90 IRICut=      82 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
          There are  90 degrees of freedom in the 1st order CPHF.
  87 vectors were produced by pass  0.
 AX will form  87 AO Fock derivatives at one time.
  87 vectors were produced by pass  1.
  87 vectors were produced by pass  2.
  87 vectors were produced by pass  3.
  87 vectors were produced by pass  4.
  87 vectors were produced by pass  5.
  87 vectors were produced by pass  6.
  40 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
 Inv2:  IOpt= 1 Iter= 1 AM= 4.48D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 652 with in-core refinement.

 ********************************************************************

            Population analysis using the SCF density.

 ********************************************************************

 Alpha  occ. eigenvalues --  -20.52761 -20.50385 -20.47995 -15.49200 -
11.32363
 Alpha  occ. eigenvalues --  -11.31259 -11.26218 -11.20107 -11.20091 -
11.19899
 Alpha  occ. eigenvalues --  -11.19816 -11.19745 -11.19726 -11.19159 -
11.18823
 Alpha  occ. eigenvalues --  -11.18425  -1.47055  -1.38995  -1.37446  -
1.25201
```

```
 Alpha  occ. eigenvalues --   -1.23184  -1.10997  -1.07980  -1.06530  -
0.96739
 Alpha  occ. eigenvalues --   -0.93713  -0.89829  -0.86486  -0.83891  -
0.80388
 Alpha  occ. eigenvalues --   -0.76271  -0.74768  -0.73549  -0.71756  -
0.69741
 Alpha  occ. eigenvalues --   -0.68978  -0.66923  -0.64411  -0.63938  -
0.61778
 Alpha  occ. eigenvalues --   -0.60990  -0.58985  -0.56658  -0.55854  -
0.54163
 Alpha  occ. eigenvalues --   -0.53156  -0.51583  -0.50035  -0.48718  -
0.47548
 Alpha  occ. eigenvalues --   -0.47158  -0.46578  -0.46017  -0.45707  -
0.44785
 Alpha  occ. eigenvalues --   -0.43521  -0.41998  -0.39094
 Alpha virt. eigenvalues --    0.05728   0.06871   0.07209   0.07481
0.09136
 Alpha virt. eigenvalues --    0.09216   0.09565   0.09673   0.10517
0.12349
 Alpha virt. eigenvalues --    0.12756   0.13192   0.14127   0.14337
0.14961
 Alpha virt. eigenvalues --    0.15917   0.16086   0.16540   0.17932
0.18508
 Alpha virt. eigenvalues --    0.18778   0.19037   0.19574   0.19704
0.20370
 Alpha virt. eigenvalues --    0.20623   0.22111   0.23236   0.23334
0.23365
 Alpha virt. eigenvalues --    0.24027   0.24386   0.24718   0.25304
0.25547
 Alpha virt. eigenvalues --    0.25750   0.25951   0.27187   0.27392
0.28179
 Alpha virt. eigenvalues --    0.28332   0.28685   0.29014   0.29788
0.30061
 Alpha virt. eigenvalues --    0.30584   0.31432   0.32244   0.33288
0.33381
 Alpha virt. eigenvalues --    0.34385   0.34575   0.35468   0.36988
0.37272
 Alpha virt. eigenvalues --    0.37606   0.38512   0.39169   0.39383
0.40783
 Alpha virt. eigenvalues --    0.41246   0.41964   0.42778   0.43150
0.44493
 Alpha virt. eigenvalues --    0.45460   0.46194   0.46286   0.47435
0.47965
 Alpha virt. eigenvalues --    0.48363   0.48734   0.49959   0.50159
0.50671
 Alpha virt. eigenvalues --    0.51089   0.51599   0.52252   0.54200
0.54859
 Alpha virt. eigenvalues --    0.55549   0.56389   0.57040   0.57815
0.58481
 Alpha virt. eigenvalues --    0.58684   0.59133   0.60778   0.61325
0.63054
 Alpha virt. eigenvalues --    0.63620   0.64606   0.65671   0.66298
0.68953
```

```
 Alpha virt. eigenvalues --    0.70299   0.72219   0.74095   0.82251
1.09131
 Alpha virt. eigenvalues --    1.10319   1.10755   1.11905   1.12623
1.14025
 Alpha virt. eigenvalues --    1.15053   1.15501   1.15823   1.16435
1.18125
 Alpha virt. eigenvalues --    1.18918   1.19439   1.20724   1.21152
1.22140
 Alpha virt. eigenvalues --    1.22703   1.24475   1.25152   1.27123
1.27750
 Alpha virt. eigenvalues --    1.30910   1.31382   1.33531   1.38265
1.39060
 Alpha virt. eigenvalues --    1.40454   1.41452   1.46523   1.48717
1.49757
 Alpha virt. eigenvalues --    1.51213   1.52301   1.53112   1.53963
1.56373
 Alpha virt. eigenvalues --    1.57360   1.58787   1.59370   1.62078
1.63844
 Alpha virt. eigenvalues --    1.65253   1.66530   1.67608   1.74161
1.75619
 Alpha virt. eigenvalues --    1.77977   1.81788   1.87175   1.91625
1.92728
 Alpha virt. eigenvalues --    2.01213   2.10092   2.13969   2.15790
2.17898
 Alpha virt. eigenvalues --    2.21822   2.25700   2.27349   2.32854
2.33597
 Alpha virt. eigenvalues --    2.37882   2.39701   2.45877   2.51401
2.52455
 Alpha virt. eigenvalues --    2.60616   2.78614   2.92158   3.14946
3.17932
 Alpha virt. eigenvalues --    3.19622   3.46760   3.69689   3.83136
3.90043
 Alpha virt. eigenvalues --    4.22926
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   13.906461  -5.328810   2.649425  -5.720732   0.832284   3.487767
  2  C   -5.328810  18.073222 -10.585440   1.789583   3.883486 -10.231361
  3  C    2.649425 -10.585440  37.015212  13.087366 -34.476637   8.774269
  4  C   -5.720732   1.789583  13.087366  32.315490 -32.260811  -2.034049
  5  C    0.832284   3.883486 -34.476637 -32.260811  70.834755  -2.368092
  6  C    3.487767 -10.231361   8.774269  -2.034049  -2.368092  20.038089
  7  C   -0.186863   3.898760  -3.302868   0.192967   2.355698  -6.475358
  8  C    0.306001  -1.301896  -4.477843  -8.971953   8.877342   1.513935
  9  C    2.236240  -3.114745   9.990033   5.035631 -12.251252   6.255740
 10  C   -3.147881   9.163409 -16.562127  -2.996644  11.459735 -12.863628
 11  C   -3.126391   0.214486   0.553500   1.310407  -1.117879  -0.259775
 12  C   -0.459695  -0.505425   1.614300   2.300785  -5.015627  -0.297714
 13  N    0.039603   0.000756  -0.065490  -0.116142   0.031201   0.047746
 14  O    0.000310   0.020723  -0.117747  -0.090543   0.156769  -0.121493
 15  O    0.017250   0.007944   1.279620   1.185390  -3.106355  -0.017468
 16  O    0.139523  -0.052287   0.916677   0.772229  -2.001961   0.010400
 17  H    0.540176  -0.140584   0.041744  -0.143604  -0.027004   0.040235
 18  H   -0.108964   0.600148  -0.128431   0.034002  -0.032588  -0.132845
 19  H    0.004083  -0.106897   0.680990   0.107243  -0.291086   0.052562
```

20	H	-0.063046	-0.003517	0.102248	0.681203	-0.276435	0.007011
21	H	-0.001986	-0.102206	0.074895	0.009210	-0.005813	0.559996
22	H	-0.024837	0.031988	-0.009129	0.045905	0.008784	-0.090112
23	H	0.022158	0.000679	0.006589	-0.131291	-0.007429	0.006307
24	H	-0.007646	0.065791	-0.074493	0.017569	-0.045682	-0.124753
25	H	-0.092980	0.025133	0.011796	0.055707	-0.034078	0.024675
26	H	-0.079667	0.013691	-0.006808	0.027211	0.004383	0.018691
27	H	0.000220	0.001034	-0.008015	-0.007667	0.033790	0.000738
28	H	0.000075	-0.001229	0.009362	0.006317	-0.034740	0.004001
29	H	0.026093	0.018177	-0.070402	-0.053941	0.175839	-0.009425

		7	8	9	10	11	12
1	C	-0.186863	0.306001	2.236240	-3.147881	-3.126391	-0.459695
2	C	3.898760	-1.301896	-3.114745	9.163409	0.214486	-0.505425
3	C	-3.302868	-4.477843	9.990033	-16.562127	0.553500	1.614300
4	C	0.192967	-8.971953	5.035631	-2.996644	1.310407	2.300785
5	C	2.355698	8.877342	-12.251252	11.459735	-1.117879	-5.015627
6	C	-6.475358	1.513935	6.255740	-12.863628	-0.259775	-0.297714
7	C	15.143494	-4.523647	-1.895241	5.136198	-3.349538	-1.217233
8	C	-4.523647	22.660032	-19.427951	6.776862	0.928250	3.813402
9	C	-1.895241	-19.427951	58.224178	-25.145624	-0.530315	-14.955931
10	C	5.136198	6.776862	-25.145624	32.338024	0.468512	2.474624
11	C	-3.349538	0.928250	-0.530315	0.468512	12.150235	-0.465653
12	C	-1.217233	3.813402	-14.955931	2.474624	-0.465653	18.531924
13	N	-0.019862	0.110212	-0.444707	0.002422	-0.025234	0.358975
14	O	0.092827	0.368492	-1.389956	0.508008	-0.010784	0.472412
15	O	0.040336	-0.528296	1.075311	-0.504318	-0.014271	-0.470815
16	O	-0.019137	-0.178269	0.222001	-0.196543	0.007699	0.073316
17	H	-0.009492	0.045386	0.012471	-0.017096	0.001008	0.004273
18	H	0.007356	0.004654	-0.004804	0.096192	0.023935	0.001008
19	H	-0.004377	-0.013818	0.011135	-0.134279	0.001544	0.042623
20	H	0.010976	-0.176757	0.052442	-0.027245	0.018739	0.016904
21	H	-0.092070	0.034181	-0.037014	-0.103486	0.029748	-0.003921
22	H	0.545946	-0.159176	-0.011992	0.038302	-0.033859	0.006489
23	H	-0.041172	0.598546	-0.183105	0.071546	0.027171	-0.023552
24	H	0.043591	0.027188	-0.182294	0.627231	0.001243	0.005549
25	H	-0.120052	0.048179	-0.021887	0.006072	0.407823	0.006401
26	H	-0.112924	0.043548	-0.012939	0.001226	0.422811	-0.000440
27	H	0.001841	-0.014248	0.123542	-0.012620	0.000128	-0.142593
28	H	0.006158	-0.051023	0.132001	-0.049409	-0.000953	-0.014484
29	H	0.012823	-0.037065	0.016527	-0.022413	-0.022322	0.011325

		13	14	15	16	17	18
1	C	0.039603	0.000310	0.017250	0.139523	0.540176	-0.108964
2	C	0.000756	0.020723	0.007944	-0.052287	-0.140584	0.600148
3	C	-0.065490	-0.117747	1.279620	0.916677	0.041744	-0.128431
4	C	-0.116142	-0.090543	1.185390	0.772229	-0.143604	0.034002
5	C	0.031201	0.156769	-3.106355	-2.001961	-0.027004	-0.032588
6	C	0.047746	-0.121493	-0.017468	0.010400	0.040235	-0.132845
7	C	-0.019862	0.092827	0.040336	-0.019137	-0.009492	0.007356
8	C	0.110212	0.368492	-0.528296	-0.178269	0.045386	0.004654
9	C	-0.444707	-1.389956	1.075311	0.222001	0.012471	-0.004804
10	C	0.002422	0.508008	-0.504318	-0.196543	-0.017096	0.096192
11	C	-0.025234	-0.010784	-0.014271	0.007699	0.001008	0.023935
12	C	0.358975	0.472412	-0.470815	0.073316	0.004273	0.001008
13	N	7.600527	0.003571	-0.074126	0.001313	-0.000020	-0.000018

14	O	0.003571	8.669596	-0.010409	-0.000050	-0.000002	0.000013
15	O	-0.074126	-0.010409	9.178614	0.040670	-0.001098	0.000100
16	O	0.001313	-0.000050	0.040670	8.558816	0.005034	0.002373
17	H	-0.000020	-0.000002	-0.001098	0.005034	0.395689	-0.000252
18	H	-0.000018	0.000013	0.000100	0.002373	-0.000252	0.370013
19	H	-0.001042	0.000024	0.000958	0.000787	-0.000006	0.000017
20	H	-0.000707	-0.000020	0.001357	0.001117	-0.000045	-0.000011
21	H	-0.000033	0.003278	0.000145	0.000007	-0.000011	-0.000505
22	H	0.000059	0.004487	-0.000051	0.000009	-0.000016	-0.000010
23	H	0.002207	0.002740	0.002772	0.000087	-0.000019	0.000000
24	H	0.000648	0.001268	0.004171	0.000212	0.000000	-0.000083
25	H	-0.000024	0.000053	0.000065	0.000111	-0.000132	-0.000029
26	H	-0.000002	0.000004	-0.000007	-0.000052	-0.000374	0.000134
27	H	0.281102	-0.001499	0.010744	0.000034	0.000000	0.000000
28	H	0.008880	0.193680	0.004390	0.000015	0.000000	0.000000
29	H	-0.000689	-0.000011	0.008007	0.160037	-0.001199	-0.000078

		19	20	21	22	23	24
1	C	0.004083	-0.063046	-0.001986	-0.024837	0.022158	-0.007646
2	C	-0.106897	-0.003517	-0.102206	0.031988	0.000679	0.065791
3	C	0.680990	0.102248	0.074895	-0.009129	0.006589	-0.074493
4	C	0.107243	0.681203	0.009210	0.045905	-0.131291	0.017569
5	C	-0.291086	-0.276435	-0.005813	0.008784	-0.007429	-0.045682
6	C	0.052562	0.007011	0.559996	-0.090112	0.006307	-0.124753
7	C	-0.004377	0.010976	-0.092070	0.545946	-0.041172	0.043591
8	C	-0.013818	-0.176757	0.034181	-0.159176	0.598546	0.027188
9	C	0.011135	0.052442	-0.037014	-0.011992	-0.183105	-0.182294
10	C	-0.134279	-0.027245	-0.103486	0.038302	0.071546	0.627231
11	C	0.001544	0.018739	0.029748	-0.033859	0.027171	0.001243
12	C	0.042623	0.016904	-0.003921	0.006489	-0.023552	0.005549
13	N	-0.001042	-0.000707	-0.000033	0.000059	0.002207	0.000648
14	O	0.000024	-0.000020	0.003278	0.004487	0.002740	0.001268
15	O	0.000958	0.001357	0.000145	-0.000051	0.002772	0.004171
16	O	0.000787	0.001117	0.000007	0.000009	0.000087	0.000212
17	H	-0.000006	-0.000045	-0.000011	-0.000016	-0.000019	0.000000
18	H	0.000017	-0.000011	-0.000505	-0.000010	0.000000	-0.000083
19	H	0.351202	-0.000022	-0.000076	0.000000	0.000000	-0.000490
20	H	-0.000022	0.355776	0.000000	-0.000017	-0.000251	0.000000
21	H	-0.000076	0.000000	0.367448	-0.000406	-0.000014	-0.000144
22	H	0.000000	-0.000017	-0.000406	0.361444	0.000047	-0.000014
23	H	0.000000	-0.000251	-0.000014	0.000047	0.357924	-0.000014
24	H	-0.000490	0.000000	-0.000144	-0.000014	-0.000014	0.350502
25	H	0.000000	0.000039	-0.000029	-0.000278	0.000070	0.000000
26	H	0.000000	-0.000034	0.000087	-0.000425	-0.000033	0.000000
27	H	-0.000001	-0.000001	0.000000	0.000000	-0.000003	-0.000005
28	H	0.000000	0.000001	0.000002	-0.000009	0.000306	0.000322
29	H	-0.000048	-0.000285	0.000000	0.000000	0.000001	0.000001

		25	26	27	28	29
1	C	-0.092980	-0.079667	0.000220	0.000075	0.026093
2	C	0.025133	0.013691	0.001034	-0.001229	0.018177
3	C	0.011796	-0.006808	-0.008015	0.009362	-0.070402
4	C	0.055707	0.027211	-0.007667	0.006317	-0.053941
5	C	-0.034078	0.004383	0.033790	-0.034740	0.175839
6	C	0.024675	0.018691	0.000738	0.004001	-0.009425
7	C	-0.120052	-0.112924	0.001841	0.006158	0.012823

8	C	0.048179	0.043548	-0.014248	-0.051023	-0.037065
9	C	-0.021887	-0.012939	0.123542	0.132001	0.016527
10	C	0.006072	0.001226	-0.012620	-0.049409	-0.022413
11	C	0.407823	0.422811	0.000128	-0.000953	-0.022322
12	C	0.006401	-0.000440	-0.142593	-0.014484	0.011325
13	N	-0.000024	-0.000002	0.281102	0.008880	-0.000689
14	O	0.000053	0.000004	-0.001499	0.193680	-0.000011
15	O	0.000065	-0.000007	0.010744	0.004390	0.008007
16	O	0.000111	-0.000052	0.000034	0.000015	0.160037
17	H	-0.000132	-0.000374	0.000000	0.000000	-0.001199
18	H	-0.000029	0.000134	0.000000	0.000000	-0.000078
19	H	0.000000	0.000000	-0.000001	0.000000	-0.000048
20	H	0.000039	-0.000034	-0.000001	0.000001	-0.000285
21	H	-0.000029	0.000087	0.000000	0.000002	0.000000
22	H	-0.000278	-0.000425	0.000000	-0.000009	0.000000
23	H	0.000070	-0.000033	-0.000003	0.000306	0.000001
24	H	0.000000	0.000000	-0.000005	0.000322	0.000001
25	H	0.433035	-0.016406	0.000000	0.000000	0.000000
26	H	-0.016406	0.431327	0.000000	0.000000	0.000001
27	H	0.000000	0.000000	0.340802	0.000090	0.000000
28	H	0.000000	0.000000	0.000090	0.286276	0.000000
29	H	0.000000	0.000001	0.000000	0.000000	0.354152

Total atomic charges:

		1
1	C	0.141829
2	C	-0.334611
3	C	-0.922594
4	C	-0.446836
5	C	0.699403
6	C	0.183912
7	C	-0.119136
8	C	-0.294268
9	C	2.222504
10	C	-1.385052
11	C	-1.610265
12	C	-0.161225
13	N	-0.741123
14	O	-0.755741
15	O	-0.130630
16	O	-0.464169
17	H	0.254938
18	H	0.268675
19	H	0.298972
20	H	0.300580
21	H	0.268715
22	H	0.286871
23	H	0.287735
24	H	0.290330
25	H	0.266736
26	H	0.266997
27	H	0.392587
28	H	0.499971
29	H	0.434896

Sum of Mulliken charges= 0.00000

```
 Atomic charges with hydrogens summed into heavy atoms:
                1
  1  C    0.396766
  2  C   -0.065936
  3  C   -0.623621
  4  C   -0.146257
  5  C    0.699403
  6  C    0.452627
  7  C    0.167735
  8  C   -0.006533
  9  C    2.222504
 10  C   -1.094721
 11  C   -1.076532
 12  C   -0.161225
 13  N   -0.348536
 14  O   -0.255770
 15  O   -0.130630
 16  O   -0.029273
 17  H    0.000000
 18  H    0.000000
 19  H    0.000000
 20  H    0.000000
 21  H    0.000000
 22  H    0.000000
 23  H    0.000000
 24  H    0.000000
 25  H    0.000000
 26  H    0.000000
 27  H    0.000000
 28  H    0.000000
 29  H    0.000000
 Sum of Mulliken charges=   0.00000
 Electronic spatial extent (au):  <R**2>=  2419.2853
 Charge=     0.0000 electrons
 Dipole moment (Debye):
    X=    -4.6573    Y=     0.2866    Z=     0.2555  Tot=     4.6731
 Quadrupole moment (Debye-Ang):
   XX=   -93.3291   YY=  -108.4218   ZZ=   -91.2561
   XY=    -2.0501   XZ=     0.1722   YZ=     0.8247
 Octapole moment (Debye-Ang**2):
  XXX=     6.0832  YYY=    -0.9446  ZZZ=     0.6281  XYY=   -27.1567
  XXY=    20.3380  XXZ=    -0.6937  XZZ=     0.9373  YZZ=     2.3660
  YYZ=    -0.0838  XYZ=     0.6454
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -1563.3339 YYYY= -1208.4725 ZZZZ=  -490.0236 XXXY=    39.2397
 XXXZ=   -18.7376 YYYX=   -67.1031 YYYZ=     5.8727 ZZZX=     2.3031
 ZZZY=    -1.4314 XXYY=  -410.8710 XXZZ=  -355.8659 YYZZ=  -265.7435
 XXYZ=   -10.9692 YYXZ=    -1.2653 ZZXY=     0.0909
 N-N= 1.246149914381D+03 E-N=-4.216143561323D+03  KE= 7.354352411121D+02
  Exact polarizability: 143.805  -4.221 117.313  -0.858   0.705 102.401
 Approx polarizability: 122.007  -4.900 110.620  -1.481   0.163  99.793
 Full mass-weighted force constant matrix:
 Low frequencies --- -210.8764   -1.0349   -0.0005   -0.0003    0.0005
0.6678
```

```
 Low frequencies ---    0.7726  128.8650  254.4648
 ******    1 imaginary frequencies (negative Signs) ******
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                      1                      2                      3
                     ?A                     ?A                     ?A
 Frequencies --  -210.8764               128.8650               254.4648
 Red. masses --     1.0773                 5.8245                 4.6214
 Frc consts  --     0.0282                 0.0570                 0.1763
 IR Inten    --   155.6196                 6.5391                 0.2208
 Raman Activ --     1.9456                 2.6304                 0.4129
 Depolar     --     0.7486                 0.7491                 0.4561
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.01    -0.04   0.00   0.07     0.08   0.11  -
0.02
   2   6     0.01   0.00   0.00     0.05   0.00   0.05     0.03   0.10
0.00
   3   6     0.01   0.00   0.00     0.07   0.00  -0.04     0.07  -0.05
0.00
   4   6    -0.01   0.01   0.00    -0.07   0.00  -0.02     0.09  -0.07  -
0.01
   5   6     0.00   0.00   0.00     0.00  -0.01  -0.08     0.03  -0.07
0.00
   6   6     0.00   0.00   0.00     0.05   0.00   0.02    -0.09   0.05
0.01
   7   6     0.00   0.00   0.00    -0.03   0.00   0.02    -0.14   0.03
0.02
   8   6     0.00   0.00   0.00    -0.06   0.01  -0.05    -0.03  -0.12
0.02
   9   6     0.00   0.00   0.00    -0.01  -0.01  -0.11     0.02  -0.07
0.00
  10   6     0.00   0.00   0.00     0.06  -0.02  -0.06    -0.03  -0.09
0.00
  11   6     0.00   0.00   0.00    -0.07   0.00   0.10    -0.07   0.17
0.00
  12   6     0.00   0.00   0.00     0.01   0.01   0.05    -0.02   0.02
0.01
  13   7     0.00   0.00   0.01     0.07   0.04   0.46    -0.02   0.03
0.00
  14   8     0.00   0.00  -0.01    -0.02  -0.01  -0.21     0.26   0.03  -
0.02
  15   8     0.00   0.00  -0.01    -0.02  -0.01  -0.15     0.02   0.03
0.03
  16   8    -0.01   0.00   0.06     0.00  -0.01  -0.08    -0.20  -0.12  -
0.03
  17   1    -0.02  -0.01   0.02    -0.05   0.00   0.11     0.18   0.19  -
0.05
  18   1     0.01   0.01   0.00     0.10   0.01   0.10     0.04   0.17  -
0.02
  19   1     0.00   0.01  -0.01     0.13   0.00  -0.06     0.14  -0.05  -
0.01
```

20	1	-0.01	-0.01	-0.01	-0.13	0.00	-0.02	0.15	-0.08	-0.01
21	1	0.00	0.00	0.00	0.08	0.00	0.03	-0.16	0.10	0.02
22	1	0.00	0.00	0.00	-0.04	0.00	0.01	-0.29	0.02	0.04
23	1	0.00	0.01	0.00	-0.11	0.01	-0.06	-0.07	-0.16	0.02
24	1	0.00	-0.01	0.00	0.10	-0.02	-0.09	-0.07	-0.13	0.01
25	1	0.00	0.00	0.00	-0.14	0.00	0.11	-0.08	0.17	0.00
26	1	0.00	0.00	0.00	-0.03	0.00	0.17	-0.11	0.27	0.01
27	1	0.00	0.00	0.01	0.09	0.05	0.64	-0.02	0.03	0.02
28	1	0.00	0.00	0.00	0.03	0.01	0.15	0.25	0.24	-0.06
29	1	0.00	-0.04	-1.00	0.00	0.00	0.06	-0.24	-0.29	-0.04

		4			5			6		
		?A			?A			?A		
Frequencies --		267.2161			300.2327			322.2371		
Red. masses --		10.3315			5.3876			4.9844		
Frc consts --		0.4347			0.2861			0.3049		
IR Inten --		1.9012			28.0906			4.0885		
Raman Activ --		0.1471			0.4592			0.5193		
Depolar --		0.7500			0.1606			0.6417		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	-0.03	0.03	-0.09	-0.03	0.02	-0.01	0.05	0.16
2	6	-0.03	-0.01	0.04	-0.08	-0.04	0.00	0.03	-0.11	0.10
3	6	-0.09	0.07	0.04	-0.08	-0.01	-0.01	0.01	-0.04	0.05
4	6	0.06	-0.05	0.04	-0.08	0.00	0.02	-0.04	0.02	0.06
5	6	0.00	0.02	0.05	-0.02	0.02	0.00	-0.01	-0.01	0.01
6	6	0.02	0.01	0.06	-0.07	-0.04	0.00	0.06	-0.10	-0.11
7	6	0.01	-0.02	0.07	-0.07	-0.03	0.00	-0.03	0.03	-0.16
8	6	-0.01	0.00	0.02	-0.05	-0.04	0.01	0.00	0.03	-0.09
9	6	-0.01	0.01	-0.05	0.00	-0.02	0.00	0.02	-0.01	-0.04
10	6	0.01	0.03	0.01	-0.06	-0.04	-0.01	0.03	-0.04	-0.08
11	6	0.01	-0.04	0.06	-0.09	-0.03	0.01	-0.07	0.14	0.01
12	6	0.01	0.01	0.09	-0.05	0.01	0.01	0.03	0.00	-0.01

13	7	-0.01	0.00	-0.07	-0.05	0.01	0.01	0.05	0.10	0.00
14	8	-0.07	-0.02	-0.35	0.31	0.12	-0.01	-0.03	-0.03	0.28
15	8	0.06	0.03	0.51	-0.04	-0.04	0.01	-0.02	-0.02	0.04
16	8	0.01	0.00	-0.42	0.35	0.09	-0.03	0.01	-0.02	-0.22
17	1	0.03	-0.03	0.00	-0.09	-0.03	0.04	0.03	0.11	0.27
18	1	-0.08	-0.03	0.00	-0.07	-0.05	0.01	0.05	-0.22	0.17
19	1	-0.10	0.04	0.07	-0.09	-0.05	0.02	0.05	-0.09	0.07
20	1	0.06	-0.02	0.05	-0.10	-0.03	0.00	-0.13	0.08	0.08
21	1	0.05	0.01	0.08	-0.06	-0.04	0.00	0.14	-0.20	-0.16
22	1	0.03	-0.02	0.08	-0.08	-0.03	-0.01	-0.12	0.04	-0.27
23	1	-0.03	-0.04	0.02	-0.08	-0.01	-0.01	0.00	0.13	-0.13
24	1	0.03	0.07	0.01	-0.09	-0.02	0.01	0.05	-0.10	-0.12
25	1	-0.01	-0.07	0.07	-0.10	-0.03	0.01	-0.17	0.29	0.01
26	1	0.02	-0.01	0.09	-0.07	-0.04	0.02	-0.03	0.08	0.05
27	1	0.01	0.01	0.09	-0.05	0.00	0.01	-0.03	0.17	0.05
28	1	-0.05	-0.03	-0.22	0.29	0.42	-0.10	-0.06	-0.14	0.02
29	1	0.01	0.00	-0.48	0.41	0.39	-0.10	0.01	-0.01	-0.26

	7			8			9		
	?A			?A			?A		
Frequencies --	351.9988			367.0225			448.1729		
Red. masses --	4.3843			3.8305			2.1197		
Frc consts --	0.3201			0.3040			0.2508		
IR Inten --	7.2372			8.2628			7.0889		
Raman Activ --	2.2083			0.7764			1.4130		
Depolar --	0.4298			0.7312			0.7475		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.02	0.01	-0.06	0.01	0.02	0.07	-0.01	0.02	-0.04
2 6	-0.01	0.05	-0.04	-0.02	-0.03	0.07	-0.01	0.01	-0.04
3 6	0.00	-0.02	-0.02	0.00	-0.02	0.09	-0.01	-0.03	0.00
4 6	0.03	-0.05	-0.03	-0.01	0.02	0.11	0.01	0.03	-0.03
5 6	0.01	-0.04	-0.01	-0.01	-0.01	0.02	0.01	-0.02	-0.02

```
   6   6    -0.06   0.03   0.03    -0.06  -0.03   0.04    -0.03  -0.02  -
0.05
   7   6    -0.07  -0.02   0.06     0.02   0.03   0.01     0.05   0.04  -
0.06
   8   6    -0.02  -0.08   0.02     0.04   0.05   0.12     0.06   0.09
0.02
   9   6     0.03  -0.07   0.00     0.01  -0.02   0.13     0.02   0.02
0.11
  10   6    -0.02  -0.03   0.00    -0.03  -0.07   0.12    -0.05  -0.06
0.08
  11   6    -0.04   0.01   0.01     0.12   0.08  -0.17    -0.07  -0.02
0.13
  12   6     0.04   0.00  -0.01    -0.02  -0.01   0.04     0.04   0.00
0.10
  13   7     0.11   0.38  -0.05    -0.01   0.05  -0.02     0.03   0.01  -
0.02
  14   8    -0.09  -0.14  -0.02     0.00  -0.03  -0.13     0.00   0.01  -
0.03
  15   8    -0.05  -0.04   0.03    -0.06  -0.04  -0.19     0.01  -0.01  -
0.06
  16   8     0.12  -0.02   0.07     0.01  -0.01  -0.14    -0.01  -0.03  -
0.03
  17   1     0.05   0.03  -0.10     0.01   0.03   0.09    -0.01   0.01  -
0.05
  18   1    -0.02   0.10  -0.07    -0.01  -0.03   0.08    -0.01   0.01  -
0.05
  19   1     0.02  -0.01  -0.03    -0.01  -0.02   0.09    -0.04  -0.01  -
0.01
  20   1     0.08  -0.08  -0.04     0.00   0.00   0.10     0.03   0.04  -
0.02
  21   1    -0.08   0.08   0.06    -0.10  -0.05  -0.01    -0.13  -0.04  -
0.12
  22   1    -0.11  -0.03   0.10     0.03   0.04  -0.03     0.09   0.05  -
0.10
  23   1    -0.06  -0.13   0.03     0.09   0.08   0.13     0.17   0.10
0.05
  24   1    -0.05  -0.02   0.03    -0.10  -0.07   0.16    -0.14  -0.07
0.12
  25   1    -0.05  -0.06   0.02     0.46   0.24  -0.21    -0.42  -0.13
0.18
  26   1    -0.05   0.07   0.04    -0.02  -0.02  -0.51     0.10   0.01
0.47
  27   1    -0.22   0.65  -0.01    -0.09   0.08  -0.19     0.00   0.00  -
0.18
  28   1    -0.07  -0.31   0.10     0.01  -0.02  -0.03    -0.06  -0.03  -
0.51
  29   1     0.15   0.08   0.02     0.01   0.01  -0.10    -0.01  -0.05
0.00
                     10                     11                     12
                     ?A                     ?A                     ?A
 Frequencies --    469.8851               484.4776               505.8644
 Red. masses --      1.2064                 6.6410                 7.7860
 Frc consts  --      0.1569                 0.9184                 1.1739
 IR Inten    --    120.3032                 2.0319                 2.1503
```

Raman Activ --		0.7190			7.8854			4.3209		
Depolar --		0.7497			0.4825			0.7499		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	-0.01	0.01	-0.21	0.02	0.05	-0.04	-0.03	0.01
2	6	0.01	0.01	0.01	-0.16	0.09	0.05	-0.06	-0.04	0.01
3	6	0.03	0.00	-0.03	-0.11	0.09	-0.01	-0.01	-0.08	0.06
4	6	-0.02	0.01	-0.01	-0.15	0.05	0.04	-0.02	-0.10	0.00
5	6	-0.01	0.01	-0.02	-0.06	-0.08	0.00	0.11	-0.17	0.01
6	6	0.00	0.02	0.03	-0.02	0.14	-0.02	-0.08	-0.06	0.04
7	6	-0.01	0.00	0.04	0.03	0.11	0.00	-0.11	-0.06	0.05
8	6	-0.03	0.00	0.00	0.00	0.10	-0.03	-0.10	-0.02	0.01
9	6	0.00	-0.02	-0.02	0.13	-0.02	-0.03	-0.06	0.24	-0.02
10	6	0.02	-0.01	-0.02	-0.01	0.14	-0.02	-0.06	0.01	0.04
11	6	0.03	-0.01	-0.04	-0.03	-0.02	-0.05	-0.06	-0.01	-0.08
12	6	-0.01	-0.01	0.02	0.23	-0.14	-0.03	0.17	0.15	-0.05
13	7	0.00	0.01	0.03	0.28	-0.04	-0.04	0.17	0.01	-0.01
14	8	0.01	-0.02	0.05	0.14	-0.05	-0.02	-0.17	0.30	0.01
15	8	0.00	0.00	0.02	0.00	-0.21	0.05	0.18	0.12	-0.04
16	8	-0.01	0.01	0.01	-0.09	-0.10	0.03	0.11	-0.27	0.01
17	1	-0.04	-0.02	0.01	-0.26	-0.03	-0.02	-0.01	0.00	0.02
18	1	0.04	0.04	0.03	-0.11	0.03	0.12	-0.05	-0.02	0.01
19	1	0.06	0.00	-0.04	-0.06	0.15	-0.07	-0.05	-0.02	0.02
20	1	-0.05	0.00	-0.02	-0.20	0.10	0.06	-0.02	-0.05	0.02
21	1	0.01	0.03	0.05	0.04	0.09	-0.03	-0.06	-0.02	0.08
22	1	0.01	0.00	0.06	0.09	0.10	0.08	-0.13	-0.06	0.04
23	1	-0.08	-0.01	-0.02	-0.08	0.15	-0.08	-0.09	-0.10	0.05
24	1	0.05	0.00	-0.04	-0.09	0.18	0.04	0.01	-0.09	-0.04
25	1	0.17	0.02	-0.06	0.10	0.05	-0.07	0.13	0.04	-0.10

26	1	-0.03	-0.03	-0.17	-0.02	-0.20	-0.17	-0.16	0.01	-0.25
27	1	-0.01	0.02	0.06	0.23	0.00	-0.01	0.30	-0.09	0.01
28	1	-0.11	-0.08	-0.93	0.16	-0.03	0.14	-0.20	0.16	-0.22
29	1	-0.01	0.01	0.01	-0.11	-0.18	0.09	0.12	-0.26	-0.01

	13	14	15
	?A	?A	?A
Frequencies --	547.3292	555.2876	586.8666
Red. masses --	5.2502	4.4104	3.2716
Frc consts --	0.9267	0.8012	0.6639
IR Inten --	3.7443	3.7633	5.2450
Raman Activ --	10.0613	8.2864	0.5691
Depolar --	0.0713	0.0645	0.7131

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.09	0.03	-0.07	0.04	-0.03	-0.07	-0.09	-0.03	0.01
2	6	-0.03	0.09	-0.01	-0.11	-0.02	-0.04	0.03	0.15	0.03
3	6	-0.03	0.05	0.18	-0.09	0.04	0.17	0.16	-0.06	0.04
4	6	0.09	-0.02	0.08	0.09	0.00	0.16	-0.04	0.06	0.05
5	6	-0.03	-0.12	0.16	0.03	0.12	0.18	0.07	0.01	0.05
6	6	0.07	0.12	-0.04	-0.06	-0.01	-0.02	-0.12	0.09	-0.04
7	6	0.11	0.04	-0.01	-0.06	-0.07	0.02	0.05	0.02	-0.01
8	6	0.02	0.01	-0.09	-0.02	-0.06	0.02	-0.03	0.06	-0.06
9	6	-0.05	0.03	-0.11	0.03	-0.03	-0.09	-0.04	-0.03	-0.04
10	6	0.02	0.09	-0.02	-0.04	0.00	-0.04	-0.07	-0.15	-0.05
11	6	0.09	-0.02	0.05	-0.05	-0.06	0.02	0.05	-0.18	-0.01
12	6	-0.14	-0.06	-0.11	0.09	0.01	-0.14	-0.03	0.02	0.02
13	7	-0.11	0.04	0.05	0.12	-0.03	0.02	-0.04	0.03	-0.01
14	8	-0.01	0.10	0.01	0.02	-0.08	0.01	0.01	-0.02	0.05
15	8	-0.15	-0.15	-0.04	0.07	0.07	-0.12	0.06	0.06	0.02
16	8	0.07	-0.19	-0.02	-0.06	0.16	-0.05	0.00	-0.01	-0.06
17	1	0.11	0.02	-0.19	0.07	-0.02	-0.14	-0.19	-0.15	-0.09
18	1	-0.13	0.00	-0.10	-0.21	-0.08	-0.13	0.13	0.24	0.11

19	1	-0.05	0.05	0.19	-0.23	-0.14	0.33	0.28	-0.16	0.08
20	1	0.27	0.17	0.18	0.25	0.05	0.19	-0.05	0.13	0.08
21	1	0.08	0.10	-0.04	-0.03	0.02	0.03	-0.24	0.11	-0.09
22	1	0.13	0.03	0.07	-0.07	-0.07	0.05	0.21	0.01	0.12
23	1	-0.02	0.05	-0.12	-0.16	0.01	-0.05	-0.09	0.11	-0.09
24	1	0.11	-0.04	-0.13	-0.03	-0.09	-0.07	-0.09	-0.30	-0.09
25	1	-0.03	-0.10	0.07	-0.17	-0.17	0.04	0.07	-0.16	-0.01
26	1	0.16	0.01	0.19	-0.02	0.06	0.15	0.07	-0.30	-0.03
27	1	-0.19	0.12	0.21	0.21	-0.08	0.14	-0.06	0.05	-0.02
28	1	-0.05	0.13	-0.31	-0.02	-0.14	-0.31	0.04	0.02	0.30
29	1	0.09	-0.11	-0.07	-0.09	0.06	-0.08	-0.01	-0.08	-0.03

	16	17	18
	?A	?A	?A
Frequencies --	639.4423	690.8883	717.5744
Red. masses --	4.5559	5.8005	6.2457
Frc consts --	1.0976	1.6313	1.8948
IR Inten --	2.1707	0.7743	15.4666
Raman Activ --	2.7187	6.1038	2.3795
Depolar --	0.7337	0.4264	0.5202

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	0.07	-0.18	0.14	0.04	0.11	-0.12	0.07	-0.08
2	6	0.06	-0.11	-0.12	-0.18	0.00	0.12	-0.07	0.00	-0.02
3	6	-0.01	-0.15	-0.02	-0.17	-0.11	-0.12	-0.06	-0.07	0.01
4	6	-0.01	0.22	-0.07	0.07	0.03	-0.08	-0.04	0.00	-0.01
5	6	0.00	0.00	0.03	-0.03	-0.01	-0.09	-0.12	-0.09	0.03
6	6	0.03	-0.11	0.13	-0.16	-0.08	0.11	0.07	0.06	0.01
7	6	-0.04	0.06	0.17	0.12	0.07	0.12	0.04	0.13	0.05
8	6	-0.14	0.18	0.07	0.07	0.01	-0.08	0.04	0.02	0.05
9	6	-0.01	0.01	-0.03	-0.01	0.00	-0.11	0.14	-0.03	-0.01
10	6	0.10	-0.10	0.04	-0.19	-0.07	-0.14	0.11	-0.02	0.01
11	6	0.01	0.01	0.00	0.27	0.09	0.17	-0.03	0.05	-0.01

12	6	0.01	-0.06	-0.04	0.03	0.02	-0.04	0.00	0.25	-0.05
13	7	0.04	0.01	0.00	0.04	-0.01	-0.01	-0.07	-0.08	0.02
14	8	0.02	0.04	0.05	0.00	0.00	0.02	0.04	-0.25	0.02
15	8	-0.02	-0.09	0.02	0.00	0.02	-0.02	-0.09	0.27	0.00
16	8	-0.03	0.00	-0.07	0.00	0.00	0.01	0.11	-0.19	-0.01
17	1	-0.12	0.01	-0.01	0.11	-0.01	0.05	-0.10	0.08	-0.11
18	1	0.03	-0.03	-0.19	-0.21	0.19	0.01	-0.06	-0.06	0.01
19	1	-0.16	-0.19	0.04	-0.01	-0.20	-0.09	-0.08	-0.03	-0.02
20	1	0.22	0.29	-0.03	-0.13	0.03	-0.09	0.08	0.03	0.01
21	1	-0.01	-0.04	0.18	-0.07	-0.24	0.01	0.08	0.02	-0.02
22	1	0.10	0.10	-0.01	0.10	0.07	0.10	0.03	0.12	0.07
23	1	-0.33	0.09	0.04	-0.10	-0.12	-0.09	-0.06	0.00	0.02
24	1	0.25	-0.05	-0.02	-0.14	0.05	-0.14	0.08	0.01	0.04
25	1	0.11	-0.27	0.01	0.24	0.07	0.18	0.00	-0.06	0.00
26	1	-0.06	0.19	0.00	0.28	0.10	0.20	0.00	0.00	0.01
27	1	-0.02	0.07	0.05	0.09	-0.05	0.03	0.37	-0.44	0.03
28	1	0.04	0.08	0.24	0.00	-0.01	0.03	0.05	-0.32	0.04
29	1	-0.05	-0.06	-0.05	0.02	0.06	-0.02	0.19	0.14	-0.04

	19			20			21		
	?A			?A			?A		
Frequencies --	743.9157			776.2316			816.3830		
Red. masses --	4.4473			3.9997			4.1404		
Frc consts --	1.4501			1.4199			1.6259		
IR Inten --	9.3448			1.2780			3.3569		
Raman Activ --	1.4195			0.9739			9.6196		
Depolar --	0.4332			0.5899			0.0246		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.05	0.00	0.06	0.02	-0.02	-0.02	-0.03	0.00	-0.02
2 6	-0.06	-0.07	-0.02	-0.06	-0.05	0.01	-0.05	0.04	0.00
3 6	-0.07	0.08	-0.09	-0.03	0.05	-0.01	0.06	-0.09	-0.22
4 6	0.03	0.08	0.04	0.05	0.05	0.04	0.07	-0.06	0.23

```
    5   6     0.18   0.01  -0.04     0.06   0.01   0.05     0.00   0.02
0.01
    6   6     0.01  -0.06   0.02     0.09   0.01   0.05    -0.02  -0.05  -
0.02
    7   6     0.04   0.03  -0.05    -0.07  -0.02   0.06    -0.01   0.01  -
0.01
    8   6    -0.06   0.06   0.03    -0.03   0.02  -0.12     0.05   0.08
0.26
    9   6    -0.08  -0.07   0.02    -0.01  -0.02  -0.03     0.06   0.01
0.02
   10   6    -0.04   0.11   0.10    -0.03   0.08  -0.16     0.01   0.06  -
0.23
   11   6     0.01  -0.02   0.00    -0.04  -0.02  -0.01    -0.05  -0.01  -
0.04
   12   6    -0.12  -0.08  -0.16     0.01   0.01   0.37    -0.02   0.00  -
0.03
   13   7    -0.10   0.07   0.03    -0.06   0.01  -0.04    -0.03   0.00
0.01
   14   8     0.07  -0.10   0.00     0.02  -0.05  -0.01    -0.03   0.06
0.00
   15   8     0.22   0.08  -0.01     0.05   0.02  -0.10    -0.03  -0.04
0.02
   16   8     0.00  -0.12   0.02     0.01  -0.07   0.00     0.00  -0.02
0.00
   17   1    -0.11  -0.03   0.12     0.01  -0.01   0.02     0.07   0.05  -
0.15
   18   1    -0.04  -0.10   0.02    -0.12  -0.08  -0.04     0.09   0.22
0.09
   19   1    -0.22   0.17  -0.12    -0.01  -0.06   0.07     0.24  -0.30  -
0.11
   20   1    -0.02   0.05   0.03     0.09   0.20   0.11     0.20  -0.26
0.15
   21   1     0.01  -0.12  -0.04     0.34  -0.01   0.18     0.19  -0.10
0.06
   22   1     0.12   0.05  -0.15    -0.07  -0.03   0.08     0.07   0.03  -
0.10
   23   1    -0.06   0.12   0.01    -0.15   0.02  -0.16     0.03   0.27
0.19
   24   1    -0.03   0.27   0.15     0.03   0.15  -0.18    -0.03   0.30  -
0.13
   25   1    -0.04   0.00   0.01     0.07  -0.07  -0.02    -0.19  -0.06  -
0.02
   26   1     0.05  -0.08   0.05    -0.12   0.08  -0.09     0.02   0.00
0.10
   27   1    -0.32   0.29   0.27    -0.20   0.04  -0.52    -0.03   0.00
0.04
   28   1     0.06   0.05  -0.10     0.04   0.00   0.10    -0.03  -0.03  -
0.01
   29   1    -0.05  -0.35   0.03    -0.01  -0.15   0.00     0.00  -0.02
0.00
                     22                    23                    24
                     ?A                    ?A                    ?A
 Frequencies --    830.8534              853.8034              884.3614
 Red. masses --      4.5484                3.6917                3.2280
```

Frc consts --		1.8499			1.5856			1.4874		
IR Inten --		0.6930			20.2218			0.5715		
Raman Activ --		11.7474			0.1550			13.3080		
Depolar --		0.0275			0.6992			0.0392		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	-0.12	-0.08	0.19	-0.11	0.07	-0.10	0.12	-0.12
2	6	-0.09	0.01	0.26	0.15	0.05	-0.04	-0.08	0.16	0.07
3	6	0.04	-0.01	0.06	0.01	0.09	-0.06	0.06	0.01	0.04
4	6	0.15	-0.02	-0.12	-0.01	0.09	0.06	-0.07	0.06	-0.02
5	6	-0.02	0.00	-0.02	-0.05	-0.01	0.02	-0.01	-0.01	0.02
6	6	-0.05	-0.05	0.22	-0.13	-0.05	0.08	0.05	-0.19	0.06
7	6	-0.04	0.14	-0.07	-0.06	-0.15	-0.08	-0.01	-0.17	-0.10
8	6	0.11	0.08	-0.09	-0.05	0.12	-0.04	-0.04	-0.08	-0.01
9	6	0.00	0.00	-0.01	-0.01	-0.01	-0.02	-0.02	0.00	0.03
10	6	0.04	0.01	0.05	-0.06	0.07	0.03	0.01	0.05	0.04
11	6	-0.19	-0.08	-0.15	-0.01	-0.05	-0.02	0.12	0.04	0.04
12	6	-0.01	-0.01	-0.05	0.04	0.07	-0.02	0.01	0.00	0.01
13	7	-0.01	0.00	0.01	0.04	-0.02	-0.01	0.01	0.00	0.00
14	8	0.00	0.00	0.00	0.03	-0.07	0.01	0.01	-0.01	-0.01
15	8	-0.01	-0.01	0.00	-0.11	0.02	0.02	0.00	0.01	0.00
16	8	0.00	0.03	0.00	0.02	-0.08	0.00	0.00	0.00	-0.01
17	1	0.18	0.01	-0.10	0.16	-0.10	0.20	-0.26	-0.08	-0.37
18	1	-0.11	0.29	0.14	0.12	0.30	-0.18	0.00	0.31	0.11
19	1	0.28	0.01	0.00	-0.04	0.17	-0.11	0.22	0.01	0.01
20	1	0.15	0.09	-0.08	-0.09	0.22	0.12	0.09	0.07	0.00
21	1	0.14	-0.32	0.08	-0.23	0.10	0.17	0.22	-0.26	0.10
22	1	0.14	0.15	-0.05	0.07	-0.13	-0.19	-0.25	-0.14	-0.37
23	1	0.19	-0.04	-0.02	-0.07	0.29	-0.11	0.06	0.01	-0.02
24	1	0.18	0.11	0.01	-0.03	0.23	0.07	0.07	0.15	0.04

```
  25   1    -0.29  -0.13  -0.13    -0.10   0.10  -0.02     0.03  -0.02
0.05
  26   1    -0.13  -0.07  -0.02    -0.05   0.12   0.01     0.14   0.06
0.09
  27   1    -0.02   0.02   0.07     0.25  -0.19   0.00     0.02  -0.01  -
0.03
  28   1     0.00   0.01   0.00     0.03   0.00   0.00     0.00   0.02  -
0.02
  29   1     0.00   0.05  -0.01     0.05   0.04   0.00     0.00   0.00  -
0.01
                     25                     26                     27
                     ?A                     ?A                     ?A
 Frequencies --    906.4410               929.3598               948.2966
 Red. masses --      2.4770                 2.6300                 2.1974
 Frc consts  --      1.1991                 1.3384                 1.1643
 IR Inten    --      1.5318                 6.6712                 2.9706
 Raman Activ --      0.7991                 1.4827                 3.5947
 Depolar     --      0.5313                 0.4884                 0.6830
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.07   0.02  -0.05    -0.09   0.03   0.05    -0.06   0.06
0.00
   2   6    -0.01  -0.08   0.11     0.06  -0.03   0.02     0.12  -0.01
0.05
   3   6     0.09   0.12   0.06    -0.01  -0.04  -0.04    -0.05   0.04  -
0.05
   4   6     0.03   0.05  -0.05     0.10   0.18  -0.08     0.11  -0.04
0.02
   5   6    -0.03  -0.01  -0.06     0.02   0.01   0.07     0.00  -0.01
0.03
   6   6     0.05  -0.02  -0.12    -0.01   0.02  -0.04    -0.05  -0.07  -
0.04
   7   6    -0.04   0.01   0.04    -0.07  -0.06   0.05     0.02   0.12  -
0.02
   8   6    -0.10   0.04   0.09     0.14  -0.08  -0.03    -0.10  -0.07
0.00
   9   6    -0.01   0.00   0.04     0.05   0.02   0.08    -0.04  -0.02  -
0.04
  10   6    -0.13   0.01  -0.05    -0.06   0.05  -0.05     0.00   0.04
0.04
  11   6     0.03  -0.05   0.00    -0.04  -0.04   0.03     0.03  -0.06
0.00
  12   6     0.01   0.01  -0.04    -0.02   0.01  -0.08     0.03   0.03
0.07
  13   7     0.03   0.00   0.00    -0.01   0.00   0.02     0.03   0.00  -
0.02
  14   8     0.01  -0.02   0.00    -0.01   0.02  -0.02     0.00   0.01
0.00
  15   8    -0.03   0.00   0.02    -0.04  -0.02   0.00    -0.05   0.00  -
0.02
  16   8     0.01  -0.03   0.01     0.00  -0.02  -0.02     0.00   0.02
0.01
  17   1     0.04   0.00  -0.02    -0.26  -0.06   0.23    -0.04   0.08
0.03
```

18	1	-0.17	-0.36	0.04	0.18	-0.06	0.17	0.33	0.05	0.27
19	1	0.47	0.23	-0.10	-0.03	-0.15	0.04	-0.24	0.11	-0.06
20	1	0.11	-0.02	-0.08	0.30	0.39	0.02	0.37	-0.04	0.03
21	1	0.25	-0.10	-0.09	0.04	0.08	0.06	-0.21	-0.20	-0.27
22	1	0.06	0.02	0.01	-0.21	-0.09	0.16	0.03	0.13	-0.08
23	1	-0.19	-0.02	0.09	0.34	-0.19	0.07	-0.32	-0.19	-0.03
24	1	-0.42	-0.18	0.05	-0.23	0.13	0.07	0.11	0.19	0.03
25	1	0.05	-0.21	0.01	0.12	0.00	0.01	0.04	-0.12	0.00
26	1	0.01	0.07	0.03	-0.11	-0.09	-0.12	0.11	-0.26	0.02
27	1	0.09	-0.05	0.02	0.04	-0.05	0.02	0.11	-0.07	-0.05
28	1	0.01	0.03	-0.01	-0.02	-0.06	-0.06	0.00	0.06	0.00
29	1	0.02	0.03	0.00	-0.01	-0.09	-0.01	0.00	0.04	0.01

	28	29	30
	?A	?A	?A
Frequencies --	989.0179	998.6531	1006.1730
Red. masses --	2.1156	1.6051	2.3374
Frc consts --	1.2192	0.9432	1.3942
IR Inten --	2.3795	88.2705	42.7103
Raman Activ --	4.6380	3.2984	8.7559
Depolar --	0.3991	0.3370	0.0396

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.05	-0.03	0.03	0.02	-0.05	-0.02	0.01	0.18	0.05
2	6	0.05	0.13	-0.03	0.00	-0.05	0.00	-0.03	0.04	0.04
3	6	-0.06	-0.06	0.01	0.05	-0.05	-0.01	-0.07	0.03	0.02
4	6	-0.01	-0.06	-0.04	-0.04	0.00	0.02	0.03	0.02	-0.03
5	6	0.01	0.00	0.04	-0.01	0.00	0.03	0.02	0.00	-0.05
6	6	0.14	-0.06	-0.05	-0.02	0.04	0.01	-0.03	-0.04	-0.02
7	6	0.00	0.05	0.03	-0.01	0.06	-0.03	0.09	-0.15	0.04
8	6	-0.05	0.05	-0.02	-0.04	-0.04	-0.02	-0.01	0.01	0.02
9	6	-0.01	0.01	0.06	-0.03	-0.01	0.04	0.05	0.03	-0.04
10	6	-0.08	0.01	0.00	0.01	0.06	0.00	0.04	-0.04	-0.01

11	6	-0.07	-0.03	0.05	0.05	0.02	-0.02	-0.09	-0.06	-0.05
12	6	0.00	-0.01	-0.06	0.00	-0.01	-0.08	-0.02	0.01	-0.04
13	7	0.01	0.00	0.03	0.03	0.01	0.10	-0.02	0.00	0.07
14	8	0.01	-0.02	0.00	0.00	0.00	-0.01	0.00	0.00	0.01
15	8	0.00	0.01	0.01	0.01	0.02	0.03	0.00	-0.02	0.02
16	8	0.00	0.02	0.00	0.00	0.00	-0.01	0.00	0.00	0.01
17	1	0.15	0.03	-0.04	-0.02	-0.07	0.00	0.16	0.32	0.09
18	1	0.10	0.39	-0.08	-0.03	-0.06	-0.03	-0.01	-0.05	0.10
19	1	-0.20	-0.19	0.13	0.13	-0.15	0.04	-0.09	0.15	-0.05
20	1	-0.07	-0.04	-0.03	-0.08	0.06	0.04	0.05	-0.07	-0.07
21	1	0.39	-0.23	-0.08	-0.07	0.02	-0.04	-0.10	0.05	0.02
22	1	0.12	0.07	-0.02	-0.10	0.05	0.01	0.39	-0.16	0.12
23	1	-0.04	-0.01	0.01	-0.05	-0.09	-0.01	-0.06	0.05	-0.01
24	1	-0.28	-0.02	0.10	0.04	0.21	0.04	0.13	-0.14	-0.10
25	1	0.30	0.09	0.00	-0.09	-0.05	0.00	-0.11	-0.03	-0.06
26	1	-0.22	-0.08	-0.28	0.13	0.03	0.13	-0.10	-0.04	-0.06
27	1	-0.03	-0.01	-0.22	-0.10	-0.06	-0.86	-0.11	-0.05	-0.61
28	1	0.01	0.03	-0.02	-0.01	0.06	-0.04	0.00	-0.10	0.01
29	1	0.00	0.03	0.00	0.01	0.05	-0.01	-0.01	-0.05	0.00

	31			32			33		
	?A			?A			?A		
Frequencies --	1011.1986			1021.3201			1031.7563		
Red. masses --	2.1593			3.3554			2.8581		
Frc consts --	1.3009			2.0621			1.7926		
IR Inten --	27.5701			25.3822			2.5411		
Raman Activ --	2.1245			1.2485			0.8623		
Depolar --	0.5194			0.4425			0.7153		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.04	0.10	0.01	0.08	-0.02	0.04	0.12	0.04	-0.02
2 6	-0.01	-0.03	-0.02	0.06	0.05	0.05	-0.05	0.03	0.14
3 6	0.08	-0.11	-0.01	-0.08	-0.06	0.16	-0.10	-0.12	-0.08

4	6	-0.07	0.01	0.01	-0.06	0.04	-0.18	0.00	0.05	0.07
5	6	0.00	-0.01	0.04	-0.03	0.04	0.01	-0.02	-0.01	-0.05
6	6	0.01	0.00	0.01	-0.10	0.01	-0.07	0.03	0.09	-0.13
7	6	0.13	-0.02	0.03	-0.05	0.02	-0.06	-0.13	-0.04	0.00
8	6	-0.04	-0.08	-0.05	-0.05	0.00	0.18	-0.04	0.02	-0.06
9	6	-0.03	-0.01	0.04	0.05	0.05	0.01	0.01	-0.01	0.05
10	6	-0.06	0.11	0.03	0.09	0.11	-0.13	0.13	0.00	0.08
11	6	-0.06	0.00	-0.08	0.05	-0.05	-0.03	0.05	-0.09	-0.01
12	6	0.01	0.00	0.03	-0.01	-0.02	0.05	0.00	-0.02	0.01
13	7	0.01	0.00	-0.05	-0.03	-0.01	-0.02	0.00	-0.01	-0.02
14	8	0.00	-0.01	-0.01	0.02	-0.04	-0.01	0.00	0.02	0.00
15	8	-0.01	0.01	-0.01	0.06	-0.01	-0.03	0.02	0.02	-0.01
16	8	0.00	0.02	-0.01	0.00	-0.05	0.00	0.00	0.00	0.00
17	1	0.17	0.25	0.16	-0.05	-0.08	0.19	0.23	0.05	-0.29
18	1	-0.03	-0.02	-0.05	-0.03	0.15	-0.10	0.08	-0.04	0.31
19	1	0.25	-0.30	0.09	-0.13	-0.29	0.34	-0.13	-0.05	-0.13
20	1	-0.13	0.09	0.04	-0.12	-0.12	-0.26	-0.23	0.11	0.09
21	1	-0.01	-0.05	-0.05	-0.06	0.03	-0.02	-0.02	0.00	-0.24
22	1	0.34	-0.04	0.21	0.01	0.03	-0.13	-0.26	-0.09	0.25
23	1	-0.08	-0.16	-0.03	-0.02	-0.23	0.28	0.09	0.21	-0.09
24	1	-0.11	0.38	0.15	0.20	0.14	-0.18	0.05	0.10	0.16
25	1	-0.19	-0.06	-0.06	-0.14	0.05	-0.01	0.08	-0.33	0.00
26	1	0.00	0.03	0.06	0.16	-0.14	0.12	-0.02	0.17	0.04
27	1	0.09	0.02	0.38	-0.17	0.14	0.14	-0.04	0.06	0.16
28	1	0.00	0.06	-0.02	0.02	-0.08	0.00	0.00	-0.02	0.01
29	1	0.00	0.06	-0.02	0.02	0.00	0.01	0.01	0.08	-0.01
			34			35			36	
			?A			?A			?A	

Frequencies --	1036.7028			1040.6712			1047.7446		
Red. masses --	2.2564			2.8244			2.0370		
Frc consts --	1.4288			1.8022			1.3175		
IR Inten --	9.7228			20.7431			91.1668		
Raman Activ --	5.9794			1.2518			3.2118		
Depolar --	0.5462			0.6462			0.6838		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.02	0.00	-0.01	0.00	-0.14	0.05	-0.04	0.03
2 6	0.06	0.00	0.05	0.17	-0.04	0.07	-0.04	0.03	-0.01
3 6	-0.09	-0.02	-0.03	-0.03	0.08	0.03	-0.01	0.05	-0.02
4 6	0.01	0.03	0.00	-0.15	-0.03	0.05	-0.06	0.08	0.04
5 6	-0.05	0.00	0.00	-0.05	0.03	0.03	0.12	0.01	-0.01
6 6	0.11	0.12	0.10	-0.05	-0.08	0.00	0.03	-0.03	0.00
7 6	0.03	-0.03	-0.08	0.03	0.01	0.11	-0.01	0.07	0.01
8 6	-0.04	-0.04	0.05	0.11	0.01	-0.03	-0.01	-0.11	0.02
9 6	-0.10	-0.04	0.02	0.04	0.03	-0.03	0.09	0.02	-0.01
10 6	-0.06	-0.08	-0.03	-0.09	0.01	-0.05	0.01	-0.05	0.01
11 6	0.04	0.00	-0.10	-0.01	0.07	-0.06	0.01	-0.01	-0.09
12 6	0.02	-0.02	-0.01	-0.02	-0.04	-0.02	-0.01	0.07	0.00
13 7	0.05	0.00	-0.01	-0.01	-0.01	0.01	-0.05	0.01	0.00
14 8	-0.01	0.01	0.00	0.01	-0.01	0.00	-0.02	0.03	0.00
15 8	0.01	0.04	-0.01	0.07	0.01	0.00	-0.05	-0.06	0.01
16 8	0.00	-0.02	0.00	0.00	-0.04	0.00	0.01	0.02	0.00
17 1	-0.04	0.02	0.11	0.04	0.03	-0.19	-0.01	-0.05	0.12
18 1	0.17	0.08	0.14	0.40	0.07	0.29	-0.05	0.27	-0.12
19 1	-0.27	-0.01	-0.01	-0.23	0.09	0.07	-0.14	0.12	-0.04
20 1	0.10	-0.01	-0.01	-0.26	-0.01	0.05	-0.27	0.13	0.05
21 1	0.37	0.23	0.35	-0.05	-0.17	-0.09	0.19	-0.24	-0.10
22 1	0.07	-0.03	-0.04	-0.03	-0.01	0.23	-0.09	0.05	0.10
23 1	0.03	-0.01	0.06	0.13	0.06	-0.05	-0.14	-0.25	0.03

```
  24   1    -0.17  -0.29  -0.04    -0.13  -0.03  -0.05    -0.09  -0.18
0.04
  25   1    -0.36  -0.01  -0.06    -0.10  -0.25  -0.02    -0.25  -0.13  -
0.05
  26   1     0.22  -0.02   0.23    -0.01   0.33   0.12     0.14   0.03
0.20
  27   1     0.03   0.03   0.02    -0.21   0.15  -0.01     0.15  -0.16  -
0.01
  28   1    -0.01   0.19  -0.01     0.01  -0.10  -0.01    -0.01  -0.18
0.01
  29   1     0.04   0.15   0.00     0.03   0.09   0.00    -0.09  -0.43
0.02
                     37                    38                    39
                     ?A                    ?A                    ?A
 Frequencies --  1069.8936             1078.6821             1107.3467
 Red. masses --     1.7341                2.1075                1.8775
 Frc consts  --     1.1695                1.4448                1.3564
 IR Inten    --     0.6573               55.6757               31.7576
 Raman Activ --     4.9448                8.1360                1.9085
 Depolar     --     0.7405                0.6054                0.6554
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.02  -0.13  -0.02    -0.03   0.04  -0.04    -0.02   0.00
0.01
   2   6    -0.01   0.02   0.07     0.04  -0.05   0.04     0.01  -0.01  -
0.01
   3   6    -0.02  -0.03  -0.02    -0.02  -0.06   0.04     0.01  -0.04
0.00
   4   6     0.04   0.02  -0.03    -0.01  -0.10  -0.04     0.03  -0.04
0.00
   5   6     0.01  -0.01   0.01     0.14  -0.01  -0.02    -0.04  -0.04
0.00
   6   6     0.00   0.04  -0.06    -0.01   0.05   0.04     0.00   0.02
0.04
   7   6     0.07  -0.07   0.01    -0.03  -0.03  -0.02    -0.02  -0.01  -
0.03
   8   6    -0.07   0.00   0.02    -0.02   0.09  -0.03    -0.05   0.02  -
0.04
   9   6     0.02   0.01  -0.01     0.01   0.04   0.00     0.20   0.04  -
0.03
  10   6     0.02   0.01   0.03    -0.06   0.06   0.00    -0.05   0.02
0.05
  11   6    -0.02   0.11   0.00     0.04   0.00   0.00     0.03  -0.01  -
0.02
  12   6     0.00   0.01   0.01     0.00   0.08  -0.02    -0.02  -0.02
0.00
  13   7    -0.01   0.00   0.00    -0.04   0.03   0.00    -0.05  -0.03
0.01
  14   8     0.00   0.00   0.00     0.01  -0.05   0.00     0.00   0.06
0.00
  15   8     0.00  -0.01  -0.01    -0.05  -0.06   0.01     0.04   0.00  -
0.01
  16   8     0.00   0.02   0.00     0.02   0.07   0.00    -0.01   0.02
0.00
```

17	1	-0.25	-0.38	-0.22	0.01	0.04	-0.16	0.00	0.03	0.09
18	1	0.09	0.01	0.18	0.16	-0.20	0.24	0.02	0.02	-0.01
19	1	-0.03	-0.03	-0.02	-0.12	-0.20	0.15	0.04	0.01	-0.04
20	1	0.17	0.04	-0.02	-0.10	-0.25	-0.12	0.14	0.01	0.02
21	1	-0.04	-0.02	-0.14	0.00	0.23	0.22	0.06	0.15	0.21
22	1	0.38	-0.08	0.19	-0.06	-0.01	-0.13	-0.10	0.01	-0.18
23	1	-0.20	-0.07	0.00	0.02	0.18	-0.05	-0.36	0.04	-0.16
24	1	-0.04	0.02	0.07	-0.11	0.07	0.03	-0.35	0.02	0.23
25	1	-0.16	0.40	-0.01	0.02	-0.08	0.01	-0.07	0.00	-0.01
26	1	-0.11	0.36	0.01	0.05	0.02	0.03	0.11	-0.11	0.06
27	1	0.00	-0.01	-0.01	0.26	-0.23	-0.01	-0.28	0.16	0.03
28	1	0.00	-0.05	0.01	0.02	0.03	0.00	0.01	-0.51	0.03
29	1	-0.02	-0.08	0.00	-0.12	-0.52	0.01	0.03	0.23	-0.01

	40			41			42		
	?A			?A			?A		
Frequencies --	1165.4696			1183.1284			1209.8774		
Red. masses --	1.6019			3.3831			2.5228		
Frc consts --	1.2820			2.7901			2.1758		
IR Inten --	20.0219			147.6703			53.9468		
Raman Activ --	2.3253			2.4714			10.3534		
Depolar --	0.7094			0.6038			0.7302		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.05	0.00	0.05	-0.02	0.01	0.01	0.00	0.00	-0.01
2 6	-0.01	0.01	-0.04	0.00	0.00	0.00	0.01	0.02	0.01
3 6	0.03	-0.05	0.04	0.01	0.01	0.02	0.01	0.00	0.04
4 6	0.04	-0.03	0.00	0.01	-0.01	-0.02	0.03	0.06	0.00
5 6	-0.01	-0.04	-0.04	0.09	0.09	-0.03	-0.03	0.21	-0.07
6 6	0.00	-0.01	-0.04	0.00	-0.01	0.00	0.05	0.01	0.02
7 6	-0.04	-0.03	0.06	-0.01	-0.01	0.02	0.01	0.00	-0.02
8 6	0.02	0.05	-0.01	0.01	0.02	-0.01	0.04	-0.03	0.02
9 6	-0.04	0.04	-0.05	0.01	-0.09	-0.02	0.03	-0.15	-0.09

```
  10   6    -0.01   0.06   0.05     0.00   0.01   0.02    -0.03  -0.01
0.06
  11   6     0.05   0.02  -0.07     0.01   0.00  -0.02    -0.03  -0.01
0.01
  12   6     0.00   0.01   0.01     0.02  -0.18   0.01    -0.01   0.04
0.02
  13   7    -0.01   0.01   0.00     0.11  -0.10  -0.01    -0.02   0.05
0.00
  14   8     0.01  -0.04   0.00     0.00   0.08   0.00    -0.04   0.07
0.01
  15   8     0.01  -0.02   0.00    -0.21   0.20   0.01     0.04  -0.06
0.00
  16   8    -0.01   0.02   0.00     0.05  -0.03   0.00    -0.01  -0.12
0.01
  17   1    -0.21  -0.05   0.38    -0.11  -0.04   0.07    -0.07  -0.07  -
0.05
  18   1    -0.01   0.27  -0.14    -0.04  -0.01  -0.03    -0.04  -0.10  -
0.01
  19   1    -0.03   0.04  -0.01    -0.03  -0.16   0.16    -0.05  -0.31
0.27
  20   1     0.24  -0.20  -0.07    -0.03  -0.30  -0.16    -0.12  -0.37  -
0.20
  21   1     0.15  -0.23  -0.17     0.02  -0.08  -0.06    -0.11  -0.03  -
0.10
  22   1    -0.20  -0.09   0.37    -0.07  -0.03   0.11    -0.10  -0.02
0.04
  23   1     0.07   0.31  -0.09    -0.01   0.15  -0.06    -0.17   0.22  -
0.15
  24   1     0.01  -0.07   0.00    -0.01   0.04   0.04    -0.11   0.20
0.19
  25   1    -0.20  -0.11  -0.03    -0.05  -0.03  -0.01     0.02   0.00
0.00
  26   1     0.14   0.10   0.18     0.03   0.01   0.03    -0.06   0.01  -
0.05
  27   1     0.02  -0.02  -0.05    -0.38   0.33   0.00     0.32  -0.26  -
0.08
  28   1     0.01   0.13   0.00     0.00  -0.24   0.02    -0.03   0.01
0.01
  29   1     0.01   0.13   0.01    -0.05  -0.51   0.01     0.09   0.25
0.00
                     43                     44                     45
                     ?A                     ?A                     ?A
 Frequencies --  1215.7877              1227.5045              1243.9874
 Red. masses --     3.0663                 2.6680                 2.7787
 Frc consts  --     2.6705                 2.3686                 2.5335
 IR Inten    --    17.2738                81.0237                98.8664
 Raman Activ --     2.2122                 1.9607                 0.6453
 Depolar     --     0.7426                 0.4637                 0.7492
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.01   0.04  -0.04    -0.06  -0.01   0.10     0.02   0.02  -
0.05
   2   6     0.00  -0.06   0.04    -0.07   0.06  -0.07    -0.07  -0.13
0.01
```

3	6	-0.03	0.14	-0.05	0.05	0.06	-0.03	0.12	-0.01	-0.06
4	6	-0.05	-0.10	-0.06	0.11	-0.08	-0.04	0.00	0.03	0.01
5	6	-0.01	0.03	0.11	0.01	0.13	0.04	0.01	0.16	0.02
6	6	-0.06	0.04	0.03	0.02	-0.09	-0.04	-0.06	0.09	0.04
7	6	0.01	-0.04	-0.03	-0.05	-0.01	0.09	0.03	-0.02	-0.07
8	6	-0.11	0.04	-0.10	-0.04	0.09	-0.09	-0.06	-0.05	0.00
9	6	0.06	-0.08	0.20	-0.01	0.07	0.11	-0.02	0.19	-0.02
10	6	0.11	-0.11	-0.10	0.04	-0.04	-0.01	0.00	0.03	0.04
11	6	0.05	0.01	0.02	0.06	0.02	-0.09	-0.01	0.00	0.08
12	6	-0.01	0.02	-0.05	0.00	-0.01	-0.03	0.01	0.02	0.01
13	7	-0.02	0.03	0.00	0.01	-0.01	0.00	0.02	-0.04	0.00
14	8	-0.02	0.05	-0.01	0.01	-0.03	0.00	0.04	-0.06	0.00
15	8	0.03	-0.02	-0.01	-0.03	-0.02	0.00	-0.04	-0.04	0.01
16	8	0.00	-0.01	0.00	-0.01	-0.07	0.00	-0.01	-0.07	0.00
17	1	-0.09	0.08	0.36	0.07	0.01	-0.21	0.16	0.12	-0.12
18	1	-0.13	0.27	-0.23	0.13	-0.21	0.27	0.14	0.31	0.07
19	1	0.02	-0.13	0.13	-0.08	-0.16	0.16	-0.34	-0.01	0.04
20	1	0.29	-0.11	-0.05	-0.35	0.08	0.01	0.03	-0.14	-0.07
21	1	0.07	-0.23	-0.16	-0.06	0.15	0.16	0.24	-0.26	-0.12
22	1	0.09	-0.08	0.28	0.04	0.01	-0.02	-0.06	-0.05	0.14
23	1	0.08	0.28	-0.13	-0.12	-0.37	0.05	0.13	0.02	0.04
24	1	-0.05	0.18	0.09	0.04	-0.03	0.00	-0.04	-0.37	-0.07
25	1	0.07	-0.03	0.02	-0.27	-0.05	-0.05	0.14	0.18	0.05
26	1	0.02	0.08	0.01	0.20	0.03	0.21	-0.03	-0.21	-0.11
27	1	0.16	-0.11	0.13	0.00	0.02	0.09	-0.18	0.13	-0.01
28	1	-0.02	-0.05	0.01	0.01	0.08	0.00	0.04	-0.14	0.00
29	1	-0.01	-0.08	0.01	0.08	0.30	-0.01	0.05	0.13	0.00

	46			47			48		
	?A			?A			?A		
Frequencies --	1256.6662			1264.2221			1269.7452		
Red. masses --	1.9371			1.5461			2.0106		
Frc consts --	1.8024			1.4559			1.9099		
IR Inten --	28.4290			21.8427			3.0114		
Raman Activ --	2.2717			7.8037			9.8206		
Depolar --	0.7129			0.7470			0.7493		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.02	-0.02	0.00	0.01	0.01	0.00	0.00	-0.03	0.02
2 6	0.03	0.06	0.02	-0.02	-0.03	-0.02	-0.09	0.00	0.02
3 6	-0.07	0.04	-0.06	0.04	0.01	-0.02	0.04	0.02	-0.07
4 6	-0.02	0.00	-0.02	-0.03	0.00	-0.08	-0.02	-0.03	-0.09
5 6	-0.02	0.03	0.07	0.00	-0.04	0.10	0.00	0.01	0.17
6 6	0.11	0.00	0.03	-0.03	-0.01	-0.01	0.03	0.05	-0.03
7 6	0.00	0.00	0.00	-0.02	-0.03	0.03	0.01	-0.04	-0.01
8 6	-0.03	0.00	0.03	0.02	0.06	0.05	0.02	0.04	0.06
9 6	-0.02	0.13	-0.05	0.00	-0.10	-0.06	-0.01	-0.04	-0.13
10 6	-0.07	-0.12	0.03	0.02	0.01	0.01	0.00	-0.02	0.05
11 6	-0.01	0.00	-0.03	0.01	0.00	0.00	0.01	0.02	0.00
12 6	0.01	0.04	0.00	0.00	-0.02	0.01	0.00	0.00	0.02
13 7	0.01	-0.03	0.00	-0.01	0.02	0.00	0.00	0.00	0.00
14 8	0.02	-0.04	0.01	-0.02	0.03	0.01	0.00	0.01	0.01
15 8	0.01	-0.03	-0.01	0.01	0.02	-0.01	0.00	0.00	-0.02
16 8	0.01	0.00	0.00	0.00	0.02	-0.01	0.00	0.00	-0.01
17 1	0.07	0.02	0.00	0.25	0.12	-0.31	0.05	0.11	0.37
18 1	-0.12	-0.24	-0.05	0.06	-0.03	0.07	0.12	0.17	0.19
19 1	0.37	-0.16	-0.01	-0.11	0.16	-0.09	-0.04	0.06	-0.08
20 1	0.14	-0.06	-0.04	-0.09	0.12	-0.03	-0.07	-0.06	-0.10
21 1	-0.28	0.01	-0.19	0.17	-0.12	0.00	-0.08	0.07	-0.08
22 1	-0.30	-0.06	0.23	-0.16	-0.08	0.30	0.02	0.01	-0.36

```
  23   1     0.12   0.12   0.04    -0.01   0.03   0.05     0.12  -0.17
0.17
  24   1     0.16   0.36   0.06    -0.13   0.05   0.12    -0.09   0.08
0.14
  25   1    -0.11   0.14  -0.03    -0.18   0.44  -0.01     0.17  -0.48
0.02
  26   1     0.10  -0.22   0.02     0.19  -0.45   0.03    -0.10   0.35
0.02
  27   1    -0.18   0.13   0.00     0.11  -0.09  -0.04    -0.01   0.00  -
0.07
  28   1     0.03  -0.12   0.02    -0.02   0.09   0.01     0.00   0.02
0.01
  29   1    -0.04  -0.21   0.00    -0.01   0.00  -0.01     0.00  -0.01
0.00
                     49                     50                     51
                     ?A                     ?A                     ?A
 Frequencies --  1301.9225              1325.6010              1344.4537
 Red. masses --     1.6996                 1.7115                 1.7293
 Frc consts  --     1.6973                 1.7720                 1.8416
 IR Inten    --     1.4807                77.3518                60.8385
 Raman Activ --     1.4217                 1.2544                 2.6594
 Depolar     --     0.7434                 0.7373                 0.7431
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.03   0.10   0.06    -0.01  -0.06   0.01    -0.07  -0.01  -
0.05
   2   6     0.00  -0.02  -0.05    -0.05   0.00  -0.03     0.07   0.00
0.04
   3   6     0.04   0.01   0.00     0.04   0.02   0.04    -0.06   0.03
0.00
   4   6    -0.01  -0.03  -0.01     0.02   0.03  -0.04     0.01  -0.04
0.04
   5   6     0.01  -0.04   0.03     0.07  -0.09  -0.04     0.10   0.00  -
0.08
   6   6     0.02   0.00   0.06     0.06   0.03   0.05    -0.03   0.04  -
0.01
   7   6    -0.11   0.05  -0.07     0.05  -0.03  -0.02    -0.03  -0.04
0.00
   8   6     0.00  -0.01   0.01    -0.07   0.01   0.04    -0.02   0.04
0.01
   9   6     0.01   0.00  -0.04     0.03  -0.03   0.05    -0.02   0.03  -
0.09
  10   6    -0.05  -0.03   0.00    -0.09   0.01  -0.05     0.03  -0.03
0.03
  11   6     0.04  -0.09   0.00    -0.01   0.03   0.00     0.02   0.03
0.02
  12   6     0.00   0.02   0.00     0.00  -0.03  -0.01     0.00  -0.05
0.02
  13   7     0.00  -0.01   0.00    -0.01   0.02   0.00    -0.01   0.02
0.00
  14   8     0.01   0.02   0.00     0.01   0.03  -0.01     0.02   0.00
0.01
  15   8     0.00   0.00   0.00    -0.02   0.02   0.01    -0.03   0.01
0.00
```

```
  16   8    -0.01   0.01   0.00    -0.03   0.01   0.00    -0.03  -0.01
0.01
  17   1    -0.31  -0.25  -0.21     0.19   0.11   0.00     0.05   0.12
0.08
  18   1     0.03  -0.16   0.03     0.16   0.00   0.21    -0.18   0.00  -
0.25
  19   1    -0.14   0.08  -0.01    -0.20  -0.04   0.13     0.15  -0.25
0.15
  20   1    -0.09  -0.08  -0.03    -0.04   0.17   0.02    -0.06   0.32
0.20
  21   1     0.08  -0.15  -0.06    -0.25  -0.10  -0.27     0.18  -0.12  -
0.04
  22   1     0.42   0.03   0.25    -0.28  -0.06   0.05     0.15  -0.03  -
0.02
  23   1     0.27  -0.03   0.11     0.08   0.17   0.04     0.31  -0.30
0.25
  24   1     0.11   0.22  -0.02     0.33   0.03  -0.29    -0.12   0.12
0.17
  25   1    -0.05   0.13   0.00     0.05  -0.15   0.00     0.03  -0.01
0.02
  26   1    -0.12   0.35   0.00     0.00   0.01   0.00     0.06  -0.08
0.02
  27   1    -0.03   0.02  -0.02     0.14  -0.11   0.02     0.14  -0.12  -
0.05
  28   1     0.01  -0.23   0.01     0.02  -0.32   0.02     0.02  -0.16
0.01
  29   1     0.02   0.17   0.00     0.05   0.31  -0.02     0.06   0.32  -
0.02
                     52                    53                    54
                     ?A                    ?A                    ?A
 Frequencies --  1352.6248             1358.2175             1361.8730
 Red. masses --     1.7463                1.4249                1.3547
 Frc consts  --     1.8825                1.5487                1.4804
 IR Inten    --    51.8713               23.0236                6.9144
 Raman Activ --     0.8119                0.4937                3.8965
 Depolar     --     0.6813                0.7498                0.7346
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.06   0.01   0.02     0.01   0.02   0.00     0.02  -0.01
0.04
   2   6    -0.02  -0.09  -0.06     0.00  -0.04  -0.02    -0.02   0.04
0.03
   3   6    -0.01   0.06   0.07    -0.08  -0.01   0.00     0.07   0.01  -
0.02
   4   6     0.08   0.00   0.01     0.02   0.01   0.00    -0.05  -0.02  -
0.01
   5   6    -0.10  -0.02  -0.09     0.04   0.01   0.06    -0.03   0.00  -
0.05
   6   6     0.05   0.03   0.02     0.04  -0.05   0.03     0.03  -0.04
0.04
   7   6    -0.04  -0.03  -0.03     0.01   0.03   0.00     0.01   0.02
0.03
   8   6    -0.01   0.01   0.02    -0.06  -0.02  -0.01    -0.04  -0.01
0.00
```

```
    9   6     0.00  -0.03  -0.02     0.00   0.00  -0.01     0.00  -0.01  -
0.04
   10   6     0.01  -0.02  -0.01     0.05   0.08  -0.02     0.05   0.03  -
0.04
   11   6     0.03   0.00   0.01    -0.01   0.00  -0.01     0.00  -0.01  -
0.02
   12   6     0.00   0.06   0.00     0.00  -0.04   0.01     0.00   0.02
0.01
   13   7     0.02  -0.03   0.00    -0.01   0.02   0.00     0.00  -0.01
0.00
   14   8    -0.01   0.00   0.01     0.01   0.01   0.00     0.00   0.00
0.01
   15   8     0.02  -0.01   0.00    -0.01   0.01  -0.01     0.01   0.00
0.01
   16   8     0.03   0.02   0.01    -0.01  -0.01  -0.01     0.01   0.01
0.01
   17   1     0.15   0.13  -0.16    -0.10  -0.09  -0.06     0.05  -0.02  -
0.10
   18   1     0.29   0.49   0.06     0.12   0.22   0.02    -0.17  -0.18  -
0.06
   19   1     0.19  -0.21   0.21     0.43   0.04  -0.14    -0.42  -0.13
0.18
   20   1    -0.23   0.23   0.09    -0.16  -0.16  -0.09     0.35   0.20
0.11
   21   1    -0.15  -0.01  -0.13    -0.38   0.16   0.00    -0.33   0.04  -
0.09
   22   1     0.13  -0.03   0.08     0.01   0.02   0.11     0.00   0.03  -
0.06
   23   1    -0.01  -0.06   0.05     0.31   0.12   0.06     0.32   0.10
0.08
   24   1    -0.10   0.10   0.10    -0.28  -0.42   0.00    -0.40  -0.14
0.16
   25   1     0.02  -0.01   0.02    -0.02   0.04  -0.01    -0.03  -0.02  -
0.02
   26   1     0.01   0.06   0.02     0.01  -0.04   0.00     0.01   0.04
0.03
   27   1    -0.18   0.15   0.00     0.12  -0.10  -0.02    -0.07   0.05  -
0.02
   28   1    -0.01   0.11   0.00     0.01  -0.11   0.00    -0.01   0.08  -
0.01
   29   1    -0.07  -0.35   0.00     0.03   0.15   0.00    -0.02  -0.10
0.00
                     55                    56                    57
                     ?A                    ?A                    ?A
 Frequencies --  1380.2647             1390.3976             1395.8645
 Red. masses --     1.7266                1.3487                1.4951
 Frc consts  --     1.9380                1.5362                1.7164
 IR Inten    --    16.2333               10.3453               51.6353
 Raman Activ --     0.7668                1.8430                7.1406
 Depolar     --     0.7098                0.7471                0.7062
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.04   0.04  -0.01    -0.01   0.00   0.00     0.02   0.05
0.00
```

2	6	-0.04	-0.07	0.05	0.00	-0.05	0.07	0.01	-0.02	0.01
3	6	0.01	0.02	-0.04	0.05	-0.02	0.04	-0.02	0.03	0.00
4	6	-0.10	-0.04	0.01	0.03	0.03	0.01	0.01	0.00	-0.01
5	6	0.03	0.02	-0.02	0.04	-0.01	0.00	0.10	-0.07	0.01
6	6	0.09	-0.01	-0.03	0.04	-0.03	-0.06	0.00	0.05	0.06
7	6	-0.06	-0.01	0.00	0.01	0.01	0.00	0.05	-0.02	0.00
8	6	0.09	0.06	-0.01	-0.02	0.00	-0.01	0.04	0.02	0.02
9	6	0.01	0.01	0.02	0.00	0.01	0.00	0.03	0.02	0.00
10	6	-0.05	0.02	0.03	-0.02	-0.05	-0.04	0.03	-0.02	-0.04
11	6	0.02	-0.05	0.00	-0.02	0.05	0.00	-0.03	-0.04	0.00
12	6	0.00	-0.06	0.00	0.00	0.01	0.00	0.01	0.04	-0.01
13	7	-0.01	0.03	0.00	0.01	-0.01	0.00	0.01	-0.03	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	-0.03	-0.03	0.01
15	8	0.00	0.02	0.01	-0.02	0.00	0.00	-0.03	0.00	0.00
16	8	0.00	-0.01	0.00	-0.01	0.00	0.00	-0.03	0.01	0.00
17	1	-0.04	-0.02	0.00	-0.06	-0.08	-0.14	-0.21	-0.16	-0.07
18	1	0.00	0.37	-0.07	-0.16	0.34	-0.26	-0.04	-0.01	-0.06
19	1	-0.01	-0.15	0.09	-0.29	0.30	-0.11	-0.01	-0.06	0.06
20	1	0.42	0.05	0.07	-0.12	-0.14	-0.06	-0.20	-0.04	-0.03
21	1	-0.31	0.23	-0.04	-0.17	0.36	0.19	-0.12	-0.18	-0.23
22	1	-0.01	-0.01	0.02	0.04	-0.01	0.14	-0.33	-0.03	-0.15
23	1	-0.33	-0.35	0.00	0.10	-0.01	0.04	-0.28	-0.05	-0.06
24	1	0.18	-0.13	-0.15	-0.01	0.42	0.11	-0.23	0.04	0.13
25	1	-0.10	0.26	-0.01	0.06	-0.16	0.00	-0.07	0.07	-0.01
26	1	-0.02	0.04	-0.01	0.06	-0.19	0.00	-0.11	0.08	-0.07
27	1	0.14	-0.11	0.01	-0.05	0.04	0.01	-0.21	0.16	0.02
28	1	0.00	0.02	0.00	0.00	0.03	-0.01	-0.04	0.48	-0.02

```
  29   1     0.01   0.05   0.00     0.02   0.12   0.00     0.05   0.32  -
0.01
                     58                     59                     60
                     ?A                     ?A                     ?A
 Frequencies --  1402.5954              1419.5636              1425.1318
 Red. masses --     1.7071                 1.6784                 1.4943
 Frc consts  --     1.9787                 1.9928                 1.7881
 IR Inten    --     6.4952                25.6922                 2.7578
 Raman Activ --     2.3245                10.2243                 2.1466
 Depolar     --     0.6697                 0.6847                 0.7226
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.07   0.01  -0.03    -0.02  -0.06  -0.10     0.00   0.03
0.07
   2   6     0.07   0.03   0.05    -0.04   0.05   0.02     0.04  -0.02
0.04
   3   6     0.02  -0.09  -0.02     0.00   0.01  -0.01     0.00   0.04  -
0.08
   4   6     0.06  -0.03   0.01    -0.02   0.02  -0.01     0.01  -0.05  -
0.06
   5   6    -0.05   0.06   0.04     0.08  -0.02   0.00     0.00  -0.02
0.04
   6   6     0.06   0.04   0.07     0.04  -0.05   0.00    -0.01  -0.02  -
0.03
   7   6    -0.04  -0.06  -0.03    -0.11   0.01  -0.04     0.01   0.00  -
0.03
   8   6     0.01   0.05   0.00     0.04  -0.05   0.02     0.02  -0.03
0.06
   9   6     0.03  -0.03   0.03     0.01  -0.01   0.01     0.00  -0.02  -
0.01
  10   6    -0.04   0.06  -0.03     0.00   0.02   0.00    -0.02   0.04
0.06
  11   6     0.03   0.01   0.00     0.04   0.03   0.04    -0.03   0.06  -
0.01
  12   6     0.00   0.00  -0.01     0.01   0.07  -0.01     0.00   0.02
0.00
  13   7     0.00   0.00   0.00     0.01  -0.04   0.00     0.00  -0.01
0.00
  14   8     0.00   0.01   0.00    -0.02  -0.01   0.00     0.00   0.00
0.00
  15   8     0.01   0.00  -0.01    -0.02  -0.01   0.00     0.00  -0.01
0.00
  16   8     0.02   0.00  -0.01    -0.02   0.00   0.00     0.00   0.00
0.00
  17   1     0.01   0.11   0.07     0.15   0.22   0.42    -0.13  -0.18  -
0.32
  18   1    -0.31  -0.13  -0.32     0.02  -0.13   0.16    -0.19   0.03  -
0.25
  19   1    -0.15   0.26  -0.24    -0.04  -0.07   0.06     0.03  -0.29
0.14
  20   1    -0.31   0.06   0.04    -0.08   0.02  -0.01    -0.12   0.30
0.08
  21   1    -0.27  -0.21  -0.36    -0.16   0.11   0.05     0.09   0.07
0.12
```

```
  22   1     0.09  -0.07   0.04     0.49   0.01   0.23     0.06  -0.02
0.15
  23   1    -0.12  -0.24   0.06    -0.14   0.24  -0.15    -0.18   0.30  -
0.13
  24   1     0.02  -0.22  -0.17    -0.02  -0.09  -0.02     0.17  -0.28  -
0.15
  25   1    -0.03  -0.02   0.01     0.06   0.09   0.04     0.11  -0.38
0.00
  26   1     0.02   0.01  -0.02     0.10  -0.14   0.02     0.03  -0.10
0.00
  27   1     0.01  -0.01   0.02    -0.20   0.16   0.01    -0.05   0.04
0.00
  28   1     0.00   0.00   0.00    -0.02   0.19  -0.01     0.00  -0.02
0.01
  29   1    -0.03  -0.19   0.01     0.03   0.21  -0.01     0.00   0.03  -
0.01
                     61                     62                     63
                     ?A                     ?A                     ?A
 Frequencies --  1433.7644              1445.1312              1453.9523
 Red. masses --     1.4425                 1.5364                 2.3418
 Frc consts  --     1.7471                 1.8905                 2.9168
 IR Inten    --     3.7694                 8.0293                64.7918
 Raman Activ --     2.0540                 0.9693                 1.0696
 Depolar     --     0.6538                 0.7027                 0.5195
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.08   0.05  -0.07    -0.06  -0.03   0.07    -0.03   0.00  -
0.02
   2   6    -0.03  -0.02   0.02     0.04  -0.03   0.01     0.02  -0.01
0.04
   3   6     0.02   0.01  -0.01    -0.01   0.01  -0.01    -0.02  -0.01  -
0.02
   4   6     0.03  -0.05   0.00    -0.03   0.08  -0.01    -0.01  -0.01
0.01
   5   6    -0.03   0.00  -0.01     0.03  -0.05   0.03     0.05   0.02
0.00
   6   6     0.02   0.04  -0.02     0.01   0.05   0.00    -0.01  -0.01  -
0.06
   7   6    -0.03  -0.02   0.12    -0.07  -0.03   0.09     0.06   0.02
0.06
   8   6     0.00  -0.02   0.00     0.04  -0.04  -0.03    -0.04   0.05  -
0.02
   9   6    -0.02  -0.01   0.00    -0.03   0.02   0.02    -0.05  -0.16
0.01
  10   6    -0.02  -0.01   0.01     0.01   0.00   0.00    -0.03   0.05
0.04
  11   6    -0.03   0.02  -0.02     0.02   0.01  -0.02     0.02  -0.07  -
0.01
  12   6     0.00   0.01   0.00     0.00   0.01   0.00     0.00   0.21  -
0.01
  13   7     0.00   0.00   0.00     0.00   0.00   0.00     0.04  -0.08
0.00
  14   8     0.01   0.01   0.00     0.01   0.00   0.00     0.01   0.04
0.00
```

15	8	0.01	0.00	0.00	0.00	0.00	0.00	0.00	-0.06	0.00
16	8	0.01	0.00	0.00	-0.01	0.00	-0.01	-0.02	-0.01	0.00
17	1	-0.37	-0.24	0.22	0.30	0.14	-0.38	0.08	0.11	0.03
18	1	0.06	0.08	0.08	-0.09	0.08	-0.19	-0.10	0.09	-0.13
19	1	-0.09	-0.02	0.03	0.04	-0.05	0.02	0.05	-0.03	-0.02
20	1	-0.25	0.18	0.10	0.17	-0.34	-0.19	0.02	-0.01	0.01
21	1	-0.04	-0.05	-0.16	-0.01	-0.16	-0.22	0.09	0.13	0.13
22	1	0.14	0.08	-0.47	0.32	0.08	-0.45	-0.27	0.03	-0.13
23	1	0.13	0.23	-0.05	-0.02	0.14	-0.12	0.25	-0.10	0.13
24	1	0.08	0.04	-0.04	0.00	0.01	0.00	0.22	-0.14	-0.17
25	1	-0.11	0.19	-0.02	-0.08	-0.02	0.00	-0.14	0.33	-0.02
26	1	0.12	-0.38	0.00	0.07	-0.02	0.06	-0.08	0.24	0.00
27	1	0.02	-0.01	0.00	0.00	0.00	0.01	-0.33	0.27	0.02
28	1	0.01	-0.13	0.01	0.01	-0.13	0.00	0.01	-0.32	0.02
29	1	-0.01	-0.05	0.00	0.01	0.08	0.00	0.02	0.13	0.00

	64			65			66		
	?A			?A			?A		
Frequencies --	1462.6662			1471.1354			1500.2930		
Red. masses --	1.5794			1.8576			1.9092		
Frc consts --	1.9908			2.3687			2.5319		
IR Inten --	6.1496			96.3061			5.3601		
Raman Activ --	2.2083			3.9118			2.1094		
Depolar --	0.7477			0.4742			0.6909		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.07	0.00	0.02	0.00	0.00	0.06	-0.01	-0.01	-0.01
2 6	-0.01	0.01	-0.04	0.00	-0.02	-0.04	0.01	-0.01	0.02
3 6	-0.02	0.00	0.01	-0.05	-0.08	0.07	0.01	0.03	-0.04
4 6	-0.05	0.03	0.05	-0.07	-0.08	-0.05	0.02	0.04	0.03
5 6	0.01	-0.01	-0.02	0.08	0.15	-0.02	-0.03	-0.03	0.01
6 6	0.00	0.02	0.03	0.01	0.03	0.01	-0.01	0.00	-0.03
7 6	-0.03	-0.05	-0.02	-0.02	0.00	0.02	-0.01	0.01	0.03

8	6	0.00	0.08	-0.05	-0.02	-0.03	0.02	-0.10	-0.02	-0.04
9	6	0.02	-0.07	0.01	0.07	-0.03	0.00	0.20	-0.02	-0.03
10	6	0.00	0.02	0.00	-0.03	-0.01	-0.02	-0.08	0.00	0.06
11	6	-0.05	0.10	-0.01	0.00	0.01	-0.02	0.01	-0.01	0.00
12	6	0.00	0.07	-0.01	0.00	0.02	0.00	0.00	-0.05	0.00
13	7	0.01	-0.03	0.00	0.01	-0.02	0.00	-0.02	0.01	0.00
14	8	-0.01	0.01	0.00	-0.03	-0.01	0.00	-0.05	-0.02	0.01
15	8	0.01	-0.02	0.00	-0.02	-0.01	0.00	0.00	0.02	0.00
16	8	0.00	0.00	0.00	-0.01	-0.03	0.00	0.00	0.01	0.00
17	1	-0.15	-0.22	-0.07	0.06	-0.02	-0.17	0.05	0.05	-0.01
18	1	0.12	-0.09	0.14	0.12	0.08	0.05	-0.06	0.02	-0.07
19	1	0.09	-0.03	0.01	0.24	0.37	-0.30	-0.01	-0.17	0.10
20	1	0.25	-0.26	-0.06	0.33	0.43	0.19	-0.05	-0.20	-0.08
21	1	0.02	-0.14	-0.10	0.03	-0.07	-0.08	0.08	0.04	0.06
22	1	0.11	-0.07	0.10	0.11	0.04	-0.13	0.04	0.04	-0.09
23	1	0.09	-0.43	0.16	0.08	0.23	-0.04	0.42	-0.02	0.13
24	1	0.03	-0.10	-0.06	0.09	0.13	-0.04	0.33	-0.09	-0.20
25	1	0.14	-0.36	0.00	0.03	-0.09	-0.01	-0.03	0.11	0.00
26	1	0.16	-0.45	0.01	0.04	0.04	0.06	0.02	0.01	0.02
27	1	-0.13	0.10	0.02	-0.07	0.06	0.01	-0.01	-0.01	0.00
28	1	-0.01	0.01	0.00	-0.03	0.30	-0.02	-0.06	0.65	-0.04
29	1	0.00	0.03	0.00	0.03	0.07	0.00	-0.01	-0.04	0.00

	67	68	69
	?A	?A	?A
Frequencies --	1639.3508	1891.5992	3211.3728
Red. masses --	1.1000	9.2129	1.0585
Frc consts --	1.7418	19.4226	6.4318
IR Inten --	6.2907	376.7859	37.9315
Raman Activ --	10.0325	72.7744	128.3630
Depolar --	0.6486	0.2284	0.2246

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z

1	6	-0.01	0.01	0.00	0.00	0.00	0.00	0.01	-0.01	0.00
2	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
4	6	0.01	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	-0.02	0.04	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	6	0.01	0.00	0.00	-0.01	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	-0.08	-0.06	0.01	0.00	0.00	0.00
10	6	0.00	0.00	0.00	-0.01	0.00	0.01	0.00	0.00	0.00
11	6	-0.07	-0.03	-0.04	0.00	0.00	0.00	-0.05	-0.02	-0.03
12	6	0.00	0.00	0.00	0.70	-0.05	-0.09	0.00	0.00	0.00
13	7	0.00	0.00	0.00	-0.43	0.04	0.05	0.00	0.00	0.00
14	8	0.00	0.00	0.00	0.01	0.02	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	-0.05	0.00	0.01	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
17	1	-0.02	0.00	-0.01	0.00	0.00	0.00	-0.12	0.13	-0.04
18	1	-0.02	0.00	-0.02	0.01	0.01	0.00	0.00	0.00	0.00
19	1	-0.01	0.00	0.00	0.01	0.02	-0.01	0.00	0.00	0.00
20	1	-0.03	-0.01	-0.01	0.00	0.02	0.00	0.00	0.00	0.00
21	1	-0.01	-0.01	-0.02	0.01	0.00	0.01	-0.01	-0.01	0.01
22	1	-0.01	-0.01	-0.01	0.00	0.00	0.00	0.00	-0.06	-0.01
23	1	-0.03	-0.01	-0.01	0.04	0.00	0.01	0.00	-0.01	-0.01
24	1	-0.01	0.00	0.00	0.03	0.00	-0.02	0.00	0.00	0.00
25	1	0.65	0.25	-0.12	-0.01	0.00	0.00	0.05	0.04	0.68
26	1	0.25	0.12	0.64	0.00	0.00	0.00	0.58	0.21	-0.32
27	1	0.00	0.00	0.00	-0.53	0.04	0.07	0.00	0.00	0.00

```
  28   1     0.00  -0.01   0.00    -0.01   0.00   0.00     0.00   0.00
0.00
  29   1     0.00   0.00   0.00     0.00  -0.01   0.00     0.00   0.00
0.00
                     70                    71                    72
                     ?A                    ?A                    ?A
 Frequencies --  3250.9102             3256.7862             3277.0680
 Red. masses --     1.0871                1.1069                1.0878
 Frc consts  --     6.7688                6.9172                6.8830
 IR Inten    --    32.0998               23.4182                8.3941
 Raman Activ --    95.1265               91.5607               57.4322
 Depolar     --     0.3485                0.7479                0.6540
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.05  -0.06   0.02     0.00   0.00   0.00    -0.01   0.01
0.00
   2   6    -0.01   0.00   0.01     0.00   0.00   0.00     0.01   0.00  -
0.01
   3   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   4   6     0.00   0.01  -0.02     0.00   0.00   0.00     0.00   0.02  -
0.06
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   7   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.01
0.00
   8   6     0.00   0.00   0.00     0.00   0.00   0.00    -0.02   0.02
0.05
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  11   6     0.01   0.00   0.00    -0.04  -0.01   0.08     0.00   0.00
0.00
  12   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  17   1    -0.59   0.70  -0.19    -0.01   0.01   0.00     0.10  -0.12
0.03
  18   1     0.14  -0.05  -0.12    -0.01   0.00   0.00    -0.10   0.03
0.09
  19   1     0.00   0.01   0.01     0.00   0.00   0.00     0.00   0.00  -
0.01
  20   1     0.00  -0.09   0.20     0.00  -0.01   0.02    -0.03  -0.29
0.66
```

21	1	-0.01	-0.01	0.01	0.00	-0.01	0.00	0.01	0.01	-0.01
22	1	0.00	0.06	0.01	0.00	0.00	0.00	-0.01	0.10	0.02
23	1	0.01	-0.01	-0.03	-0.01	0.01	0.02	0.20	-0.21	-0.58
24	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01
25	1	-0.01	-0.01	-0.11	-0.08	-0.05	-0.70	0.00	0.00	0.02
26	1	-0.11	-0.04	0.06	0.59	0.21	-0.30	0.01	0.01	-0.01
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

		73			74			75		
		?A			?A			?A		
Frequencies --		3284.7468			3291.9416			3297.5353		
Red. masses --		1.0888			1.0876			1.0883		
Frc consts --		6.9218			6.9445			6.9713		
IR Inten --		16.7546			22.9123			36.8634		
Raman Activ --		60.0453			124.2159			88.6789		
Depolar --		0.6474			0.2693			0.6644		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.01	0.00	-0.01	0.01	0.00	0.00	0.00	0.00
2	6	-0.05	0.02	0.04	-0.01	0.00	0.01	-0.03	0.01	0.03
3	6	0.00	-0.01	-0.02	0.00	-0.01	-0.01	0.00	-0.01	-0.01
4	6	0.00	0.00	0.01	0.00	0.02	-0.05	0.00	0.00	0.01
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.02	0.03	-0.03	0.00	0.00	0.00	-0.02	-0.04	0.04
7	6	0.00	-0.01	0.00	0.00	0.02	0.00	0.00	0.03	0.00
8	6	-0.01	0.01	0.02	0.02	-0.02	-0.05	-0.01	0.01	0.02
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.01	0.00	0.01	0.00	0.00	0.00	-0.01	0.01	-0.02
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  14   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  17   1     0.10  -0.12   0.04     0.09  -0.11   0.03     0.04  -0.05
0.01
  18   1     0.54  -0.19  -0.48     0.13  -0.05  -0.12     0.35  -0.12  -
0.31
  19   1     0.03   0.13   0.18     0.02   0.08   0.11     0.03   0.10
0.14
  20   1     0.00   0.03  -0.08    -0.02  -0.26   0.58     0.00   0.03  -
0.06
  21   1    -0.20  -0.33   0.34    -0.03  -0.04   0.05     0.27   0.45  -
0.46
  22   1    -0.01   0.15   0.02     0.02  -0.28  -0.05     0.02  -0.36  -
0.05
  23   1     0.06  -0.07  -0.18    -0.20   0.22   0.58     0.06  -0.07  -
0.18
  24   1    -0.07   0.05  -0.13     0.00   0.00  -0.01     0.11  -0.07
0.19
  25   1     0.00   0.00   0.02     0.00   0.00   0.03     0.00   0.00  -
0.02
  26   1     0.02   0.01  -0.01     0.00   0.00   0.00     0.01   0.00
0.00
  27   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  29   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     76                     77                     78
                     ?A                     ?A                     ?A
 Frequencies --  3306.8779              3312.5834              3323.5040
 Red. masses --     1.0887                 1.0896                 1.0918
 Frc consts  --     7.0142                 7.0448                 7.1054
 IR Inten    --    11.5227                35.2909                20.1449
 Raman Activ --    92.5125                90.0143               336.4376
 Depolar     --     0.4999                 0.3029                 0.0369
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   2   6     0.02   0.00  -0.01     0.00   0.00   0.00     0.02  -0.01  -
0.01
   3   6    -0.01  -0.03  -0.05    -0.01  -0.02  -0.03    -0.01  -0.03  -
0.04
   4   6     0.00   0.00   0.01     0.00   0.00  -0.01     0.00   0.00
0.01
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00  -0.01   0.01    -0.01  -0.02   0.02     0.01   0.02  -
0.02
```

7	6	0.00	0.01	0.00	0.00	-0.07	-0.01	0.00	0.02	0.00
8	6	0.00	0.00	0.00	0.01	-0.01	-0.02	0.00	0.00	0.01
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.03	-0.01	0.05	-0.01	0.01	-0.02	-0.03	0.02	-0.05
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	1	-0.04	0.04	-0.01	0.03	-0.04	0.01	-0.04	0.04	-0.01
18	1	-0.18	0.06	0.16	0.01	-0.01	-0.01	-0.17	0.06	0.15
19	1	0.12	0.39	0.56	0.07	0.23	0.32	0.09	0.29	0.41
20	1	0.00	0.03	-0.06	0.00	-0.03	0.06	0.00	0.03	-0.07
21	1	0.04	0.07	-0.07	0.11	0.18	-0.19	-0.14	-0.24	0.24
22	1	0.01	-0.15	-0.02	-0.05	0.78	0.12	0.02	-0.28	-0.04
23	1	0.02	-0.02	-0.05	-0.07	0.07	0.19	0.03	-0.04	-0.10
24	1	-0.31	0.18	-0.53	0.12	-0.07	0.20	0.32	-0.19	0.55
25	1	0.00	0.00	-0.02	0.01	0.00	0.05	0.00	0.00	-0.02
26	1	-0.01	0.00	0.01	0.04	0.01	-0.02	-0.02	-0.01	0.01
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	79	80	81
	?A	?A	?A
Frequencies --	3670.2860	3773.7908	3885.6121
Red. masses --	1.0765	1.0657	1.0673
Frc consts --	8.5443	8.9423	9.4939
IR Inten --	47.2213	138.6366	64.8589
Raman Activ --	168.5803	52.2839	67.3197
Depolar --	0.3240	0.1729	0.2258

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	7	-0.05	-0.05	0.01	0.00	0.00	0.00	0.00	0.00	0.00
14	8	0.00	0.00	0.00	-0.06	0.00	0.01	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.00	0.00	0.00	0.06	-0.02	0.00
17	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
18	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
22	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
23	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
25	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
26	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  27   1     0.64   0.75  -0.14     0.01   0.02   0.00     0.00   0.00
0.00
  28   1    -0.02   0.00   0.00     0.99   0.00  -0.12     0.00   0.00
0.00
  29   1     0.00   0.00   0.00     0.00   0.00   0.00    -0.97   0.24  -
0.01

 -------------------
 - Thermochemistry -
 -------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Atom  1 has atomic number  6 and mass  12.00000
 Atom  2 has atomic number  6 and mass  12.00000
 Atom  3 has atomic number  6 and mass  12.00000
 Atom  4 has atomic number  6 and mass  12.00000
 Atom  5 has atomic number  6 and mass  12.00000
 Atom  6 has atomic number  6 and mass  12.00000
 Atom  7 has atomic number  6 and mass  12.00000
 Atom  8 has atomic number  6 and mass  12.00000
 Atom  9 has atomic number  6 and mass  12.00000
 Atom 10 has atomic number  6 and mass  12.00000
 Atom 11 has atomic number  6 and mass  12.00000
 Atom 12 has atomic number  6 and mass  12.00000
 Atom 13 has atomic number  7 and mass  14.00307
 Atom 14 has atomic number  8 and mass  15.99491
 Atom 15 has atomic number  8 and mass  15.99491
 Atom 16 has atomic number  8 and mass  15.99491
 Atom 17 has atomic number  1 and mass   1.00783
 Atom 18 has atomic number  1 and mass   1.00783
 Atom 19 has atomic number  1 and mass   1.00783
 Atom 20 has atomic number  1 and mass   1.00783
 Atom 21 has atomic number  1 and mass   1.00783
 Atom 22 has atomic number  1 and mass   1.00783
 Atom 23 has atomic number  1 and mass   1.00783
 Atom 24 has atomic number  1 and mass   1.00783
 Atom 25 has atomic number  1 and mass   1.00783
 Atom 26 has atomic number  1 and mass   1.00783
 Atom 27 has atomic number  1 and mass   1.00783
 Atom 28 has atomic number  1 and mass   1.00783
 Atom 29 has atomic number  1 and mass   1.00783
 Molecular mass:   219.08954 amu.
 Principal axes and moments of inertia in atomic units:
                          1         2         3
     EIGENVALUES --  1951.39712 2511.56200 3451.27208
           X            0.99998  -0.00111   0.00587
           Y            0.00108   0.99999   0.00536
           Z           -0.00587  -0.00535   0.99997
 THIS MOLECULE IS AN ASYMMETRIC TOP.
 ROTATIONAL SYMMETRY NUMBER  1.
 WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
           MAY CAUSE SIGNIFICANT ERROR
 ROTATIONAL TEMPERATURES (KELVIN)      0.04439     0.03449     0.02510
 ROTATIONAL CONSTANTS (GHZ)            0.92485     0.71857     0.52292
    1 IMAGINARY FREQUENCIES IGNORED.
```

Zero-point vibrational energy 668127.9 (Joules/Mol)
159.68641 (Kcal/Mol)
WARNING-- EXPLICIT CONSIDERATION OF 14 DEGREES OF FREEDOM AS VIBRATIONS MAY CAUSE SIGNIFICANT ERROR

VIBRATIONAL TEMPERATURES: (KELVIN)	185.41	366.12	384.46	431.97	463.62
	506.44	528.06	644.82	676.06	697.05
	727.82	787.48	798.93	844.37	920.01
	994.03	1032.42	1070.32	1116.82	1174.59
	1195.41	1228.43	1272.39	1304.16	1337.13
	1364.38	1422.97	1436.83	1447.65	1454.88
	1469.44	1484.46	1491.58	1497.29	1507.46
	1539.33	1551.97	1593.22	1676.84	1702.25
	1740.73	1749.24	1766.10	1789.81	1808.05
	1818.92	1826.87	1873.17	1907.23	1934.36
	1946.11	1954.16	1959.42	1985.88	2000.46
	2008.33	2018.01	2042.42	2050.43	2062.86
	2079.21	2091.90	2104.44	2116.62	2158.57
	2358.65	2721.57	4620.42	4677.31	4685.76
	4714.94	4725.99	4736.34	4744.13	4757.83
	4766.04	4781.75	5280.69	5429.61	5590.50

Zero-point correction= 0.254476
(Hartree/Particle)
Thermal correction to Energy= 0.263579
Thermal correction to Enthalpy= 0.264524
Thermal correction to Gibbs Free Energy= 0.220272
Sum of electronic and zero-point Energies= -736.740360
Sum of electronic and thermal Energies= -736.731257
Sum of electronic and thermal Enthalpies= -736.730313
Sum of electronic and thermal Free Energies= -736.774564

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	165.399	41.835	93.134
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	42.056
ROTATIONAL	0.889	2.981	31.204
VIBRATIONAL	163.621	35.874	19.874
VIBRATION 1	0.611	1.924	2.963
VIBRATION 2	0.665	1.755	1.699
VIBRATION 3	0.672	1.733	1.614
VIBRATION 4	0.693	1.673	1.416
VIBRATION 5	0.707	1.631	1.299
VIBRATION 6	0.729	1.571	1.157
VIBRATION 7	0.740	1.540	1.092
VIBRATION 8	0.807	1.365	0.801
VIBRATION 9	0.827	1.317	0.738
VIBRATION 10	0.841	1.284	0.698
VIBRATION 11	0.861	1.237	0.644
VIBRATION 12	0.903	1.146	0.550
VIBRATION 13	0.911	1.128	0.533
VIBRATION 14	0.944	1.060	0.473

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.481258-101	-101.317622	-233.292447

TOTAL V=0		0.540313D+16	15.732646	36.225756
VIB (BOT)		0.256449-115	-115.590999	-266.158111
VIB (BOT)	1	0.158246D+01	0.199334	0.458983
VIB (BOT)	2	0.765359D+00	-0.116135	-0.267411
VIB (BOT)	3	0.724266D+00	-0.140102	-0.322596
VIB (BOT)	4	0.633352D+00	-0.198355	-0.456729
VIB (BOT)	5	0.582588D+00	-0.234638	-0.540275
VIB (BOT)	6	0.523470D+00	-0.281108	-0.647275
VIB (BOT)	7	0.497052D+00	-0.303598	-0.699061
VIB (BOT)	8	0.383206D+00	-0.416568	-0.959183
VIB (BOT)	9	0.359006D+00	-0.444898	-1.024416
VIB (BOT)	10	0.343884D+00	-0.463588	-1.067450
VIB (BOT)	11	0.323203D+00	-0.490525	-1.129475
VIB (BOT)	12	0.287461D+00	-0.541421	-1.246669
VIB (BOT)	13	0.281181D+00	-0.551015	-1.268758
VIB (BOT)	14	0.257868D+00	-0.588603	-1.355308
VIB (V=0)		0.287918D+02	1.459269	3.360091
VIB (V=0)	1	0.215958D+01	0.334368	0.769912
VIB (V=0)	2	0.141421D+01	0.150513	0.346569
VIB (V=0)	3	0.138009D+01	0.139908	0.322150
VIB (V=0)	4	0.130693D+01	0.116252	0.267680
VIB (V=0)	5	0.126773D+01	0.103027	0.237228
VIB (V=0)	6	0.122389D+01	0.087743	0.202037
VIB (V=0)	7	0.120503D+01	0.080996	0.186500
VIB (V=0)	8	0.112996D+01	0.053062	0.122180
VIB (V=0)	9	0.111554D+01	0.047484	0.109336
VIB (V=0)	10	0.110684D+01	0.044085	0.101510
VIB (V=0)	11	0.109537D+01	0.039559	0.091088
VIB (V=0)	12	0.107674D+01	0.032112	0.073942
VIB (V=0)	13	0.107364D+01	0.030859	0.071054
VIB (V=0)	14	0.106258D+01	0.026361	0.060700
ELECTRONIC		0.100000D+01	0.000000	0.000000
TRANSLATIONAL		0.127466D+09	8.105393	18.663357
ROTATIONAL		0.147226D+07	6.167984	14.202307

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000003447	0.000000295	0.000004447
2	6	0.000005292	0.000004072	0.000001116
3	6	0.000005524	-0.000003144	0.000003472
4	6	-0.000000731	-0.000006986	-0.000003599
5	6	-0.000014417	0.000023233	0.000003659
6	6	0.000001361	-0.000000897	-0.000000991
7	6	0.000003502	-0.000001261	0.000000836
8	6	-0.000000369	0.000007508	-0.000004716
9	6	-0.000006981	-0.000007250	-0.000000101
10	6	-0.000001663	0.000006077	0.000002007
11	6	0.000004010	0.000000814	-0.000006137
12	6	-0.000011756	0.000006126	0.000003029
13	7	-0.000004907	0.000002874	0.000003913
14	8	0.000004766	-0.000002471	0.000001142
15	8	0.000013474	-0.000011035	-0.000000915

16	8	-0.000001265	-0.000013484	-0.000001315
17	1	0.000000315	-0.000000632	-0.000000152
18	1	0.000001223	-0.000000164	-0.000000055
19	1	-0.000000184	0.000000849	0.000000466
20	1	-0.000001608	0.000001856	-0.000001021
21	1	0.000000293	0.000000459	0.000000560
22	1	0.000000569	0.000000212	-0.000001301
23	1	0.000000418	-0.000000080	-0.000000330
24	1	-0.000000341	-0.000000218	0.000001046
25	1	-0.000000723	-0.000001159	-0.000000513
26	1	0.000001431	0.000000316	0.000000249
27	1	-0.000000061	-0.000000739	-0.000003342
28	1	0.000004825	-0.000006934	-0.000001513
29	1	0.000001449	0.000001761	0.000000058

Cartesian Forces: Max 0.000023233 RMS 0.000004926

Internal Coordinate Forces (Hartree/Bohr or radian)

Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	C	-0.000003(	1)	0.000000(	30)	0.000004(	59)	
2	C	0.000005(	2)	0.000004(	31)	0.000001(	60)	
3	C	0.000006(	3)	-0.000003(	32)	0.000003(	61)	
4	C	-0.000001(	4)	-0.000007(	33)	-0.000004(	62)	
5	C	-0.000014(	5)	0.000023(	34)	0.000004(	63)	
6	C	0.000001(	6)	-0.000001(	35)	-0.000001(	64)	
7	C	0.000004(	7)	-0.000001(	36)	0.000001(	65)	
8	C	0.000000(	8)	0.000008(	37)	-0.000005(	66)	
9	C	-0.000007(	9)	-0.000007(	38)	0.000000(	67)	
10	C	-0.000002(	10)	0.000006(	39)	0.000002(	68)	
11	C	0.000004(	11)	0.000001(	40)	-0.000006(	69)	
12	C	-0.000012(	12)	0.000006(	41)	0.000003(	70)	
13	N	-0.000005(	13)	0.000003(	42)	0.000004(	71)	
14	O	0.000005(	14)	-0.000002(	43)	0.000001(	72)	
15	O	0.000013(	15)	-0.000011(	44)	-0.000001(	73)	
16	O	-0.000001(	16)	-0.000013(	45)	-0.000001(	74)	
17	H	0.000000(	17)	-0.000001(	46)	0.000000(	75)	
18	H	0.000001(	18)	0.000000(	47)	0.000000(	76)	
19	H	0.000000(	19)	0.000001(	48)	0.000000(	77)	
20	H	-0.000002(	20)	0.000002(	49)	-0.000001(	78)	
21	H	0.000000(	21)	0.000000(	50)	0.000001(	79)	
22	H	0.000001(	22)	0.000000(	51)	-0.000001(	80)	
23	H	0.000000(	23)	0.000000(	52)	0.000000(	81)	
24	H	0.000000(	24)	0.000000(	53)	0.000001(	82)	
25	H	-0.000001(	25)	-0.000001(	54)	-0.000001(	83)	
26	H	0.000001(	26)	0.000000(	55)	0.000000(	84)	
27	H	0.000000(	27)	-0.000001(	56)	-0.000003(	85)	
28	H	0.000005(	28)	-0.000007(	57)	-0.000002(	86)	
29	H	0.000001(	29)	0.000002(	58)	0.000000(	87)	

Internal Forces: Max 0.000023233 RMS 0.000004926

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

```
Search for a local minimum.
Step number   1 out of a maximum of  97
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
    Eigenvalues ---   -0.00206   0.00350   0.00935   0.01075   0.01234
    Eigenvalues ---    0.01617   0.01764   0.02262   0.02676   0.03940
    Eigenvalues ---    0.04079   0.04458   0.04500   0.04687   0.04706
    Eigenvalues ---    0.04795   0.04840   0.04959   0.05059   0.05165
    Eigenvalues ---    0.05231   0.05324   0.05476   0.05574   0.05981
    Eigenvalues ---    0.06487   0.06829   0.06999   0.08498   0.09480
    Eigenvalues ---    0.10575   0.10877   0.12125   0.14333   0.15090
    Eigenvalues ---    0.16367   0.18353   0.19075   0.19369   0.20422
    Eigenvalues ---    0.23268   0.24329   0.25646   0.27630   0.29462
    Eigenvalues ---    0.32988   0.36457   0.38119   0.38681   0.40451
    Eigenvalues ---    0.41681   0.49307   0.50342   0.50826   0.52395
    Eigenvalues ---    0.53457   0.57884   0.58956   0.61869   0.63576
    Eigenvalues ---    0.66896   0.67620   0.72250   0.75120   0.77738
    Eigenvalues ---    0.81984   0.87456   0.88815   0.90198   0.94328
    Eigenvalues ---    0.95217   0.96699   0.97898   0.99327   1.01950
    Eigenvalues ---    1.05262   1.06613   1.09571   1.10198   1.15942
    Eigenvalues ---    1.81143
Eigenvalue   1 out of range, new value =    0.002064 Eigenvector:
                          1
          X1          -0.00634
          Y1           0.00730
          Z1           0.03499
          X2           0.00970
          Y2          -0.01434
          Z2           0.02614
          X3           0.01173
          Y3          -0.02825
          Z3           0.02418
          X4          -0.00849
          Y4           0.02681
          Z4           0.02712
          X5           0.00010
          Y5           0.00233
          Z5           0.04189
          X6           0.00364
          Y6          -0.01612
          Z6           0.00134
          X7           0.00145
          Y7           0.01013
          Z7          -0.00458
          X8          -0.00131
          Y8           0.02370
          Z8           0.00446
          X9           0.00108
          Y9           0.00004
          Z9          -0.00239
          X10          0.00560
          Y10         -0.02493
          Z10          0.00498
          X11         -0.00177
```

Y11	0.01303
Z11	0.01174
X12	0.00221
Y12	0.00119
Z12	0.01134
X13	0.00221
Y13	0.00039
Z13	0.01066
X14	-0.00442
Y14	-0.00082
Z14	-0.03961
X15	0.00052
Y15	0.00013
Z15	0.01256
X16	-0.00697
Y16	0.00078
Z16	0.16381
X17	-0.02450
Y17	0.00236
Z17	0.05946
X18	0.01790
Y18	-0.01562
Z18	0.03407
X19	0.00957
Y19	-0.02432
Z19	0.01929
X20	-0.01189
Y20	0.02404
Z20	0.02232
X21	0.00092
Y21	-0.02579
Z21	-0.00974
X22	0.00703
Y22	0.01334
Z22	-0.02387
X23	-0.00391
Y23	0.04257
Z23	-0.00332
X24	0.00657
Y24	-0.04214
Z24	-0.00359
X25	-0.00422
Y25	0.02866
Z25	0.01141
X26	0.00020
Y26	0.00313
Z26	0.01040
X27	0.00378
Y27	0.00031
Z27	0.01924
X28	-0.00187
Y28	-0.00007
Z28	-0.02180
X29	-0.01778

```
          Y29         -0.00995
          Z29         -0.97278
 Angle between quadratic step and forces=  71.70 degrees.
 Linear search not attempted -- first point.
 TrRot= -0.000002  0.000000  0.000009  0.000000 -0.000001  0.000000
```

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
X1	-3.76911	0.00000	0.00000	-0.00001	-0.00001	-3.76911
Y1	1.46357	0.00000	0.00000	-0.00001	-0.00001	1.46356
Z1	-0.80273	0.00000	0.00000	0.00001	0.00001	-0.80272
X2	-3.20035	0.00001	0.00000	0.00000	0.00000	-3.20035
Y2	0.90111	0.00000	0.00000	0.00001	0.00001	0.90112
Z2	2.02965	0.00000	0.00000	0.00001	0.00001	2.02966
X3	-0.35477	0.00001	0.00000	0.00000	-0.00001	-0.35477
Y3	1.56835	0.00000	0.00000	0.00001	0.00001	1.56836
Z3	2.51367	0.00000	0.00000	0.00002	0.00003	2.51370
X4	-1.06637	0.00000	0.00000	0.00000	0.00000	-1.06637
Y4	1.44154	-0.00001	0.00000	0.00001	0.00001	1.44154
Z4	-1.94213	0.00000	0.00000	0.00001	0.00002	-1.94211
X5	0.56297	-0.00001	0.00000	-0.00003	-0.00003	0.56293
Y5	2.76355	0.00002	0.00000	0.00005	0.00004	2.76360
Z5	0.05286	0.00000	0.00000	0.00002	0.00003	0.05289
X6	-2.50661	0.00000	0.00000	0.00000	0.00000	-2.50661
Y6	-1.99235	0.00000	0.00000	0.00000	0.00000	-1.99235
Z6	2.00451	0.00000	0.00000	0.00000	0.00000	2.00451
X7	-2.76122	0.00000	0.00000	0.00004	0.00004	-2.76118
Y7	-2.71947	0.00000	0.00000	0.00000	0.00000	-2.71947
Z7	-0.82038	0.00000	0.00000	-0.00001	-0.00001	-0.82038
X8	-0.37685	0.00000	0.00000	0.00003	0.00003	-0.37682
Y8	-1.45286	0.00001	0.00000	0.00002	0.00002	-1.45283
Z8	-1.95628	0.00000	0.00000	0.00001	0.00001	-1.95627
X9	1.70049	-0.00001	0.00000	-0.00001	-0.00001	1.70048
Y9	-1.95596	-0.00001	0.00000	-0.00002	-0.00003	-1.95598
Z9	0.01324	0.00000	0.00000	0.00005	0.00006	0.01330
X10	0.32875	0.00000	0.00000	-0.00002	-0.00002	0.32873
Y10	-1.31305	0.00001	0.00000	0.00001	0.00001	-1.31304
Z10	2.48507	0.00000	0.00000	0.00003	0.00004	2.48511
X11	-4.93452	0.00000	0.00000	0.00004	0.00004	-4.93448
Y11	-1.02754	0.00000	0.00000	-0.00001	-0.00001	-1.02755
Z11	-1.75120	-0.00001	0.00000	-0.00004	-0.00004	-1.75124
X12	3.90586	-0.00001	0.00000	-0.00005	-0.00005	3.90580
Y12	-0.21947	0.00001	0.00000	0.00000	-0.00001	-0.21947
Z12	-0.37548	0.00000	0.00000	0.00003	0.00004	-0.37544
X13	6.11886	0.00000	0.00000	-0.00007	-0.00007	6.11879
Y13	-0.98564	0.00000	0.00000	-0.00001	-0.00001	-0.98566
Z13	-0.68523	0.00000	0.00000	-0.00007	-0.00006	-0.68528
X14	2.45970	0.00000	0.00000	0.00002	0.00002	2.45972
Y14	-4.54429	0.00000	0.00000	-0.00003	-0.00003	-4.54432
Z14	-0.04474	0.00000	0.00000	0.00008	0.00009	-0.04464
X15	3.21471	0.00001	0.00000	0.00000	0.00000	3.21471
Y15	2.28039	-0.00001	0.00000	-0.00002	-0.00002	2.28038
Z15	-0.34839	0.00000	0.00000	0.00003	0.00004	-0.34835
X16	0.39989	0.00000	0.00000	0.00002	0.00002	0.39991
Y16	5.44499	-0.00001	0.00000	0.00000	0.00000	5.44499

Z16	0.00355	0.00000	0.00000	-0.00001	0.00000	0.00355
X17	-4.84963	0.00000	0.00000	-0.00001	-0.00001	-4.84964
Y17	3.16103	0.00000	0.00000	-0.00002	-0.00002	3.16101
Z17	-1.16673	0.00000	0.00000	-0.00001	0.00000	-1.16673
X18	-4.59769	0.00000	0.00000	0.00001	0.00000	-4.59769
Y18	1.55802	0.00000	0.00000	0.00000	0.00000	1.55802
Z18	3.36089	0.00000	0.00000	0.00002	0.00002	3.36091
X19	0.16082	0.00000	0.00000	-0.00002	-0.00003	0.16079
Y19	2.63303	0.00000	0.00000	0.00002	0.00002	2.63305
Z19	4.17154	0.00000	0.00000	0.00003	0.00004	4.17158
X20	-0.89225	0.00000	0.00000	-0.00004	-0.00003	-0.89229
Y20	2.31509	0.00000	0.00000	0.00003	0.00003	2.31512
Z20	-3.77935	0.00000	0.00000	0.00001	0.00002	-3.77933
X21	-3.44097	0.00000	0.00000	-0.00001	-0.00002	-3.44098
Y21	-3.22978	0.00000	0.00000	0.00000	0.00000	-3.22978
Z21	3.32632	0.00000	0.00000	-0.00001	-0.00001	3.32632
X22	-2.89486	0.00000	0.00000	0.00007	0.00007	-2.89479
Y22	-4.71828	0.00000	0.00000	0.00000	0.00000	-4.71828
Z22	-1.19306	0.00000	0.00000	-0.00003	-0.00003	-1.19309
X23	0.14218	0.00000	0.00000	0.00006	0.00006	0.14224
Y23	-2.14324	0.00000	0.00000	0.00003	0.00003	-2.14321
Z23	-3.80547	0.00000	0.00000	0.00001	0.00002	-3.80545
X24	1.25377	0.00000	0.00000	-0.00004	-0.00005	1.25372
Y24	-2.06918	0.00000	0.00000	0.00002	0.00002	-2.06916
Z24	4.13386	0.00000	0.00000	0.00005	0.00006	4.13393
X25	-5.17693	0.00000	0.00000	0.00007	0.00007	-5.17685
Y25	-1.07349	0.00000	0.00000	-0.00001	-0.00001	-1.07350
Z25	-3.78540	0.00000	0.00000	-0.00005	-0.00004	-3.78545
X26	-6.72161	0.00000	0.00000	0.00004	0.00004	-6.72157
Y26	-1.45552	0.00000	0.00000	-0.00004	-0.00004	-1.45556
Z26	-0.84453	0.00000	0.00000	-0.00007	-0.00007	-0.84459
X27	7.46297	0.00000	0.00000	-0.00009	-0.00009	7.46288
Y27	0.34777	0.00000	0.00000	-0.00003	-0.00003	0.34774
Z27	-0.92690	0.00000	0.00000	-0.00023	-0.00021	-0.92711
X28	4.27613	0.00000	0.00000	0.00000	-0.00001	4.27613
Y28	-4.68235	-0.00001	0.00000	-0.00009	-0.00009	-4.68244
Z28	-0.29874	0.00000	0.00000	-0.00013	-0.00012	-0.29886
X29	-1.31802	0.00000	0.00000	0.00005	0.00005	-1.31797
Y29	6.06310	0.00000	0.00000	0.00009	0.00009	6.06319
Z29	0.01596	0.00000	0.00000	0.00002	0.00003	0.01599

Item	Value	Threshold	Converged?
Maximum Force	0.000023	0.000450	YES
RMS Force	0.000005	0.000300	YES
Maximum Displacement	0.000212	0.001800	YES
RMS Displacement	0.000044	0.001200	YES

Predicted change in Energy=-2.998824D-09
Optimization completed.
   -- Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1|1|UNPC-UNK|Freq|RHF|3-21+G*|C12H13N1O3|PCUSER|05-Mar-2002|0||#N RHF/
3-21+G* FREQ||Freq calc of output of mech1s10ts2||0,1|C,-1.9945250259,
0.774488931,-0.4247869052|C,-1.6935510259,0.476847931,1.0740450948|C,-
0.1877350259,0.829935931,1.3301760948|C,-0.5643000259,0.762827931,-1.0

277309052|C,0.2979089741,1.462407931,0.0279700948|C,-1.3264410259,-1.0
54307069,1.0607400948|C,-1.4611740259,-1.439084069,-0.4341239052|C,-0.
1994200259,-0.768818069,-1.0352189052|C,0.8998609741,-1.035049069,0.00
70050948|C,0.1739649741,-0.694836069,1.3150430948|C,-2.6112380259,-0.5
43749069,-0.9266969052|C,2.0668899741,-0.116136069,-0.1986969052|N,3.2
379629741,-0.521580069,-0.3626069052|O,1.3016189741,-2.404735069,-0.02
36729052|O,1.7011539741,1.206732931,-0.1843589052|O,0.2116129741,2.881
363931,0.0018810948|H,-2.5663130259,1.672742931,-0.6174059052|H,-2.432
9940259,0.824469931,1.7785090948|H,0.0851009741,1.393338931,2.20748509
48|H,-0.4721610259,1.225091931,-1.9999469052|H,-1.8208810259,-1.709127
069,1.7602140948|H,-1.5318930259,-2.496806069,-0.6313419052|H,0.075235
9741,-1.134156069,-2.0137679052|H,0.6634659741,-1.094963069,2.18754709
48|H,-2.7395110259,-0.568065069,-2.0031489052|H,-3.5569210259,-0.77022
6069,-0.4469039052|H,3.9492329741,0.184029931,-0.4904949052|H,2.262830
9741,-2.477793069,-0.1580879052|H,-0.6974650259,3.208453931,0.00844609
48||Version=x86-Win32-G98RevA.7|HF=-736.9948362|RMSD=6.818e-009|RMSF=4
.926e-006|Dipole=-1.8022989,0.3399502,0.1277163|DipoleDeriv=0.0474974,
-0.0554142,0.0203838,-0.0996406,0.1007132,-0.0293652,0.0045862,-0.0416
732,0.0131903,0.0875661,-0.0047335,-0.0699874,0.0174961,-0.0197801,0.0
287291,-0.0344425,0.0567225,0.0712069,-0.0909368,0.0264652,0.0165944,-
0.003235,-0.112937,0.0725569,0.0141458,0.1171558,-0.0131066,-0.1018796
,0.0163851,0.0112319,0.007086,-0.1197323,-0.0828633,-0.0123322,-0.1502
267,0.0126088,1.1234377,-0.2588947,-0.0688365,-0.1519247,1.2097779,-0.
0057076,-0.0680902,-0.0164069,0.5811733,0.0713171,0.0259776,-0.0556755
,0.017214,0.0687162,-0.0642093,0.0229329,-0.0851844,0.0533993,0.039023
7,-0.009514,0.0204287,0.0454516,0.095297,0.0232382,-0.0202125,0.036048
,0.029556,0.0126511,-0.0257,-0.0079354,-0.0825144,0.0426036,0.0680687,
0.0050419,0.0861564,0.0725272,0.1948164,-0.2469861,0.0135784,-0.246335
9,0.5139993,0.0224624,0.0261422,0.0430538,0.2579852,-0.0139713,0.00066
85,0.0319646,-0.0675566,0.0463475,-0.0278606,-0.0249008,-0.0539622,0.0
725498,0.0561155,0.0522656,-0.0459042,0.0346106,-0.0169863,-0.003101,-
0.0587903,-0.0082807,0.1496551,1.6556547,-0.3039585,-0.1873155,-0.8266
846,0.9910618,0.0953527,-0.1935151,0.0192938,0.2538581,-1.5803992,0.26
69272,0.1190381,0.3565209,-0.5161741,-0.0530832,0.1367619,-0.0421764,-
0.6235264,-0.6119394,0.2839355,-0.0136864,0.3224658,-0.9081832,-0.0268
728,-0.0086356,-0.0275872,-0.5987601,-1.260138,0.2098194,0.0971964,0.8
349112,-1.0573333,-0.0971462,0.1008963,-0.0035794,-0.4019968,-0.368001
8,0.0960567,-0.0009248,0.0713721,-1.2240638,0.0087369,-0.0167707,0.019
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 ,-0.00003262,-0.00002968,-0.00005644,0.00007002,0.00005932,-0.00014375
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 00000022,-0.00000105,0.00000072,0.00000116,0.00000051,-0.00000143,-0.0
 0000032,-0.00000025,0.00000006,0.00000074,0.00000334,-0.00000482,0.000
 00693,0.00000151,-0.00000145,-0.00000176,-0.00000006|||@


 HICKORY, DICKORY, DOCK
 TWO MICE RAN UP THE CLOCK
 THE CLOCK STRUCK ONE...
 THE OTHER ESCAPED WITH MINOR INJURIES.
 Job cpu time:  0 days 20 hours 13 minutes  1.0 seconds.
 File lengths (MBytes):  RWF=  218 Int=    0 D2E=    0 Chk=    6 Scr=
1
 Normal termination of Gaussian 98.
```

```
%nproc=2
%chk=mech1s8ts
%nosave

#N RHF/3-21+G* OPT=(TS,NOEIGENTEST,GDIIS) OPTCYC=200

TS search from mech1s8@1.83A

-1   1
 C                 -0.418738   -0.423296   -2.192870
 C                 -0.417627    1.070219   -1.766007
 C                  0.810680    1.296352   -0.832437
 C                  0.432528   -1.067584   -1.076089
 C                  1.506978   -0.058457   -0.663816
 C                 -1.367081    1.082341   -0.505197
 C                 -1.802663   -0.399155   -0.376415
 C                 -0.519461   -1.049741    0.183404
 C                  0.151094   -0.021212    1.143246
 C                 -0.132606    1.319306    0.419366
 C                 -1.849370   -0.875128   -1.845176
 O                  2.777259   -0.202355   -1.303007
 C                  0.085048   -0.153903    2.582548
 N                  0.553316   -0.360113    3.662138
 O                  1.637679   -0.224607    0.737955
 H                 -0.068218   -0.614776   -3.199059
 H                 -0.606141    1.779451   -2.560391
 H                  1.480256    2.123675   -1.006052
 H                  0.840860   -2.040646   -1.308706
 H                 -2.171281    1.803585   -0.475805
 H                 -2.683888   -0.567797    0.215970
 H                 -0.659268   -2.016091    0.644100
 H                 -0.118628    2.178884    1.066362
 H                 -1.988982   -1.948867   -1.938098
 H                 -2.609630   -0.362559   -2.429920
 H                  3.445570   -0.377895   -0.625431
 O                 -1.362196    0.178310    2.152726
 H                 -2.028510    0.234588    2.857314
```

```
%chk=mech1s10ts2

#N RHF/3-21+G* OPT=(TS,NOEIGENTEST,GDIIS) OPTCYC=200

TS search for mech1str10 using input@1.2964A from m1s10S2 optcyc=200

0   1
 C                    -1.97597   0.75064  -0.45984
 C                    -1.69146   0.47912   1.04625
 C                    -0.18942   0.83524   1.30743
 C                    -0.54177   0.72104  -1.04702
 C                     0.29255   1.45708  -0.00411
 C                    -1.3302   -1.05254   1.0695
 C                    -1.4527   -1.46754  -0.41959
 C                    -0.17897  -0.81695  -1.02027
 C                     0.90639  -1.09586   0.04084
 C                     0.17143  -0.69551   1.33028
 C                    -2.5921   -0.57428  -0.9415
 C                     2.07825  -0.22557  -0.17461
 N                     3.3014   -0.1458   -0.37117
 O                     1.24611  -2.48987   0.05639
 O                     1.70939   1.17551  -0.18045
 O                     0.081     2.84748  -0.11859
 H                    -2.5193    1.65869  -0.66873
 H                    -2.43411   0.84839   1.73526
 H                     0.06991   1.40139   2.18938
 H                    -0.44118   1.16381  -2.02627
 H                    -1.83053  -1.6938    1.77725
 H                    -1.52838  -2.52872  -0.59508
 H                     0.10131  -1.19871  -1.99113
 H                     0.64726  -1.07078   2.22172
 H                    -2.70922  -0.62059  -2.01862
 H                    -3.54386  -0.78986  -0.46864
 H                     2.97706   0.98999  -0.37855
 H                     2.19037  -2.66084  -0.075
 H                     0.64249   3.36747   0.47358
```

```
%nproc=2
# opt=(calcfc,gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity
optcyc=200

TS search for mech1s8 using input@1.73A from mech1st8.out
optcyc=200&calcfc

-1  1
 C                  -2.004865   -0.451353   -0.472354
 C                  -1.623268   -0.466960    1.039985
 C                  -0.621791    0.708529    1.263803
 C                  -0.822957    0.352455   -1.065675
 C                  -0.621758    1.498558   -0.052012
 C                  -0.433302   -1.495562    1.088687
 C                  -0.304316   -1.945961   -0.398177
 C                   0.375574   -0.679634   -1.023239
 C                   1.433955   -0.340532    0.054975
 C                   0.573438   -0.302818    1.320262
 C                  -1.747730   -1.894546   -0.918230
 O                  -1.941322    2.228591   -0.057165
 C                   2.405958    0.725715   -0.205055
 N                   3.314001    1.391849   -0.396231
 O                   0.389125    2.353582   -0.262189
 H                  -2.967975   -0.020539   -0.688700
 H                  -2.449352   -0.600345    1.723487
 H                  -0.742905    1.341993    2.127301
 H                  -0.991395    0.733789   -2.062007
 H                  -0.456025   -2.293449    1.817293
 H                   0.203252   -2.889262   -0.562097
 H                   0.822311   -0.848420   -1.994988
 H                   1.168261   -0.317724    2.219833
 H                  -1.814106   -2.026493   -1.994436
 H                  -2.389474   -2.620074   -0.424692
 H                  -1.689443    3.154666   -0.180641
 O                   2.358792   -1.494525    0.213984
 H                   2.002457   -2.305612   -0.161599

 1  2 1.0  4 1.0  11 1.0  16 1.0
 2  3 1.0  6 1.0  17 1.0
 3  5 1.0  10 1.0  18 1.0
 4  5 1.0  8 1.0  19 1.0
 5  12 1.0  15 1.5
 6  7 1.0  10 1.0  20 1.0
 7  8 1.0  11 1.0  21 1.0
 8  9 1.0  22 1.0
 9  10 1.0  13 1.0  27 1.0
 10  23 1.0
 11  24 1.0  25 1.0
 12  26 1.0
 13  14 3.0
 14
 15
 16
 17
```

```
18
19
20
21
22
23
24
25
26
27  28 1.0
28
```

```
%chk=mech1s10ts3
# opt=(calcfc,gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity
optcyc=200

TS search for mech1str10 using input@1.2964A from m1s10S2
optcyc=200&calcfc

0  1
 C                  0.000000    0.000000    0.000000
 C                  0.000000    0.000000    1.557673
 C                  1.495807    0.000000    2.018499
 C                  1.426546   -0.532911   -0.301406
 C                  2.293215    0.180827    0.729771
 C                 -0.106176   -1.528451    1.914422
 C                 -0.160720   -2.211471    0.522071
 C                  1.313977   -2.068257    0.061051
 C                  2.112547   -2.404747    1.342441
 C                  1.393350   -1.527803    2.374862
 C                 -0.912197   -1.188311   -0.346365
 C                  3.549304   -2.081457    1.177199
 N                  4.710546   -2.394367    1.048354
 O                  1.923848   -3.785905    1.702143
 O                  3.552919   -0.515919    0.914861
 O                  2.509319    1.516974    0.333055
 H                 -0.221004    0.950464   -0.459643
 H                 -0.682740    0.692462    2.023622
 H                  1.799616    0.653450    2.822627
 H                  1.771943   -0.359500   -1.309469
 H                 -0.854476   -1.847188    2.621940
 H                 -0.522832   -3.226482    0.525203
 H                  1.585460   -2.710244   -0.764994
 H                  1.621053   -1.803388    3.391406
 H                 -0.902042   -1.437624   -1.401809
 H                 -1.936697   -1.036952   -0.024579
 H                  4.696295   -0.904499    0.740884
 H                  2.693056   -4.341843    1.510196
 H                  3.024795    2.027286    0.973567

 1  2 1.0  4 1.0  11 1.0  17 1.0
 2  3 1.0  6 1.0  18 1.0
 3  5 1.0  10 1.0  19 1.0
 4  5 1.0  8 1.0  20 1.0
 5  15 1.0  16 1.0
 6  7 1.0  10 1.0  21 1.0
 7  8 1.0  11 1.0  22 1.0
 8  9 1.0  23 1.0
 9  10 1.0  12 1.0  14 1.0
 10  24 1.0
 11  25 1.0  26 1.0
 12  13 2.0
 13
 14  28 1.0
 15
 16  29 1.0
```

```
 Entering Gaussian System, Link 0=g98
 Input=mech1s8ts2F.gjf
 Output=mech1s8ts2F.out
 Initial command:
 /usr/g98/l1.exe /usr/scratch/Singh/Gau-15000.inp -
scrdir=/usr/scratch/Singh/
 Default is to use a total of   2 processors:
                                2 via shared-memory
                                1 via Linda
 Entering Link 1 = /usr/g98/l1.exe PID=     13798.
```

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

Cite this work as:
Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

****
Gaussian 98: DEC-AXP-OSF/1-G98RevA.7 11-Apr-1999
                  20-Mar-2002
****
%nproc=2
Will use up to   2 processors via shared memory.
%chk=mech1s8ts2F
%nosave

#N RHF/3-21+G* FREQ

1/10=4,30=1,38=1/1,3;
2/17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;

```
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;
-------------------------------------
Freq calc of output str of mech1s8ts2
-------------------------------------
Symbolic Z-matrix:
Charge = -1 Multiplicity = 1
C                    -2.00487  -0.45135  -0.47235
C                    -1.62327  -0.46696   1.03998
C                    -0.62179   0.70853   1.2638
C                    -0.82296   0.35246  -1.06567
C                    -0.62176   1.49856  -0.05201
C                    -0.4333   -1.49556   1.08869
C                    -0.30432  -1.94596  -0.39818
C                     0.37557  -0.67963  -1.02324
C                     1.43396  -0.34053   0.05498
C                     0.57344  -0.30282   1.32026
C                    -1.74773  -1.89455  -0.91823
O                    -1.94132   2.22859  -0.05717
C                     2.40596   0.72572  -0.20506
N                     3.314     1.39185  -0.39623
O                     0.38913   2.35358  -0.26219
H                    -2.96798  -0.02054  -0.6887
H                    -2.44935  -0.60035   1.72349
H                    -0.74291   1.34199   2.1273
H                    -0.9914    0.73379  -2.06201
H                    -0.45603  -2.29345   1.81729
H                     0.20325  -2.88926  -0.5621
H                     0.82231  -0.84842  -1.99499
H                     1.16826  -0.31772   2.21983
H                    -1.81411  -2.02649  -1.99444
H                    -2.38947  -2.62007  -0.42469
H                    -1.68944   3.15467  -0.18064
O                     2.35879  -1.49453   0.21398
H                     2.00246  -2.30561  -0.1616

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  94 maximum allowed number of steps= 168.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

--------------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
--------------------------------------------------------------------------
  1   1  C     0  -2.004865         -0.451353         -0.472354
  2   2  C     0  -1.623268         -0.466960          1.039985
  3   3  C     0  -0.621791          0.708529          1.263803
  4   4  C     0  -0.822957          0.352455         -1.065675
```

5	5	C	0	-0.621758	1.498558	-0.052012
6	6	C	0	-0.433302	-1.495562	1.088687
7	7	C	0	-0.304316	-1.945961	-0.398177
8	8	C	0	0.375574	-0.679634	-1.023239
9	9	C	0	1.433955	-0.340532	0.054975
10	10	C	0	0.573438	-0.302818	1.320262
11	11	C	0	-1.747730	-1.894546	-0.918230
12	12	O	0	-1.941322	2.228591	-0.057165
13	13	C	0	2.405958	0.725715	-0.205055
14	14	N	0	3.314001	1.391849	-0.396231
15	15	O	0	0.389125	2.353582	-0.262189
16	16	H	0	-2.967975	-0.020539	-0.688700
17	17	H	0	-2.449352	-0.600345	1.723487
18	18	H	0	-0.742905	1.341993	2.127301
19	19	H	0	-0.991395	0.733789	-2.062007
20	20	H	0	-0.456025	-2.293449	1.817293
21	21	H	0	0.203252	-2.889262	-0.562097
22	22	H	0	0.822311	-0.848420	-1.994988
23	23	H	0	1.168261	-0.317724	2.219833
24	24	H	0	-1.814106	-2.026493	-1.994436
25	25	H	0	-2.389474	-2.620074	-0.424692
26	26	H	0	-1.689443	3.154666	-0.180641
27	27	O	0	2.358792	-1.494525	0.213984
28	28	H	0	2.002457	-2.305612	-0.161599

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.004865	-0.451353	-0.472354
2	6	0	-1.623268	-0.466960	1.039985
3	6	0	-0.621791	0.708529	1.263803
4	6	0	-0.822957	0.352455	-1.065675
5	6	0	-0.621758	1.498558	-0.052012
6	6	0	-0.433302	-1.495562	1.088687
7	6	0	-0.304316	-1.945961	-0.398177
8	6	0	0.375574	-0.679634	-1.023239
9	6	0	1.433955	-0.340532	0.054975
10	6	0	0.573438	-0.302818	1.320262
11	6	0	-1.747730	-1.894546	-0.918230
12	8	0	-1.941322	2.228591	-0.057165
13	6	0	2.405958	0.725715	-0.205055
14	7	0	3.314001	1.391849	-0.396231
15	8	0	0.389125	2.353582	-0.262189
16	1	0	-2.967975	-0.020539	-0.688700
17	1	0	-2.449352	-0.600345	1.723487
18	1	0	-0.742905	1.341993	2.127301
19	1	0	-0.991395	0.733789	-2.062007
20	1	0	-0.456025	-2.293449	1.817293
21	1	0	0.203252	-2.889262	-0.562097
22	1	0	0.822311	-0.848420	-1.994988
23	1	0	1.168261	-0.317724	2.219833
24	1	0	-1.814106	-2.026493	-1.994436

25	1	0	-2.389474	-2.620074	-0.424692
26	1	0	-1.689443	3.154666	-0.180641
27	8	0	2.358792	-1.494525	0.213984
28	1	0	2.002457	-2.305612	-0.161599

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.559817	0.000000			
3	C	2.504488	1.560393	0.000000		
4	C	1.547593	2.397028	2.365106	0.000000	
5	C	2.427308	2.461451	1.534769	1.543226	0.000000
6	C	2.448884	1.573662	2.219056	2.865008	3.209589
7	C	2.265220	2.448548	3.147902	2.448930	3.476393
8	C	2.453992	2.880537	2.855222	1.582241	2.585048
9	C	3.480782	3.214474	2.605357	2.613377	2.760372
10	C	3.143753	2.220589	1.566711	2.841126	2.560583
11	C	1.532230	2.426540	3.578408	2.434329	3.678492
12	O	2.712659	2.927609	2.407635	2.405768	1.508053
13	C	4.572997	4.382609	3.365279	3.362422	3.128542
14	N	5.629700	5.467587	4.325864	4.317744	3.952224
15	O	3.693646	3.701465	2.461057	2.473710	1.340569
16	H	1.077027	2.235147	3.138214	2.209601	2.866664
17	H	2.245325	1.080454	2.294437	3.366365	3.301195
18	H	3.401006	2.286833	1.077763	3.343754	2.188286
19	H	2.226809	3.385767	3.346380	1.080030	2.182105
20	H	3.321853	2.302765	3.057074	3.930261	4.230967
21	H	3.290476	3.430800	4.118095	3.437357	4.493750
22	H	3.235584	3.916303	3.889632	2.238890	3.371765
23	H	4.163467	3.034295	2.274088	3.899827	3.415308
24	H	2.198679	3.417056	4.417927	2.739410	4.197700
25	H	2.203077	2.714452	4.129808	3.420638	4.497426
26	H	3.631523	3.822366	3.034779	3.063735	1.974637
27	O	4.538807	4.194636	3.852200	3.895175	4.232373
28	H	4.426452	4.239142	4.243052	3.983169	4.622794

		6	7	8	9	10
6	C	0.000000				
7	C	1.558930	0.000000			
8	C	2.404215	1.567334	0.000000		
9	C	2.426789	2.409219	1.548453	0.000000	
10	C	1.577907	2.534443	2.381835	1.530641	0.000000
11	C	2.432000	1.535103	2.448562	3.672221	3.596146
12	O	4.178088	4.496995	3.841755	4.243284	3.824834
13	C	3.830044	3.810608	2.601325	1.466045	2.596652
14	N	4.958266	4.922723	3.649457	2.596017	3.650881
15	O	4.161389	4.357227	3.127264	2.906977	3.097512
16	H	3.429193	3.299505	3.424273	4.475761	4.081325
17	H	2.295396	3.303531	3.940939	4.234561	3.064045
18	H	3.037481	4.169058	3.906901	3.444437	2.255986
19	H	3.899788	3.228230	2.223827	3.393833	3.868204
20	H	1.080744	2.247681	3.371139	3.239085	2.295527
21	H	2.252263	1.083657	2.263803	2.896797	3.220249
22	H	3.391815	2.241359	1.082755	2.198728	3.369051
23	H	2.287312	3.416667	3.358102	2.181221	1.078547

24	H	3.419672	2.198635	2.748081	4.194335	4.433807
25	H	2.716883	2.191578	3.430606	4.477164	4.146491
26	H	4.981336	5.289829	4.435778	4.693351	4.396309
27	O	2.925901	2.769599	2.475464	1.487383	2.414851
28	H	2.855226	2.346597	2.456212	2.057095	2.872141
		11	12	13	14	15
11	C	0.000000				
12	O	4.216535	0.000000			
13	C	4.962611	4.602103	0.000000		
14	N	6.057557	5.332309	1.142289	0.000000	
15	O	4.800326	2.342785	2.592456	3.081850	0.000000
16	H	2.248018	2.551752	5.447014	6.445433	4.133822
17	H	3.024219	3.381079	5.389967	6.455872	4.552532
18	H	4.556327	2.644646	3.966739	4.777990	2.830983
19	H	2.964526	2.675105	3.871736	4.663077	2.787276
20	H	3.051346	5.115520	4.625602	5.717885	5.160758
21	H	2.218698	5.571945	4.248229	5.294543	5.254703
22	H	2.976390	4.567365	2.861765	3.712593	3.666478
23	H	4.564736	4.619302	2.915603	3.790861	3.728721
24	H	1.086294	4.677066	5.346538	6.366852	5.199996
25	H	1.087109	4.883182	5.851386	6.973232	5.699498
26	H	5.103134	0.967628	4.761587	5.309280	2.229087
27	O	4.278487	5.694392	2.259930	3.100958	4.349052
28	H	3.847774	6.010266	3.058373	3.930193	4.931637
		16	17	18	19	20
16	H	0.000000				
17	H	2.534520	0.000000			
18	H	3.838918	2.616812	0.000000		
19	H	2.522271	4.270306	4.240514	0.000000	
20	H	4.213789	2.617012	3.659897	4.949723	0.000000
21	H	4.278116	4.183222	5.102117	4.099196	2.539909
22	H	4.093659	4.959070	4.923523	2.407780	4.272673
23	H	5.065208	3.662425	2.532939	4.909577	2.589176
24	H	2.657106	4.032417	5.429814	2.881072	4.055235
25	H	2.676181	2.949163	4.992177	3.985451	2.978491
26	H	3.460447	4.278232	3.083555	3.144432	5.932539
27	O	5.600171	5.118242	4.618132	4.622691	3.336476
28	H	5.495870	5.126411	5.106966	4.670402	3.155994
		21	22	23	24	25
21	H	0.000000				
22	H	2.569328	0.000000			
23	H	3.909371	4.262163	0.000000		
24	H	2.620248	2.887655	5.438241	0.000000	
25	H	2.610282	3.990006	4.995178	1.774115	0.000000
26	H	6.344830	5.062160	5.097670	5.490884	5.822132
27	O	2.682153	2.767270	2.612595	4.751125	4.921463
28	H	1.933439	2.622493	3.212289	4.243036	4.411027
		26	27	28		
26	H	0.000000				
27	O	6.177290	0.000000			
28	H	6.591292	0.962237	0.000000		

Interatomic angles:

C1-C2-C3=106.771 C2-C1-C4=100.9572 C1-C4-C3= 76.4406

C2-C3-C4= 71.984 C2-C1-C5= 72.5867 C1-C5-C3= 74.6295

C2-C3-C5=105.3562 C1-C4-C5=103.5021 C2-C4-C5= 73.7638
C3-C5-C4=100.419 C1-C2-C6=102.7994 C1-C6-C3= 64.6762
C3-C2-C6= 90.1513 C4-C1-C6= 88.6105 C4-C2-C6= 89.8946
C4-C3-C6= 77.2887 C5-C1-C6= 82.3267 C5-C2-C6=103.1793
C5-C3-C6=116.3354 C5-C4-C6= 88.1313 C2-C1-C7= 77.1729
C3-C1-C7= 82.4318 C3-C2-C7=101.1606 C4-C1-C7= 77.4038
C4-C2-C7= 60.7041 C3-C4-C7= 81.6526 C5-C1-C7= 95.5433
C5-C2-C7= 90.1482 C5-C4-C7=119.3653 C1-C7-C6= 77.2022
C2-C6-C7=102.8203 C3-C6-C7=111.6701 C4-C7-C6= 88.3546
C2-C1-C8= 88.8203 C3-C1-C8= 70.3066 C2-C3-C8= 75.1104
C1-C4-C8=103.263 C2-C4-C8= 90.3646 C3-C4-C8= 90.4217
C5-C1-C8= 63.9517 C2-C5-C8= 69.5625 C3-C5-C8= 83.5913
C5-C4-C8=111.5963 C1-C6-C8= 60.7414 C2-C6-C8= 90.3092
C3-C6-C8= 76.1614 C4-C8-C6= 89.4317 C5-C8-C6= 79.9869
C1-C7-C8= 77.2618 C2-C7-C8= 88.8471 C3-C8-C7= 85.5172
C4-C8-C7=102.0713 C5-C8-C7=111.3211 C6-C7-C8=100.5348
C1-C3-C9= 85.8496 C2-C3-C9= 97.8474 C1-C4-C9=110.9413
C2-C4-C9= 79.6884 C4-C3-C9= 63.2244 C1-C5-C9= 84.0219
C2-C5-C9= 75.7475 C5-C3-C9= 79.016 C5-C4-C9= 78.6195
C1-C6-C9= 91.1064 C2-C6-C9=104.9246 C3-C6-C9= 68.0517
C4-C9-C6= 69.1685 C5-C9-C6= 76.1485 C1-C7-C9= 96.2079
C2-C7-C9= 82.8579 C3-C9-C7= 77.6598 C4-C7-C9= 65.0806
C5-C9-C7= 84.2236 C6-C7-C9= 71.8068 C1-C8-C9=119.1001
C2-C8-C9= 87.672 C3-C9-C8= 82.6422 C4-C8-C9=113.1773
C5-C8-C9= 79.4883 C6-C8-C9= 72.0985 C7-C8-C9=101.2879
C1-C2-C10=111.3243 C1-C3-C10= 98.4718 C2-C3-C10= 90.4876
C1-C4-C10= 86.1931 C4-C2-C10= 75.8371 C4-C3-C10= 90.1832
C1-C5-C10= 78.0907 C5-C2-C10= 66.0755 C5-C3-C10=111.2947
C4-C5-C10= 83.7081 C1-C6-C10=100.4095 C2-C6-C10= 89.594
C3-C10-C6= 89.7663 C4-C10-C6= 74.7821 C5-C10-C6= 98.9353
C1-C7-C10= 81.6298 C7-C2-C10= 65.538 C3-C10-C7= 97.4616
C4-C7-C10= 69.493 C5-C10-C7= 86.0474 C7-C6-C10=107.793
C1-C8-C10= 81.0828 C2-C10-C8= 77.405 C3-C10-C8= 90.1887
C4-C8-C10= 89.2046 C5-C10-C8= 62.9495 C6-C10-C8= 71.5192
C7-C8-C10= 76.7894 C2-C10-C9=116.743 C3-C10-C9=114.5198
C4-C9-C10= 82.0927 C5-C10-C9= 80.6034 C6-C10-C9=102.6356
C7-C9-C10= 76.4835 C8-C9-C10=101.346 C2-C1-C11=103.3949
C3-C1-C11=123.0424 C3-C2-C11=126.29 C4-C1-C11=104.447
C4-C2-C11= 60.6157 C3-C4-C11= 96.4089 C5-C1-C11=135.3498
C5-C2-C11= 97.6221 C5-C4-C11=134.048 C1-C11-C6= 72.3046
C6-C2-C11= 71.2895 C3-C6-C11=100.4957 C4-C11-C6= 72.1354
C1-C11-C7= 95.2072 C2-C11-C7= 72.4274 C4-C11-C7= 72.1959
C6-C7-C11=103.6293 C1-C11-C8= 71.9808 C2-C11-C8= 72.4355
C3-C8-C11= 84.4893 C8-C4-C11= 71.581 C5-C8-C11= 93.8653
C8-C6-C11= 60.8318 C8-C7-C11=104.2239 C9-C4-C11= 93.2869
C9-C6-C11= 98.1887 C9-C7-C11=136.0392 C9-C8-C11=132.1838
C10-C2-C11=101.3081 C10-C4-C11= 85.5814 C10-C6-C11=126.1536
C10-C7-C11=122.2511 C10-C8-C11= 96.2195 C2-C1-O12= 81.7066
C1-C3-O12= 67.0077 C2-C3-O12= 92.5887 C1-C4-O12= 83.6448
C2-C4-O12= 75.1156 C3-C4-O12= 60.6095 C1-C5-O12= 83.6672
C2-C5-O12= 91.8366 C3-C5-O12=104.6017 C4-C5-O12=104.0751
C6-C1-O12=107.9786 C6-C2-O12=134.073 C6-C3-O12=129.0758
C6-C4-O12=104.5383 C7-C1-O12=128.995 C7-C2-O12=113.2384
C7-C4-O12=135.7341 C8-C1-O12= 95.943 C8-C2-O12= 82.8157

C8-C3-O12= 93.3778 C8-C4-O12=148.1663 C8-C5-O12=138.0906
C9-C3-O12=115.6007 C9-C4-O12=115.3719 C9-C5-O12=166.9815
C10-C2-O12= 94.9745 C10-C3-O12=147.7184 C10-C4-O12= 93.2275
C10-C5-O12=138.6611 C11-C1-O12=166.2011 C11-C2-O12=103.5141
C11-C4-O12=121.1881 C1-C8-C13=129.5137 C2-C8-C13=106.048
C3-C8-C13= 75.9984 C4-C8-C13=104.3162 C5-C8-C13= 74.2015
C6-C8-C13= 99.7678 C7-C8-C13=130.514 C3-C9-C13=108.2155
C4-C9-C13=107.6777 C5-C9-C13= 90.1333 C6-C9-C13=158.7252
C7-C9-C13=158.3808 C8-C9-C13=119.2711 C2-C10-C13=130.7887
C3-C10-C13=105.1609 C4-C10-C13= 76.2432 C5-C10-C13= 74.689
C6-C10-C13=131.5651 C7-C10-C13= 95.9077 C8-C10-C13= 62.8274
C10-C9-C13=120.0953 C11-C8-C13=158.6547 C3-C9-N14=112.5427
C4-C9-N14=111.9587 C5-C9-N14= 95.0482 C6-C9-N14=161.5998
C7-C9-N14=159.1493 C8-C9-N14=121.3399 C10-C9-N14=122.3016
C8-C13-N14=151.9902 C9-C13-N14=168.7721 C10-C13-N14=152.9113
C1-C3-O15= 96.1178 C2-C3-O15=132.7066 C1-C4-O15=132.0551
C2-C4-O15= 98.9055 C4-C3-O15= 61.6314 C1-C5-O15=156.1904
C2-C5-O15=152.3342 C3-C5-O15=117.5644 C4-C5-O15=117.97
C6-C3-O15=125.4578 C6-C4-O15=102.1762 C7-C4-O15=124.5368
C8-C3-O15= 71.6289 C8-C4-O15= 98.5 C8-C5-O15=100.8123
C9-C3-O15= 69.9612 C9-C4-O15= 69.6396 C9-C5-O15= 82.498
C6-C9-O15=102.1822 C7-C9-O15=109.7385 C8-C9-O15= 83.184
C10-C3-O15= 98.0747 C10-C4-O15= 70.9121 C10-C5-O15=100.4132
C10-C9-O15= 82.2582 C11-C4-O15=155.9475 C1-O12-O15= 93.5899
C2-O12-O15= 88.5016 C3-O12-O15= 62.3883 C4-O12-O15= 62.7741
O12-C5-O15=110.5197 C9-O15-O12=107.3697 C3-O15-C13= 83.4638
C4-O15-C13= 83.1301 C5-O15-C13=100.5264 C8-C13-O15= 74.0431
C9-C13-O15= 86.8356 C10-C13-O15= 73.3 O12-O15-C13=137.5983
N14-C9-O15= 67.8442 N14-C13-O15=104.3923 C2-C1-H16=114.6786
C3-C1-H16=116.6044 C3-C2-H16=110.2795 C4-C1-H16=113.4632
C2-H16-C4= 65.2683 C3-C4-H16= 86.5571 C5-C1-H16=102.8851
C5-C2-H16= 75.0595 C3-C5-H16= 85.2746 C5-C4-H16= 98.0402
C6-C1-H16=150.7479 C6-C2-H16=127.5472 C6-C4-H16= 83.9645
C7-C1-H16=160.3595 C7-C2-H16= 89.4528 C7-C4-H16= 90.0378
C8-C1-H16=149.2655 C8-C2-H16= 83.007 C8-C4-H16=128.3645
C8-C5-H16= 77.6316 C9-C4-H16=136.0906 C9-C5-H16=105.3711
C10-C2-H16=132.6878 C10-C4-H16=107.1528 C10-C5-H16= 97.3688
C11-C1-H16=117.9287 C2-H16-C11= 65.5377 C4-H16-C11= 66.1939
C5-H16-C11= 91.1557 C6-C11-H16= 94.1493 C7-C11-H16=120.2463
C8-C11-H16= 93.5236 C1-H16-O12= 86.7366 C2-H16-O12= 75.0829
C3-O12-H16= 78.4522 O12-C4-H16= 66.9735 C5-O12-H16= 85.7684
C11-H16-O12=122.7956 O15-C4-H16=123.8352 O15-C5-H16=156.9746
O15-O12-H16=115.1873 C1-C2-H17=115.3115 C1-H17-C3= 66.9543
C3-C2-H17=119.5361 C4-C1-H17=124.0961 C4-C2-H17=148.5597
C4-C3-H17= 92.5044 C5-C1-H17= 89.8138 C5-C2-H17=133.6551
C5-C3-H17=117.7378 C1-H17-C6= 65.2633 C6-C2-H17=118.547
C6-C3-H17= 61.1093 C4-C6-H17= 80.6153 C7-C1-H17= 94.1752
C7-C2-H17=135.1408 C7-C6-H17=116.6872 C8-C1-H17=113.9157
C8-C2-H17=167.0444 C8-C3-H17= 99.2862 C8-C6-H17=113.9582
C9-C3-H17=119.4556 C9-C6-H17=127.4431 C10-C2-H17=133.285
C10-C3-H17=103.4263 C10-C6-H17=103.0019 C11-C1-H17=104.7917
C11-C2-H17=113.4948 C11-C6-H17= 79.4846 O12-C1-H17= 85.4408
O12-C2-H17=105.5263 O12-C3-H17= 91.922 O15-C3-H17=146.3791
H16-C1-H17= 92.6346 H16-C2-H17= 93.0921 C3-H17-H16= 80.8981

C4-H16-H17= 90.1345 C5-H16-H17= 75.0706 C6-H17-H16= 90.3286
C11-H16-H17= 78.1939 O12-H16-H17= 83.3249 C1-C2-H18=123.1793
C1-C3-H18=139.9558 C2-C3-H18=119.05 C4-C2-H18= 91.0732
C4-C3-H18=150.2335 C1-C5-H18= 94.7864 C2-H18-C5= 66.696
C5-C3-H18=112.6031 C4-C5-H18=126.4272 C6-C2-H18=102.1942
C6-C3-H18=131.0384 C7-C2-H18=123.3467 C8-C2-H18= 97.5752
C8-C3-H18=165.1884 C8-C5-H18=109.5872 C9-C3-H18=134.1924
C9-C5-H18= 87.4186 C2-C10-H18= 61.4341 C10-C3-H18=115.866
C4-C10-H18= 81.1111 C5-H18-C10= 70.342 C6-C10-H18=103.376
C7-C10-H18=120.8746 C8-C10-H18=114.7619 C9-C10-H18=129.9197
C11-C2-H18=150.3227 C1-O12-H18= 78.8043 C2-H18-O12= 72.4225
O12-C3-H18= 90.396 C4-O12-H18= 82.7712 O12-C5-H18= 89.4039
C10-H18-O12=102.3183 C13-C10-H18=109.4588 C2-H18-O15= 92.0216
O15-C3-H18= 98.6309 C4-O15-H18= 77.8285 O15-C5-H18=104.0943
C9-O15-H18= 73.7679 C10-H18-O15= 74.0534 O15-O12-H18= 68.8635
C13-O15-H18= 93.9054 H16-C2-H18=116.1898 H16-C5-H18= 97.9301
H16-O12-H18= 95.236 C1-H17-H18= 88.4281 H17-C2-H18= 95.2331
H17-C3-H18= 94.8912 C5-H18-H17= 86.3033 C6-H17-H18= 76.0787
C10-H18-H17= 77.5333 O12-H18-H17= 79.9719 O15-H18-H17=113.312
H16-H17-H18= 96.3443 C2-C1-H19=125.8825 C3-C1-H19= 89.8311
C1-C4-H19=114.7054 C2-C4-H19=151.5217 C3-C4-H19=150.3098
C1-H19-C5= 66.8 C2-C5-H19= 93.4321 C3-C5-H19=127.5393
C5-C4-H19=111.3496 C6-C1-H19=112.9496 C6-C4-H19=160.4997
C7-C1-H19= 91.8834 C7-C4-H19=128.0137 C1-H19-C8= 66.9234
C2-C8-H19= 82.016 C3-C8-H19= 81.3978 C8-C4-H19=111.9124
C5-H19-C8= 71.8421 C6-C8-H19=114.7849 C7-C8-H19=115.6681
C9-C4-H19=128.6009 C9-C5-H19= 85.8913 C9-C8-H19=127.3163
C10-C4-H19=158.8741 C10-C5-H19=109.036 C10-C8-H19=114.2113
C11-C1-H19=102.5432 C2-C11-H19= 77.0952 C11-C4-H19=108.8164
C5-H19-C11= 89.9172 C6-C11-H19= 92.0083 C7-C11-H19= 85.4408
C11-C8-H19= 78.6006 C1-H19-O12= 66.4702 C2-O12-H19= 74.2044
C3-O12-H19= 82.1711 O12-C4-H19= 92.2278 O12-C5-H19= 91.048
C8-H19-O12=102.9063 C11-H19-O12= 96.6421 C13-C8-H19=106.4589
C1-H19-O15= 94.2291 C3-O15-H19= 78.9588 O15-C4-H19= 95.1884
O15-C5-H19=101.938 C8-H19-O15= 76.3072 C9-O15-H19= 73.1352
C11-H19-O15=113.1078 O15-O12-H19= 67.1075 C13-O15-H19= 91.9851
H16-C1-H19= 92.9061 C2-H16-H19= 90.537 H16-C4-H19= 93.7607
C5-H19-H16= 74.6944 C8-H19-H16= 92.1373 C11-H16-H19= 76.6055
O12-H16-H19= 63.6319 O15-H19-H16=102.1432 H17-C1-H19=145.4417
H17-H16-H19=115.2301 H18-C5-H19=151.9938 H18-O12-H19=105.7117
H18-O15-H19= 98.0082 C1-C2-H20=117.3369 C3-C2-H20=102.9309
C4-C2-H20=113.48 C5-C2-H20=125.231 C1-C6-H20=136.9753
C2-C6-H20=119.1783 C3-C6-H20=132.7117 C4-C6-H20=168.6078
C1-C7-H20= 94.7962 C2-H20-C7= 65.0942 C4-C7-H20=113.5446
C7-C6-H20=115.5594 C8-C2-H20= 80.2983 C8-C6-H20=148.1937
C8-C7-H20=123.1804 C9-C6-H20=130.8991 C9-C7-H20= 88.0701
C2-C10-H20= 61.2876 C3-C10-H20=103.0297 C4-C10-H20= 99.2893
C5-C10-H20=121.116 C10-C6-H20=118.1991 C7-H20-C10= 67.8055
C8-C10-H20= 92.2116 C9-C10-H20=114.1887 C11-C2-H20= 80.3148
C11-C6-H20=115.078 C11-C7-H20=105.9997 O12-C2-H20=155.7652
C13-C10-H20=141.9218 H16-C2-H20=136.4223 C1-H17-H20= 85.8253
H17-C2-H20= 94.3641 C3-H17-H20= 76.6765 H17-C6-H20= 94.7622
C7-H20-H17= 85.1849 C10-H20-H17= 76.8675 H16-H17-H20=109.7535
H18-C2-H20=105.7708 H18-C10-H20=107.0447 H18-H17-H20= 88.7382

C1-C6-H21= 88.7404 C2-C6-H21=126.5485 C3-C6-H21=134.1448
C4-C6-H21= 83.4795 C1-C7-H21=157.0759 C2-C7-H21=150.1058
C4-C7-H21=151.0384 C6-C7-H21=115.7549 C1-C8-H21= 88.3514
C2-C8-H21= 82.7233 C3-C8-H21=106.5465 C4-C8-H21=125.7669
C5-C8-H21=135.7701 C6-H21-C8= 64.3308 C8-C7-H21=116.091
C3-C9-H21= 96.77 C4-C9-H21= 77.0008 C5-C9-H21=105.1616
C9-C6-H21= 76.3995 C9-C7-H21=105.6981 C9-C8-H21= 97.1196
C10-C6-H21=113.2658 C10-C7-H21=120.3115 C10-C8-H21= 87.7258
C10-C9-H21= 87.6457 C1-C11-H21=121.5431 C2-C11-H21= 95.1133
C4-C11-H21= 95.1352 C6-H21-C11= 65.9015 C11-C7-H21=114.7285
C8-H21-C11= 66.2112 C9-H21-C11= 90.7629 C13-C8-H21=121.5108
C13-C9-H21=152.1046 N14-C9-H21=149.0698 O15-C9-H21=129.7528
H16-C11-H21=146.581 H17-C6-H21=133.8098 H19-C8-H21=131.9692
H19-C11-H21=103.5961 C2-H20-H21= 90.081 H20-C6-H21= 92.4775
H20-C7-H21= 92.6444 C8-H21-H20= 88.9469 C9-H21-H20= 72.8021
C10-H20-H21= 83.349 C11-H21-H20= 79.4527 H17-H20-H21=108.4147
C1-C4-H22=116.2165 C2-C4-H22=115.2532 C3-C4-H22=115.282
C5-C4-H22=125.1122 C6-C4-H22= 82.3108 C1-C7-H22= 91.7725
C2-C7-H22=113.1681 C4-H22-C7= 66.2689 C6-C7-H22=125.4231
C1-C8-H22=128.039 C2-C8-H22=160.1599 C3-C8-H22=159.8503
C4-C8-H22=112.9637 C5-C8-H22=128.8824 C6-C8-H22=150.9596
C7-C8-H22=114.2645 C3-C9-H22=107.8242 C4-H22-C9= 72.1536
C5-C9-H22= 84.8706 C6-C9-H22= 94.1953 C7-H22-C9= 65.7143
C9-C8-H22=112.1515 C10-C4-H22= 82.1656 C10-C7-H22= 89.5129
C10-C8-H22=150.8586 C10-C9-H22=128.3167 C1-C11-H22= 85.3614
C2-C11-H22= 92.3426 C11-C4-H22= 79.0011 C6-C11-H22= 76.9494
C11-C7-H22=102.4083 C11-C8-H22=108.5981 C9-H22-C11= 89.089
O12-C4-H22=159.0517 C4-H22-C13= 81.4893 C7-H22-C13= 95.8491
C13-C8-H22= 92.5482 C13-C9-H22=100.7817 C10-C13-H22= 76.0542
C11-H22-C13=116.4163 N14-C9-H22=101.1605 N14-C13-H22=130.9949
O15-C4-H22=102.0434 O15-C9-H22= 90.7088 O15-C13-H22= 84.3242
H16-C4-H22=133.92 H16-C11-H22=102.2772 C1-H19-H22= 88.4659
H19-C4-H22= 85.4733 C5-H19-H22= 94.4199 C7-H22-H19= 87.8781
H19-C8-H22= 86.1856 C9-H22-H19= 94.8016 C11-H19-H22= 66.3492
O12-H19-H22=127.8658 C13-H22-H19= 94.1747 O15-H19-H22= 89.4738
H16-H19-H22=112.2483 H20-C7-H22=144.2771 C4-H22-H21= 91.0028
C6-H21-H22= 89.1597 H21-C7-H22= 94.764 H21-C8-H22= 93.5586
C9-H22-H21= 74.3683 C11-H21-H22= 76.4812 C13-H22-H21=102.7932
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C2-C3-H23=103.0347 C4-C3-H23=114.3984 C5-C3-H23=126.3494
C1-C6-H23=123.0255 C2-C6-H23=102.0163 C6-C3-H23= 61.1889
C4-C6-H23= 97.7552 C7-C6-H23=124.2296 C8-C3-H23= 80.931
C8-C6-H23= 91.3796 C3-H23-C9= 71.5398 C4-C9-H23=108.5196
C5-C9-H23= 86.6053 C6-H23-C9= 65.7377 C7-C9-H23= 96.071
C8-C9-H23=127.5986 C2-C10-H23=130.5283 C3-C10-H23=117.3687
C4-C10-H23=167.0787 C5-C10-H23=135.5725 C6-C10-H23=117.6347
C7-C10-H23=138.3796 C8-C10-H23=149.7986 C9-C10-H23=112.2762
C11-C6-H23=150.576 O12-C3-H23=161.259 C3-H23-C13= 79.8051
C6-H23-C13= 94.0271 C8-C13-H23= 74.7465 C13-C9-H23=104.4298
C13-C10-H23= 96.0966 N14-C9-H23=104.699 N14-C13-H23=133.2632
O15-C3-H23=103.8269 O15-C9-H23= 93.1422 O15-C13-H23= 84.9975
H17-C3-H23=106.5779 H17-C6-H23=106.1043 C2-H18-H23= 77.8492
H18-C3-H23= 90.967 C5-H18-H23= 92.378 C6-H23-H18= 77.9385
C9-H23-H18= 93.5835 H18-C10-H23= 91.92 O12-H18-H23=126.2817

C13-H23-H18= 93.1767 O15-H18-H23= 87.8946 H17-H18-H23= 90.6478
C2-H20-H23= 76.4215 C3-H23-H20= 77.5956 H20-C6-H23= 93.5256
C7-H20-H23= 89.5949 C9-H23-H20= 85.0741 H20-C10-H23= 93.1387
C13-H23-H20=114.2108 H17-H20-H23= 89.4113 H18-H23-H20= 91.2024
H21-C6-H23=118.8957 H21-C9-H23= 99.7221 H21-H20-H23= 99.312
H22-C9-H23=153.3645 H22-C13-H23= 95.073 C2-C1-H24=130.0014
C3-C1-H24=139.7972 C4-C1-H24= 92.3171 C2-C4-H24= 83.1172
C3-C4-H24=119.6992 C5-C1-H24=130.2367 C5-C4-H24=156.1789
C6-C1-H24= 94.5963 C6-C4-H24= 75.1668 C1-H24-C7= 62.0133
C2-C7-H24= 94.5114 C4-C7-H24= 72.0045 C6-C7-H24=130.2577
C8-C1-H24= 72.1692 C2-C8-H24= 74.7167 C3-C8-H24=104.0655
C8-C4-H24= 73.5426 C5-C8-H24=103.7884 C6-C8-H24= 82.8791
C8-C7-H24= 92.1738 C9-C4-H24=103.1538 C9-C7-H24=131.0275
C9-C8-H24=153.9013 C10-C4-H24=105.204 C10-C7-H24=138.924
C10-C8-H24=119.436 C1-C11-H24=113.1069 C2-C11-H24=150.9385
C4-C11-H24= 94.3198 C6-C11-H24=150.5169 C7-C11-H24=112.8931
C8-C11-H24= 94.058 O12-C1-H24=144.2611 O12-C4-H24=130.6295
C13-C8-H24=176.2463 O15-C4-H24=171.8567 H16-C1-H24=103.0081
C2-H16-H24= 88.1676 C4-H16-H24= 67.7923 C5-H16-H24= 98.8461
C7-H24-H16= 85.0534 C8-H24-H16= 78.6002 H16-C11-H24= 99.7439
O12-H16-H24=127.7569 H17-C1-H24=130.2896 H17-H16-H24=101.8958
H19-C1-H24= 81.2341 H19-C4-H24= 86.4126 C5-H19-H24=111.2567
C7-H24-H19= 77.634 H19-C8-H24= 69.918 C11-H24-H19= 83.6509
O12-H19-H24=114.6061 O15-H19-H24=133.0835 H19-H16-H24= 67.5368
H20-C7-H24=131.5755 C1-H24-H21= 85.6564 C4-H24-H21= 79.7496
C6-H21-H24= 88.8143 H21-C7-H24=100.3657 C8-H21-H24= 68.029
C9-H21-H24= 98.8493 H21-C11-H24= 99.1081 H16-H24-H21=108.3181
H19-H24-H21= 96.2249 H20-H21-H24=103.5923 C1-H24-H22= 77.7062
H22-C4-H24= 70.0842 H22-C7-H24= 81.1334 H22-C8-H24= 86.2833
C9-H22-H24=110.3673 C11-H24-H22= 83.9641 C13-H22-H24=136.8463
H16-H24-H22= 95.0818 H22-H19-H24= 65.4728 H22-H21-H24= 67.6108
C2-C1-H25= 90.6809 C3-C1-H25=122.5008 C3-C2-H25=148.8818
C4-C1-H25=130.7616 C4-C2-H25= 83.7654 C5-C1-H25=152.4398
C5-C2-H25=120.5877 C6-C1-H25= 71.2458 C6-C2-H25= 73.2425
C3-C6-H25=113.1978 C4-C6-H25= 75.5338 C1-H25-C7= 62.0543
C2-C7-H25= 71.3608 C4-C7-H25= 94.8123 C6-C7-H25= 91.2426
C8-C1-H25= 94.7397 C8-C2-H25= 75.5711 C8-C6-H25= 83.8805
C8-C7-H25=131.0272 C9-C6-H25=120.9121 C9-C7-H25=153.3443
C10-C2-H25=113.952 C10-C6-H25=148.649 C10-C7-H25=122.4889
C1-C11-H25=113.4178 C2-C11-H25= 93.2418 C4-C11-H25=150.2027
C6-C11-H25= 93.0899 C7-C11-H25=112.2661 C8-C11-H25=149.6004
O12-C1-H25=166.7331 O12-C2-H25=119.8314 H16-C1-H25=104.0045
C2-H16-H25= 66.3996 C4-H16-H25= 88.3355 C5-H16-H25=108.4157
C6-H25-H16= 78.9625 C7-H25-H16= 84.7259 H16-C11-H25=100.9277
O12-H16-H25=138.1399 H17-C1-H25= 83.0479 H17-C2-H25= 91.5819
C3-H17-H25=103.2129 H17-C6-H25= 71.5237 C7-H25-H17= 78.4543
C11-H25-H17= 83.4317 H17-H16-H25= 68.8793 H18-C2-H25=173.0577
H18-H17-H25=127.4086 H19-C1-H25=128.2296 H19-C11-H25=156.5596
H19-H16-H25=100.0679 C1-H25-H20= 78.171 H20-C2-H25= 72.3062
H20-C6-H25= 93.1427 H20-C7-H25= 84.2697 C10-H20-H25=102.8988
C11-H25-H20= 83.4162 H16-H25-H20= 96.2034 H20-H17-H25= 64.3784
C1-H25-H21= 85.8122 C2-H25-H21= 80.2025 C6-H21-H25= 67.4727
H21-C7-H25=100.1402 C8-H21-H25= 89.1791 C9-H21-H25=108.6656
H21-C11-H25= 98.4534 H16-H25-H21=108.0407 H17-H25-H21= 97.4196

H20-H21-H25= 70.6507
H22-H21-H25=100.764
C1-H24-H25= 66.3612
C6-H25-H24= 96.9424
H24-C11-H25=109.4291
H19-H24-H25=115.7161
H22-H24-H25=115.643
C3-C5-H26=119.18
C9-C5-H26=164.5732
C2-O12-H26=154.2552
C5-O12-H26=103.6486
O15-C5-H26= 82.102
C13-O15-H26=161.8577
H18-C5-H26= 95.4482
H19-C5-H26= 98.1835
C1-C6-O27=114.9407
C4-C6-O27= 84.5347
C4-C7-O27= 96.3675
C2-C8-O27=102.8411
C5-C8-O27=113.4963
C3-C9-O27=138.8875
C6-C9-O27= 93.6477
C2-C10-O27=129.5738
C5-C10-O27=116.5353
C8-C10-O27= 62.1346
C11-C7-O27=166.7896
C7-O27-C13= 98.0026
C10-O27-C13= 67.3904
O15-C9-O27=162.5905
H18-C10-O27=162.7591
H20-C7-O27= 82.6597
C7-H21-O27= 83.1078
C10-O27-H21= 78.1711
H20-H21-O27= 79.3713
C7-H22-O27= 66.1755
C10-O27-H22= 80.7915
H19-H22-O27=126.4332
C6-H23-O27= 72.9888
H23-C9-O27= 88.725
H18-H23-O27=127.6568
H22-O27-H23=104.7548
H24-H21-O27=127.2789
H25-C7-O27=165.3909
C2-C6-H28=144.783
C1-C7-H28=147.3952
C6-C7-H28= 91.6882
C3-C8-H28=105.7966
C6-C8-H28= 71.9426
C4-C9-H28=116.5403
C7-H28-C9= 65.9542
C3-C10-H28=144.2049
C10-C6-H28= 74.5993
C10-C9-H28=105.4226
C11-C8-H28=103.348
H22-C7-H25=128.3342
H23-C6-H25=173.0944
C2-H25-H24= 96.9206
C7-H25-H24= 66.3735
H16-H24-H25= 71.1524
H20-H25-H24=114.7589
C1-C5-H26=110.7543
C4-C5-H26=120.6363
C10-C5-H26=151.3197
C3-O12-H26=122.1128
C3-O15-H26= 80.4742
C9-O15-H26=131.6227
H16-C5-H26= 89.28
H18-O12-H26=107.9563
H19-O12-H26=110.2867
C2-C6-O27=135.407
C1-C7-O27=128.4292
C6-C7-O27= 79.7266
C3-C8-O27= 92.2672
C6-C8-O27= 73.6675
C4-C9-O27=142.0503
C7-C9-O27= 87.2331
C3-C10-O27=150.0054
C6-C10-O27= 91.8017
C10-C9-O27=106.2787
C11-C8-O27=120.6612
C8-O27-C13= 66.462
N14-C9-O27= 94.935
O15-C13-O27=127.2106
H19-C8-O27=159.2514
H20-C10-O27= 90.1608
H21-C8-O27= 68.7686
C11-H21-O27=121.332
C4-H22-O27=101.649
H22-C8-O27= 93.8239
C11-H22-O27= 96.2339
H22-H21-O27= 63.5566
C7-O27-H23= 78.7523
H23-C10-O27= 88.1395
H20-H23-O27= 79.7929
H24-C7-O27=145.7646
H24-H22-O27=114.3004
H25-H21-O27=136.8359
C3-C6-H28=112.8807
C2-C7-H28=124.2557
C1-C8-H28=128.7067
C4-C8-H28=160.5524
C8-C7-H28= 74.7882
C5-C9-H28=146.9482
C8-C9-H28= 84.6286
C4-C10-H28= 88.4005
C10-C7-H28= 71.9742
C11-C6-H28= 93.0479
C13-C8-H28= 74.3546
H22-C11-H25=155.3042
H23-H20-H25=127.4402
C4-H24-H25= 96.195
C8-H24-H25= 96.2978
H17-H25-H24=114.9573
H21-H25-H24= 70.4759
C2-C5-H26=118.5947
C8-C5-H26=152.9768
C1-O12-H26=158.7616
C4-O12-H26=124.8799
C4-O15-H26= 81.1241
O12-H26-O15= 84.4596
H16-O12-H26=156.4488
H18-O15-H26= 74.0181
H19-O15-H26= 76.7396
C3-C6-O27= 95.9866
C2-C7-O27=106.8387
C1-C8-O27=134.0721
C4-C8-O27=146.6153
C7-C8-O27= 83.2372
C5-C9-O27=169.7738
C8-C9-O27=109.2403
C4-C10-O27= 95.3059
C7-C10-O27= 68.006
C11-C6-O27=105.6116
C6-O27-C13= 94.3412
C13-C9-O27= 99.8451
N14-C13-O27=128.3555
H17-C6-O27=157.0247
H20-C6-O27=102.8189
C6-H21-O27= 72.1383
C9-O27-H21= 82.6928
C13-O27-H21=118.2939
C6-O27-H22= 73.0749
H22-C9-O27= 95.3607
C13-O27-H22= 68.5429
C3-H23-O27=103.8394
C8-O27-H23= 82.5518
C13-O27-H23= 73.1029
H21-O27-H23= 95.1729
H24-C8-O27=130.8176
H25-C6-O27=121.3793
C1-C6-H28=112.9112
C4-C6-H28= 88.2664
C4-C7-H28=112.3035
C2-C8-H28=104.9055
C5-C8-H28=132.9641
C3-C9-H28=130.6589
C6-C9-H28= 78.6283
C2-C10-H28=112.057
C5-C10-H28=116.5063
C10-C8-H28= 72.8156
C11-C7-H28=164.4938
C13-C9-H28=119.5286

C13-C10-H28= 67.7904 N14-C9-H28=114.7735 O15-C9-H28=166.6963
H17-C6-H28=168.8183 H18-C10-H28=169.51 H19-C8-H28=172.636
H20-C6-H28= 95.9521 H20-C7-H28= 86.7486 H20-C10-H28= 74.3444
C6-H21-H28= 85.6634 C7-H21-H28= 98.1497 C8-H21-H28= 71.1381
C9-H28-H21= 93.0382 C10-H28-H21= 81.6264 C11-H21-H28=135.7414
H20-H21-H28= 88.6638 C4-H22-H28=109.7884 C6-H28-H22= 76.3843
H22-C7-H28= 69.681 H22-C8-H28= 86.466 H22-C9-H28= 75.999
C10-H28-H22= 75.4829 C11-H22-H28= 86.581 C13-H22-H28= 67.6261
H19-H22-H28=136.3499 H22-H21-H28= 69.6061 H23-C6-H28= 76.4271
H23-C9-H28= 98.5194 H23-C10-H28= 98.4121 H24-C7-H28=137.9553
H24-C8-H28=109.1048 H24-H21-H28=136.9111 H24-H22-H28=100.6048
H25-C6-H28=104.6482 H25-C7-H28=152.7943 H25-H21-H28=151.9185
C6-H28-O27= 84.5977 C7-H28-O27=105.9141 C8-H28-O27= 79.8752
C9-O27-H28=112.4573 C10-O27-H28=108.7234 C13-O27-H28=139.771
H21-H28-O27=132.837 H22-H28-O27= 88.347 H23-O27-H28=120.704
Stoichiometry C12H12NO3(1-)
Framework group C1[X(C12H12NO3)]
Deg. of freedom 78
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.048887	-0.183358	-0.463424
2	6	0	-1.664417	-0.264675	1.046079
3	6	0	-0.518215	0.769057	1.275084
4	6	0	-0.776189	0.467458	-1.056485
5	6	0	-0.423109	1.566805	-0.032611
6	6	0	-0.617147	-1.438865	1.076333
7	6	0	-0.555424	-1.885864	-0.415861
8	6	0	0.279090	-0.711227	-1.032589
9	6	0	1.378182	-0.523519	0.041873
10	6	0	0.536546	-0.388788	1.313234
11	6	0	-1.982846	-1.642712	-0.925650
12	8	0	-1.637248	2.461214	-0.021480
13	6	0	2.478447	0.410994	-0.213845
14	7	0	3.463939	0.956281	-0.404347
15	8	0	0.688673	2.286310	-0.240887
16	1	0	-2.949376	0.370615	-0.668905
17	1	0	-2.497141	-0.297684	1.733729
18	1	0	-0.551807	1.403377	2.145765
19	1	0	-0.899255	0.878232	-2.047738
20	1	0	-0.738912	-2.235051	1.796936
21	1	0	-0.174929	-2.884984	-0.592760
22	1	0	0.695053	-0.925676	-2.008983
23	1	0	1.129260	-0.490256	2.208588
24	1	0	-2.071482	-1.753198	-2.002670
25	1	0	-2.710336	-2.284604	-0.435202
26	1	0	-1.268443	3.348281	-0.137237
27	8	0	2.146934	-1.788995	0.182935
28	1	0	1.686743	-2.543090	-0.198461

```
 ----------------------------------------------------------------------
 Rotational constants (GHZ):      0.8663030      0.7010088      0.4951943
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,O-16,C-
12,N-14,
 O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,O-16,H-1
 Standard basis: 3-21+G* (6D, 7F)
 There are   232 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    131072 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
   232 basis functions      340 primitive gaussians
    58 alpha electrons       58 beta electrons
       nuclear repulsion energy      1201.9600982272 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   232 RedAO= T  NBF=   232
 NBsUse=   232 1.00D-04 NBFU=   232
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -736.406235895     A.U. after   18 cycles
             Convg  =    0.6460D-08             -V/T =  2.0022
             S**2   =   0.0000
 Range of M.O.s used for correlation:     1   232
 NBasis=   232 NAE=    58 NBE=    58 NFC=     0 NFV=     0
 NROrb=    232 NOA=    58 NOB=    58 NVA=   174 NVB=   174

 **** Warning!!: The largest alpha MO coefficient is  0.11510104D+03

          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   3 vectors were produced by pass 12.
   2 vectors were produced by pass 13.
 Inv2:  IOpt= 1 Iter= 1 AM= 7.76D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  41 with in-core refinement.
 PrsmSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
```

```
 G2DrvN: will do   10 atoms at a time, making    3 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  44 IRICut=      44 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
          There are  87 degrees of freedom in the 1st order CPHF.
  84 vectors were produced by pass  0.
 AX will form  42 AO Fock derivatives at one time.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  84 vectors were produced by pass  1.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  84 vectors were produced by pass  2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  84 vectors were produced by pass  3.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  84 vectors were produced by pass  4.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  84 vectors were produced by pass  5.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  84 vectors were produced by pass  6.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  45 vectors were produced by pass  7.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
   3 vectors were produced by pass  8.
 Inv2:  IOpt= 1 Iter= 1 AM= 4.74D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 636 with in-core refinement.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.

 ******************************************************************

           Population analysis using the SCF density.

 ******************************************************************

 Alpha  occ. eigenvalues --  -20.36953 -20.29868 -20.19507 -15.35446 -
11.15784
 Alpha  occ. eigenvalues --  -11.10823 -11.08390 -11.07999 -11.07828 -
11.06915
 Alpha  occ. eigenvalues --  -11.06416 -11.06383 -11.05436 -11.05092 -
11.03834
```

```
 Alpha  occ. eigenvalues --  -11.03374  -1.25815  -1.19861  -1.10862  -
1.09692
 Alpha  occ. eigenvalues --   -1.07047  -0.96965  -0.93923  -0.90489  -
0.82716
 Alpha  occ. eigenvalues --   -0.78032  -0.75515  -0.70660  -0.66525  -
0.62144
 Alpha  occ. eigenvalues --   -0.60611  -0.59386  -0.56969  -0.53915  -
0.52338
 Alpha  occ. eigenvalues --   -0.49989  -0.48597  -0.46002  -0.45605  -
0.44230
 Alpha  occ. eigenvalues --   -0.41858  -0.40490  -0.39833  -0.38575  -
0.37390
 Alpha  occ. eigenvalues --   -0.36977  -0.36001  -0.34333  -0.33980  -
0.32702
 Alpha  occ. eigenvalues --   -0.32338  -0.31805  -0.31013  -0.29731  -
0.28720
 Alpha  occ. eigenvalues --   -0.28123  -0.19170  -0.17285
 Alpha virt. eigenvalues --    0.14536   0.16347   0.16683   0.17970
0.18753
 Alpha virt. eigenvalues --    0.19346   0.20245   0.20875   0.21105
0.22341
 Alpha virt. eigenvalues --    0.23037   0.24129   0.24371   0.24964
0.25925
 Alpha virt. eigenvalues --    0.26480   0.27709   0.28280   0.28654
0.29142
 Alpha virt. eigenvalues --    0.29553   0.30187   0.30360   0.30825
0.31250
 Alpha virt. eigenvalues --    0.32659   0.32900   0.33421   0.34231
0.34674
 Alpha virt. eigenvalues --    0.34960   0.35464   0.35816   0.35917
0.36648
 Alpha virt. eigenvalues --    0.37145   0.38242   0.38695   0.39056
0.39300
 Alpha virt. eigenvalues --    0.39950   0.40501   0.40736   0.41475
0.41722
 Alpha virt. eigenvalues --    0.42367   0.44402   0.44886   0.45556
0.46977
 Alpha virt. eigenvalues --    0.47351   0.47918   0.48469   0.50290
0.50431
 Alpha virt. eigenvalues --    0.51432   0.52303   0.53326   0.54064
0.54088
 Alpha virt. eigenvalues --    0.54956   0.55605   0.56128   0.56778
0.58236
 Alpha virt. eigenvalues --    0.58585   0.59458   0.59929   0.60747
0.61580
 Alpha virt. eigenvalues --    0.61705   0.62443   0.63042   0.63449
0.63588
 Alpha virt. eigenvalues --    0.65232   0.66157   0.67038   0.68185
0.68369
 Alpha virt. eigenvalues --    0.68974   0.70119   0.70695   0.71323
0.73141
 Alpha virt. eigenvalues --    0.73697   0.75010   0.75557   0.76136
0.77263
```

```
 Alpha virt. eigenvalues --    0.77844   0.78968   0.80026   0.82041
0.85583
 Alpha virt. eigenvalues --    0.86595   0.93791   1.09292   1.22117
1.22769
 Alpha virt. eigenvalues --    1.24663   1.27094   1.28558   1.28614
1.29831
 Alpha virt. eigenvalues --    1.30491   1.31688   1.31859   1.32974
1.34168
 Alpha virt. eigenvalues --    1.34887   1.35156   1.35890   1.37140
1.37390
 Alpha virt. eigenvalues --    1.39645   1.40487   1.42442   1.43564
1.44679
 Alpha virt. eigenvalues --    1.47688   1.48087   1.51254   1.54266
1.55444
 Alpha virt. eigenvalues --    1.56740   1.58048   1.61998   1.62544
1.64372
 Alpha virt. eigenvalues --    1.65552   1.66853   1.67030   1.70167
1.71351
 Alpha virt. eigenvalues --    1.73147   1.73866   1.76788   1.77926
1.82482
 Alpha virt. eigenvalues --    1.83407   1.86562   1.87115   1.92814
1.93183
 Alpha virt. eigenvalues --    1.96864   1.99853   2.04472   2.15393
2.20258
 Alpha virt. eigenvalues --    2.27956   2.29933   2.33743   2.39729
2.43380
 Alpha virt. eigenvalues --    2.43761   2.46034   2.48137   2.49292
2.52866
 Alpha virt. eigenvalues --    2.57547   2.64460   2.66241   2.67870
2.92683
 Alpha virt. eigenvalues --    3.04951   3.21618   3.29340   3.48084
3.64143
 Alpha virt. eigenvalues --    3.85444   3.92499   4.00478   4.21729
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   15.083266  -4.277179   0.895067  -7.033776   3.453587   2.376261
  2  C   -4.277179  18.448241 -11.999802  -1.578677   7.597921  -9.310181
  3  C    0.895067 -11.999802  33.365038  13.057196 -31.162761   9.155858
  4  C   -7.033776  -1.578677  13.057196  29.037942 -29.413351   0.498233
  5  C    3.453587   7.597921 -31.162761 -29.413351  64.517041  -4.450974
  6  C    2.376261  -9.310181   9.155858   0.498233  -4.450974  18.441062
  7  C   -0.208917   2.275675  -3.799443  -1.392528   4.273353  -4.091187
  8  C    2.269716   0.937379  -5.427206  -9.718575   9.381615  -1.282886
  9  C   -2.243549  -5.677676  13.809149  11.437853 -20.242975  10.493235
 10  C   -0.060602  10.975981 -19.075398  -8.461244  15.866909 -14.716317
 11  C   -3.850406   0.125962   1.279288   2.467246  -3.197148   0.078084
 12  O   -0.140769  -0.189577   0.766065   0.702333  -1.954349   0.085626
 13  C   -0.719898  -0.793432   3.455966   4.382983  -5.439777  -1.556579
 14  N    0.021850  -0.047419  -0.109264  -0.160021   0.178037   0.148261
 15  O   -0.105238  -0.204073   1.032678   1.048597  -2.520314   0.128274
 16  H    0.558411  -0.099063   0.032384  -0.185439  -0.003678   0.057427
 17  H   -0.102052   0.606751  -0.152598   0.032193  -0.030191  -0.155524
 18  H    0.015558  -0.099266   0.672300   0.085007  -0.253163   0.051398
 19  H   -0.074066   0.003215   0.102602   0.662909  -0.238830   0.001694
```

20	H	0.007541	-0.140752	0.105744	0.004403	-0.002019	0.634747
21	H	-0.018070	0.045943	-0.007175	0.054794	0.000494	-0.137271
22	H	0.055820	0.002305	-0.022215	-0.189523	0.032526	-0.012152
23	H	-0.017950	0.115371	-0.153004	0.000211	0.007367	-0.171832
24	H	-0.126313	0.033277	0.010214	0.040367	-0.036992	0.026777
25	H	-0.089370	0.017842	-0.015763	0.025681	0.015342	0.010142
26	H	0.036352	0.015250	-0.109453	-0.132041	0.278668	-0.007544
27	O	0.045349	0.022587	-0.117698	-0.208330	0.317105	-0.160469
28	H	-0.000538	-0.009334	-0.002166	0.000078	-0.009000	-0.008910

		7	8	9	10	11	12
1	C	-0.208917	2.269716	-2.243549	-0.060602	-3.850406	-0.140769
2	C	2.275675	0.937379	-5.677676	10.975981	0.125962	-0.189577
3	C	-3.799443	-5.427206	13.809149	-19.075398	1.279288	0.766065
4	C	-1.392528	-9.718575	11.437853	-8.461244	2.467246	0.702333
5	C	4.273353	9.381615	-20.242975	15.866909	-3.197148	-1.954349
6	C	-4.091187	-1.282886	10.493235	-14.716317	0.078084	0.085626
7	C	16.479671	-4.576935	-1.321746	6.791771	-3.384466	-0.048462
8	C	-4.576935	30.280086	-30.949685	15.434972	0.826924	-0.142832
9	C	-1.321746	-30.949685	97.747169	-41.172900	-0.227161	0.440130
10	C	6.791771	15.434972	-41.172900	50.136743	0.353364	-0.261800
11	C	-3.384466	0.826924	-0.227161	0.353364	13.123525	0.097154
12	O	-0.048462	-0.142832	0.440130	-0.261800	0.097154	9.162345
13	C	-5.503322	0.387819	-32.202178	-7.865830	-0.819733	0.009162
14	N	0.194082	-0.141353	1.551309	0.063119	-0.007744	-0.001280
15	O	-0.092486	-0.265951	0.956277	-0.415693	0.086076	-0.041008
16	H	-0.048971	0.069411	0.015198	-0.021803	-0.027408	0.002996
17	H	0.001704	0.019686	-0.027924	0.133124	0.041024	0.004113
18	H	-0.014346	-0.007893	0.006517	-0.121533	0.005242	-0.002204
19	H	0.019523	-0.172023	0.031220	-0.005105	0.029921	0.000618
20	H	-0.136740	0.060100	-0.042126	-0.148055	0.036207	0.000018
21	H	0.482091	-0.162809	0.051877	0.019829	-0.034232	0.000048
22	H	-0.061385	0.754618	-0.323430	0.153131	0.008539	-0.000125
23	H	0.020806	0.092858	-0.268358	0.742146	0.004038	-0.000137
24	H	-0.121980	0.045850	-0.009546	0.002116	0.443607	-0.000027
25	H	-0.117532	0.061280	-0.027337	0.005171	0.434800	-0.000223
26	H	0.002189	0.002357	-0.029687	0.016998	-0.005846	0.151867
27	O	0.330116	0.634237	-1.836130	1.153215	0.047728	-0.000188
28	H	0.007207	-0.055696	0.126623	-0.131083	0.014472	-0.000012

		13	14	15	16	17	18
1	C	-0.719898	0.021850	-0.105238	0.558411	-0.102052	0.015558
2	C	-0.793432	-0.047419	-0.204073	-0.099063	0.606751	-0.099266
3	C	3.455966	-0.109264	1.032678	0.032384	-0.152598	0.672300
4	C	4.382983	-0.160021	1.048597	-0.185439	0.032193	0.085007
5	C	-5.439777	0.178037	-2.520314	-0.003678	-0.030191	-0.253163
6	C	-1.556579	0.148261	0.128274	0.057427	-0.155524	0.051398
7	C	-5.503322	0.194082	-0.092486	-0.048971	0.001704	-0.014346
8	C	0.387819	-0.141353	-0.265951	0.069411	0.019686	-0.007893
9	C	-32.202178	1.551309	0.956277	0.015198	-0.027924	0.006517
10	C	-7.865830	0.063119	-0.415693	-0.021803	0.133124	-0.121533
11	C	-0.819733	-0.007744	0.086076	-0.027408	0.041024	0.005242
12	O	0.009162	-0.001280	-0.041008	0.002996	0.004113	-0.002204
13	C	54.594840	-1.861555	-0.225925	0.006267	-0.004652	0.016852
14	N	-1.861555	7.845069	0.005685	-0.000024	0.000026	-0.000555
15	O	-0.225925	0.005685	9.316224	-0.000268	0.000437	0.004528

16	H	0.006267	-0.000024	-0.000268	0.371711	-0.000467	0.000007
17	H	-0.004652	0.000026	0.000437	-0.000467	0.403288	-0.000122
18	H	0.016852	-0.000555	0.004528	0.000007	-0.000122	0.388097
19	H	-0.011658	-0.000217	0.004756	0.000117	-0.000010	-0.000019
20	H	-0.019951	-0.000051	-0.000018	-0.000016	-0.000443	-0.000119
21	H	0.056130	-0.000860	-0.000028	-0.000019	-0.000019	0.000001
22	H	-0.057735	-0.000172	0.001538	-0.000024	0.000001	0.000001
23	H	-0.015782	-0.001869	0.001736	0.000001	-0.000126	-0.000669
24	H	0.007371	-0.000041	0.000044	-0.000187	-0.000048	0.000000
25	H	-0.003971	0.000009	-0.000019	-0.000416	0.000182	0.000000
26	H	0.000833	-0.000307	-0.001307	-0.000067	-0.000008	0.000519
27	O	-0.326903	-0.092307	-0.007155	0.000017	0.000088	-0.000313
28	H	0.114871	0.006152	0.000120	0.000000	0.000000	0.000000

		19	20	21	22	23	24
1	C	-0.074066	0.007541	-0.018070	0.055820	-0.017950	-0.126313
2	C	0.003215	-0.140752	0.045943	0.002305	0.115371	0.033277
3	C	0.102602	0.105744	-0.007175	-0.022215	-0.153004	0.010214
4	C	0.662909	0.004403	0.054794	-0.189523	0.000211	0.040367
5	C	-0.238830	-0.002019	0.000494	0.032526	0.007367	-0.036992
6	C	0.001694	0.634747	-0.137271	-0.012152	-0.171832	0.026777
7	C	0.019523	-0.136740	0.482091	-0.061385	0.020806	-0.121980
8	C	-0.172023	0.060100	-0.162809	0.754618	0.092858	0.045850
9	C	0.031220	-0.042126	0.051877	-0.323430	-0.268358	-0.009546
10	C	-0.005105	-0.148055	0.019829	0.153131	0.742146	0.002116
11	C	0.029921	0.036207	-0.034232	0.008539	0.004038	0.443607
12	O	0.000618	0.000018	0.000048	-0.000125	-0.000137	-0.000027
13	C	-0.011658	-0.019951	0.056130	-0.057735	-0.015782	0.007371
14	N	-0.000217	-0.000051	-0.000860	-0.000172	-0.001869	-0.000041
15	O	0.004756	-0.000018	-0.000028	0.001538	0.001736	0.000044
16	H	0.000117	-0.000016	-0.000019	-0.000024	0.000001	-0.000187
17	H	-0.000010	-0.000443	-0.000019	0.000001	-0.000126	-0.000048
18	H	-0.000019	-0.000119	0.000001	0.000001	-0.000669	0.000000
19	H	0.387369	0.000000	-0.000027	-0.000034	0.000000	0.000197
20	H	0.000000	0.401540	-0.000040	-0.000016	0.000094	-0.000036
21	H	-0.000027	-0.000040	0.447667	0.000249	-0.000004	0.000012
22	H	-0.000034	-0.000016	0.000249	0.395424	-0.000028	0.000147
23	H	0.000000	0.000094	-0.000004	-0.000028	0.381419	0.000000
24	H	0.000197	-0.000036	0.000012	0.000147	0.000000	0.462268
25	H	-0.000067	0.000152	-0.000245	-0.000049	0.000000	-0.020655
26	H	0.000420	0.000000	0.000000	0.000001	0.000001	0.000000
27	O	-0.000196	0.002428	-0.005117	0.009711	0.004946	-0.000065
28	H	0.000002	-0.000057	0.000208	-0.001126	0.000042	-0.000004

		25	26	27	28
1	C	-0.089370	0.036352	0.045349	-0.000538
2	C	0.017842	0.015250	0.022587	-0.009334
3	C	-0.015763	-0.109453	-0.117698	-0.002166
4	C	0.025681	-0.132041	-0.208330	0.000078
5	C	0.015342	0.278668	0.317105	-0.009000
6	C	0.010142	-0.007544	-0.160469	-0.008910
7	C	-0.117532	0.002189	0.330116	0.007207
8	C	0.061280	0.002357	0.634237	-0.055696
9	C	-0.027337	-0.029687	-1.836130	0.126623
10	C	0.005171	0.016998	1.153215	-0.131083
11	C	0.434800	-0.005846	0.047728	0.014472

12	O	-0.000223	0.151867	-0.000188	-0.000012
13	C	-0.003971	0.000833	-0.326903	0.114871
14	N	0.000009	-0.000307	-0.092307	0.006152
15	O	-0.000019	-0.001307	-0.007155	0.000120
16	H	-0.000416	-0.000067	0.000017	0.000000
17	H	0.000182	-0.000008	0.000088	0.000000
18	H	0.000000	0.000519	-0.000313	0.000000
19	H	-0.000067	0.000420	-0.000196	0.000002
20	H	0.000152	0.000000	0.002428	-0.000057
21	H	-0.000245	0.000000	-0.005117	0.000208
22	H	-0.000049	0.000001	0.009711	-0.001126
23	H	0.000000	0.000001	0.004946	0.000042
24	H	-0.020655	0.000000	-0.000065	-0.000004
25	H	0.465418	0.000000	-0.000009	-0.000001
26	H	0.000000	0.344440	0.000000	0.000000
27	O	-0.000009	0.000000	8.805192	0.158501
28	H	-0.000001	0.000000	0.158501	0.362932

Total atomic charges:

		1
1	C	0.249916
2	C	-0.797268
3	C	0.414400
4	C	0.935480
5	C	-0.964443
6	C	-0.125252
7	C	0.042261
8	C	-2.355064
9	C	5.935851
10	C	-3.391225
11	C	-1.949054
12	O	-0.639482
13	C	0.395788
14	N	-0.588558
15	O	-0.707487
16	H	0.273906
17	H	0.231565
18	H	0.254174
19	H	0.257689
20	H	0.237465
21	H	0.206575
22	H	0.254005
23	H	0.258723
24	H	0.243647
25	H	0.239639
26	H	0.436366
27	O	-0.776338
28	H	0.426720

Sum of Mulliken charges= -1.00000

Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.523822
2	C	-0.565702
3	C	0.668574
4	C	1.193169

```
  5  C   -0.964443
  6  C    0.112213
  7  C    0.248836
  8  C   -2.101059
  9  C    5.935851
 10  C   -3.132502
 11  C   -1.465767
 12  O   -0.203117
 13  C    0.395788
 14  N   -0.588558
 15  O   -0.707487
 16  H    0.000000
 17  H    0.000000
 18  H    0.000000
 19  H    0.000000
 20  H    0.000000
 21  H    0.000000
 22  H    0.000000
 23  H    0.000000
 24  H    0.000000
 25  H    0.000000
 26  H    0.000000
 27  O   -0.349618
 28  H    0.000000
 Sum of Mulliken charges=  -1.00000
 Electronic spatial extent (au):  <R**2>=  2531.1835
 Charge=    -1.0000 electrons
 Dipole moment (Debye):
    X=    -6.8541    Y=    -9.1446    Z=     0.5045  Tot=    11.4392
 Quadrupole moment (Debye-Ang):
   XX=  -139.5381   YY=  -119.3219   ZZ=   -97.4710
   XY=    -4.6659   XZ=     2.0676   YZ=     4.6367
 Octapole moment (Debye-Ang**2):
  XXX=  -101.5988  YYY=   -38.7382  ZZZ=     0.6862  XYY=   -17.4809
  XXY=   -30.0520  XXZ=     9.2054  XZZ=    -0.2493  YZZ=     0.8062
  YYZ=     0.2734  XYZ=    12.7128
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -2160.6656 YYYY= -1268.4672 ZZZZ=  -527.4640 XXXY=   -59.7491
 XXXZ=    38.2583 YYYX=   -92.7077 YYYZ=    13.2147 ZZZX=     6.0256
 ZZZY=     2.0029 XXYY=  -605.8473 XXZZ=  -379.9462 YYZZ=  -311.9466
 XXYZ=    18.6279 YYXZ=    -1.6674 ZZXY=   -13.1877
 N-N= 1.201960098227D+03 E-N=-4.145335630561D+03  KE= 7.347681317159D+02
  Exact polarizability: 142.418   6.751 132.475  -0.881   0.200 110.968
 Approx polarizability: 126.143   6.873 118.198  -1.915  -0.769 107.071
 Full mass-weighted force constant matrix:
 Low frequencies --- -306.8491   -0.2999    0.0005    0.0009    0.0013
1.1584
 Low frequencies ---    1.8588  116.2043  152.2613
 ******    1 imaginary frequencies (negative Signs) ******
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                      1                      2                      3
                    ?A                     ?A                     ?A
```

Frequencies --		-306.8491			116.2043			152.2613		
Red. masses --		1.1119			9.2502			8.6497		
Frc consts --		0.0617			0.0736			0.1181		
IR Inten --		127.5425			0.2516			14.2247		
Raman Activ --		1.3950			1.0218			0.2891		
Depolar --		0.7284			0.7496			0.6309		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	-0.05	-0.01	0.09	0.08	0.08	-0.03
2	6	0.00	0.00	0.00	0.07	0.03	0.06	0.07	0.09	-0.02
3	6	0.00	0.00	0.00	0.12	0.02	-0.06	0.11	0.04	-0.03
4	6	0.00	0.00	0.00	-0.10	-0.03	-0.03	0.10	0.03	-0.02
5	6	0.00	0.00	0.00	0.00	-0.01	-0.11	0.00	0.08	-0.02
6	6	0.01	0.00	0.00	0.04	0.01	0.02	0.01	0.04	0.00
7	6	0.00	0.00	0.01	-0.04	0.00	0.01	-0.01	0.02	0.01
8	6	0.00	0.00	0.00	-0.07	0.01	-0.06	0.06	-0.02	0.00
9	6	0.00	0.01	0.00	0.00	-0.02	-0.10	0.05	-0.11	0.01
10	6	0.00	0.00	0.00	0.07	-0.03	-0.07	0.06	-0.01	-0.01
11	6	0.01	0.00	0.00	-0.08	-0.02	0.12	0.02	0.08	-0.01
12	8	0.00	0.00	0.00	0.01	0.00	0.03	-0.28	-0.23	0.09
13	6	0.00	0.01	-0.01	0.02	0.03	0.16	0.10	-0.18	0.01
14	7	0.00	0.00	0.00	0.06	0.09	0.56	0.08	-0.15	0.00
15	8	0.00	0.00	0.00	-0.03	-0.03	-0.30	-0.23	0.41	-0.05
16	1	0.00	0.00	0.00	-0.07	-0.01	0.15	0.11	0.11	-0.04
17	1	0.00	0.00	0.00	0.13	0.08	0.13	0.06	0.15	-0.03
18	1	0.00	0.00	0.00	0.19	0.05	-0.08	0.13	0.03	-0.02
19	1	0.00	0.00	0.00	-0.18	-0.06	-0.03	0.13	0.01	-0.04
20	1	0.02	0.00	0.00	0.06	0.01	0.02	-0.03	0.05	0.01
21	1	0.02	0.00	0.04	-0.06	0.00	0.00	-0.05	0.00	0.02
22	1	-0.01	0.01	-0.01	-0.12	-0.01	-0.07	0.05	-0.05	0.01
23	1	0.00	-0.01	0.00	0.11	-0.02	-0.09	0.04	-0.03	0.00

24	1	0.00	0.00	0.00	-0.17	-0.04	0.13	0.02	0.07	-0.01
25	1	0.01	0.00	0.00	-0.04	-0.01	0.19	-0.02	0.12	-0.01
26	1	0.00	0.00	0.00	0.00	-0.01	-0.07	-0.52	-0.12	0.15
27	8	-0.05	-0.02	0.06	0.00	-0.03	-0.25	-0.03	-0.16	0.04
28	1	0.42	0.16	-0.89	-0.03	0.00	-0.28	-0.07	-0.13	0.02

	4			5			6		
	?A			?A			?A		
Frequencies --	192.6984			242.6688			310.4316		
Red. masses --	7.5742			11.2235			5.7986		
Frc consts --	0.1657			0.3894			0.3292		
IR Inten --	4.7205			0.2195			9.8960		
Raman Activ --	1.7342			0.5974			3.0256		
Depolar --	0.7174			0.7482			0.7085		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.07	-0.10	0.05	-0.02	-0.02	-0.08	0.00	-0.02	0.10
2 6	-0.02	-0.09	0.03	-0.01	0.00	-0.08	0.10	-0.09	0.06
3 6	-0.12	0.03	0.01	0.05	-0.03	-0.03	0.03	0.00	0.00
4 6	-0.15	0.04	0.02	-0.06	0.03	-0.02	-0.04	0.02	0.02
5 6	-0.15	0.02	0.01	0.01	-0.01	-0.04	-0.02	0.03	0.00
6 6	0.11	0.02	-0.03	-0.04	-0.03	-0.05	0.16	-0.04	-0.09
7 6	0.11	0.06	-0.06	0.03	0.02	-0.07	0.04	0.01	-0.13
8 6	-0.02	0.15	-0.04	0.03	0.04	0.03	0.01	0.02	-0.11
9 6	0.00	0.15	-0.03	0.00	0.00	0.11	0.02	-0.05	-0.08
10 6	0.00	0.14	-0.03	-0.04	-0.04	0.05	0.07	0.05	-0.10
11 6	0.07	-0.08	0.00	0.05	0.00	-0.14	-0.02	0.01	0.03
12 8	-0.08	0.10	0.02	0.08	0.07	0.52	0.02	0.09	-0.09
13 6	0.17	-0.06	-0.02	-0.02	0.01	0.04	0.05	-0.10	-0.06
14 7	0.35	-0.36	0.02	-0.07	0.03	-0.11	-0.10	0.21	0.05
15 8	-0.07	-0.08	-0.01	-0.02	-0.09	-0.49	-0.01	0.03	0.04
16 1	-0.13	-0.18	0.08	-0.04	-0.05	-0.08	-0.01	-0.01	0.19
17 1	0.01	-0.21	0.06	0.00	0.03	-0.07	0.15	-0.19	0.12

18	1	-0.16	0.02	0.01	0.00	-0.02	-0.04	0.06	-0.04
0.02									
19	1	-0.22	0.05	0.03	0.00	0.01	-0.03	-0.14	0.02
0.03									
20	1	0.22	-0.02	-0.05	-0.11	-0.05	-0.09	0.27	-0.08
0.11									
21	1	0.17	0.10	-0.10	0.07	0.03	-0.08	0.00	0.01
0.23									
22	1	-0.02	0.22	-0.06	0.09	0.10	0.04	-0.03	0.10
0.14									
23	1	0.01	0.18	-0.03	-0.09	-0.08	0.08	0.12	0.05
0.14									
24	1	0.05	-0.06	0.00	0.13	0.07	-0.15	-0.14	0.06
0.03									
25	1	0.16	-0.17	0.01	0.04	-0.06	-0.23	0.05	-0.03
0.08									
26	1	-0.05	0.08	-0.03	0.06	0.01	0.01	0.10	0.06
0.05									
27	8	-0.10	0.08	0.03	0.00	0.02	0.28	-0.22	-0.16
0.27									
28	1	-0.13	0.09	0.07	0.05	-0.03	0.30	-0.30	-0.16
0.36									

	7			8			9		
	?A			?A			?A		
Frequencies --	335.0221			348.1930			368.1315		
Red. masses --	5.3446			4.1231			5.0630		
Frc consts --	0.3534			0.2945			0.4043		
IR Inten --	4.8368			7.8123			39.7638		
Raman Activ --	2.3557			1.9698			2.1257		
Depolar --	0.7162			0.7064			0.2141		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	-0.09	-0.04	-0.01	0.07	0.13	0.02	0.03	-0.06
2 6	-0.01	-0.04	-0.01	0.02	-0.05	0.11	0.00	0.09	-0.04
3 6	-0.05	0.03	0.01	0.02	-0.02	0.10	0.01	0.04	-0.01
4 6	0.00	0.02	0.03	-0.01	0.02	0.12	0.03	0.01	-0.05
5 6	-0.04	0.08	0.01	0.00	-0.04	0.02	0.05	-0.09	-0.02
6 6	0.01	-0.01	0.09	0.00	-0.06	-0.02	0.01	0.10	0.04
7 6	0.11	0.00	0.09	-0.01	0.07	-0.08	0.05	0.07	0.05
8 6	0.04	0.06	0.10	0.03	0.09	0.06	0.02	0.07	0.00
9 6	0.01	-0.05	0.09	0.02	0.01	0.10	-0.01	0.08	0.01
10 6	0.00	0.00	0.10	0.00	-0.07	0.09	0.01	0.10	0.04
11 6	0.18	-0.10	-0.04	0.00	0.17	-0.10	0.07	0.01	0.01

12	8	0.05	0.20	-0.01	-0.06	-0.10	-0.19	-0.07	-0.25
0.07									
13	6	0.01	-0.09	0.08	0.02	0.02	0.09	0.06	0.02
0.01									
14	7	-0.10	0.05	-0.07	0.00	0.00	-0.08	0.01	0.11
-0.03									
15	8	-0.05	0.09	-0.04	-0.01	-0.08	-0.15	0.11	-0.21
0.03									
16	1	-0.02	-0.18	-0.07	0.02	0.13	0.18	0.02	-0.01
-0.11									
17	1	-0.04	-0.03	-0.04	0.05	-0.09	0.14	-0.02	0.11
-0.06									
18	1	-0.11	-0.01	0.03	0.04	-0.02	0.11	-0.02	0.13
-0.08									
19	1	0.03	-0.03	0.01	-0.05	0.04	0.13	0.06	0.06
-0.03									
20	1	-0.02	0.00	0.09	0.00	-0.13	-0.10	-0.01	0.12
0.05									
21	1	0.16	0.02	0.10	-0.04	0.07	-0.16	0.03	0.06
0.08									
22	1	0.08	0.06	0.12	0.07	0.19	0.06	0.06	0.02
0.03									
23	1	-0.04	0.06	0.13	-0.04	-0.14	0.11	0.03	0.11
0.03									
24	1	0.34	-0.08	-0.06	0.09	0.42	-0.14	0.11	-0.05
0.01									
25	1	0.16	-0.16	-0.16	-0.03	0.05	-0.31	0.07	0.01
0.02									
26	1	0.18	0.11	-0.33	-0.13	-0.10	-0.40	-0.27	-0.11
0.53									
27	8	-0.14	-0.17	-0.24	0.01	-0.01	-0.03	-0.25	-0.05
-0.08									
28	1	-0.35	-0.05	-0.21	-0.03	0.03	-0.06	-0.46	0.05
-0.02									

	10			11			12		
	?A			?A			?A		
Frequencies --	404.1093			421.5327			432.8940		
Red. masses --	1.2326			9.5188			2.1903		
Frc consts --	0.1186			0.9965			0.2418		
IR Inten --	116.0744			2.9519			0.2701		
Raman Activ --	1.9581			3.5875			1.1144		
Depolar --	0.6719			0.0644			0.7156		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.02	0.01	-0.02	-0.11	0.03	-0.03	0.00	0.02	-0.04
2 6	-0.01	0.01	-0.01	-0.13	0.06	0.00	0.00	0.00	-0.05
3 6	-0.02	0.01	0.02	-0.11	0.04	-0.04	-0.01	-0.03	0.00
4 6	0.04	-0.01	0.01	-0.07	0.00	0.02	0.02	0.02	-0.04
5 6	0.01	-0.01	0.05	-0.14	-0.01	0.01	0.01	0.00	-0.01

6	6	0.00	0.02	0.00	-0.11	0.09	0.01	-0.01	-0.03	-0.07
7	6	-0.01	-0.01	0.01	-0.09	0.04	0.06	0.02	0.04	-0.09
8	6	0.00	-0.02	-0.02	0.03	-0.04	0.04	0.04	0.08	-0.01
9	6	-0.01	0.01	-0.04	0.24	-0.12	-0.01	0.02	0.02	0.08
10	6	0.00	0.03	-0.02	0.00	0.03	-0.05	-0.03	-0.06	0.05
11	6	0.00	0.00	0.00	-0.09	0.05	-0.03	-0.09	-0.05	0.17
12	8	0.00	-0.03	0.06	-0.15	0.12	0.05	0.01	-0.01	-0.01
13	6	0.00	0.01	-0.04	0.39	-0.15	-0.03	0.05	0.01	0.12
14	7	0.01	0.01	0.02	0.16	0.30	-0.05	0.01	0.02	-0.07
15	8	0.01	-0.01	0.02	-0.05	-0.21	0.05	0.00	0.02	-0.01
16	1	0.03	0.02	-0.03	-0.08	0.06	-0.08	0.00	0.02	-0.04
17	1	-0.02	0.00	-0.03	-0.13	0.08	0.00	-0.01	-0.03	-0.07
18	1	-0.02	0.00	0.03	-0.05	0.03	-0.03	-0.04	-0.03	-0.01
19	1	0.05	0.02	0.02	-0.01	-0.04	-0.01	0.03	0.04	-0.03
20	1	0.01	0.03	0.01	-0.10	0.12	0.04	-0.06	-0.08	-0.13
21	1	-0.02	-0.02	0.02	-0.12	0.01	0.15	0.03	0.05	-0.13
22	1	-0.01	-0.04	-0.02	-0.12	-0.07	-0.02	0.13	0.13	0.02
23	1	0.02	0.02	-0.04	-0.15	0.06	0.06	-0.10	-0.10	0.09
24	1	0.00	-0.02	0.01	-0.02	0.07	-0.04	-0.46	-0.34	0.23
25	1	-0.01	0.02	0.01	-0.11	0.03	-0.09	0.08	0.08	0.59
26	1	-0.11	-0.12	-0.97	-0.09	0.09	-0.05	0.00	-0.02	-0.17
27	8	-0.03	0.01	0.00	0.25	-0.21	0.00	0.00	-0.01	-0.02
28	1	-0.04	0.01	0.00	0.27	-0.18	-0.12	-0.04	0.03	-0.05

	13	14	15
	?A	?A	?A
Frequencies --	498.6725	540.3318	567.0434
Red. masses --	6.5179	3.5804	4.5857
Frc consts --	0.9550	0.6159	0.8687
IR Inten --	6.4382	18.5161	3.7363
Raman Activ --	6.7978	0.7046	1.4836
Depolar --	0.6843	0.7433	0.7226

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.03	-0.03	0.00	0.13	0.06	-0.09	0.13	0.07	-0.02
2	6	-0.06	-0.07	0.01	-0.04	-0.04	-0.04	0.14	-0.10	-0.03
3	6	-0.02	-0.08	0.04	-0.10	0.00	0.18	-0.01	-0.04	-0.11
4	6	0.03	-0.11	0.02	0.15	0.02	0.11	0.07	-0.04	-0.13
5	6	0.05	-0.05	0.01	-0.02	0.02	0.14	-0.08	-0.01	-0.10
6	6	-0.08	-0.09	0.03	0.01	-0.01	-0.02	0.13	-0.11	0.06
7	6	-0.12	-0.12	0.06	0.01	-0.03	0.01	-0.07	-0.10	0.04
8	6	-0.04	-0.09	0.04	0.04	-0.05	0.01	0.05	-0.09	0.06
9	6	0.03	0.12	0.00	-0.01	-0.01	-0.07	0.01	0.03	0.07
10	6	-0.04	-0.04	0.04	-0.01	0.02	0.01	0.07	0.04	0.02
11	6	-0.11	-0.01	-0.06	0.00	0.03	0.06	-0.10	0.16	0.00
12	8	0.20	-0.05	-0.01	-0.05	0.06	-0.05	-0.13	0.15	0.06
13	6	0.23	0.15	-0.04	-0.03	-0.01	-0.18	-0.04	0.10	0.10
14	7	0.26	0.16	-0.05	0.01	0.00	0.07	0.02	-0.04	-0.03
15	8	-0.08	0.20	-0.05	-0.05	-0.06	-0.14	-0.04	-0.10	0.05
16	1	0.02	0.04	0.00	0.18	0.13	-0.14	0.19	0.23	0.14
17	1	-0.07	-0.06	-0.01	-0.15	-0.17	-0.18	0.10	-0.10	-0.09
18	1	-0.08	-0.08	0.04	-0.18	-0.14	0.28	-0.06	0.01	-0.15
19	1	0.03	-0.11	0.02	0.31	0.18	0.16	0.09	-0.18	-0.19
20	1	-0.07	-0.05	0.08	0.02	0.02	0.01	0.18	-0.05	0.13
21	1	-0.20	-0.15	0.05	-0.03	-0.05	0.00	-0.22	-0.14	-0.08
22	1	-0.05	-0.16	0.05	-0.01	-0.03	-0.01	0.14	-0.17	0.12
23	1	-0.05	-0.10	0.04	0.05	-0.04	-0.04	0.05	0.18	0.04
24	1	0.01	0.06	-0.08	-0.14	-0.17	0.09	-0.06	0.16	-0.01
25	1	-0.21	0.00	-0.19	0.00	0.19	0.27	-0.25	0.29	-0.04
26	1	0.35	-0.09	0.18	0.04	0.08	0.39	-0.04	0.10	-0.06

27	8	-0.19	0.07	-0.01	-0.02	0.00	-0.02	-0.06	0.02	-0.03
28	1	-0.35	0.17	0.01	-0.02	0.00	-0.01	-0.16	0.09	-0.06

		16			17			18		
		?A			?A			?A		
Frequencies --		611.2967			632.5800			644.3440		
Red. masses --		4.7291			5.8036			4.6550		
Frc consts --		1.0412			1.3683			1.1387		
IR Inten --		0.5042			3.6072			17.0570		
Raman Activ --		6.7583			6.5029			3.4258		
Depolar --		0.1341			0.2090			0.3816		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	0.01	0.10	-0.04	0.10	-0.15	-0.04	-0.02	0.03
2	6	-0.07	0.01	0.08	0.06	-0.06	-0.09	-0.02	-0.17	-0.05
3	6	-0.13	0.09	0.00	0.01	-0.14	-0.05	-0.18	0.04	-0.05
4	6	0.08	-0.16	0.00	-0.08	0.12	-0.12	-0.01	0.03	0.02
5	6	-0.07	-0.13	-0.03	-0.09	-0.13	-0.02	0.11	0.11	-0.05
6	6	0.05	0.13	-0.06	0.08	-0.04	0.10	0.10	-0.06	0.03
7	6	0.04	0.04	-0.10	0.00	0.15	0.11	-0.04	-0.04	-0.03
8	6	0.14	-0.06	-0.07	-0.11	0.15	0.09	-0.05	0.02	0.07
9	6	0.01	-0.01	0.02	-0.01	0.01	0.02	-0.02	0.01	0.06
10	6	-0.07	0.18	-0.03	0.13	-0.01	0.13	-0.04	0.16	0.09
11	6	-0.02	0.10	0.01	0.01	0.10	0.02	-0.11	0.01	-0.03
12	8	0.18	-0.07	0.06	0.17	-0.09	-0.04	0.00	-0.09	0.04
13	6	-0.03	-0.07	0.07	0.00	-0.13	-0.17	0.05	-0.18	-0.08
14	7	-0.08	-0.04	-0.01	-0.04	0.01	0.07	-0.06	0.03	0.04
15	8	-0.17	0.01	0.02	-0.19	-0.02	0.03	0.22	0.10	-0.05
16	1	0.13	0.14	0.01	-0.10	0.05	-0.01	-0.04	0.02	0.15
17	1	-0.07	-0.12	0.08	0.03	-0.02	-0.13	-0.02	-0.31	-0.05
18	1	-0.09	0.25	-0.12	-0.12	-0.06	-0.12	-0.41	0.03	-0.04
19	1	-0.03	-0.20	0.00	0.07	0.22	-0.09	-0.05	-0.08	-0.03
20	1	0.20	0.09	-0.08	-0.01	-0.06	0.07	0.19	-0.05	0.05

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  21   1    -0.07  -0.02   0.00     0.07   0.21  -0.06    -0.03  -0.02  -
0.15
  22   1     0.25   0.00  -0.04    -0.14   0.04   0.10     0.00   0.06
0.08
  23   1    -0.12   0.21   0.01     0.18   0.11   0.11    -0.08   0.31
0.14
  24   1    -0.12   0.23   0.01     0.11  -0.10   0.04    -0.12   0.01  -
0.03
  25   1     0.05   0.01   0.01    -0.03   0.19   0.08    -0.13   0.04  -
0.02
  26   1     0.43  -0.16   0.15     0.41  -0.20  -0.16    -0.35   0.05
0.05
  27   8     0.04  -0.02  -0.06     0.05   0.01   0.04     0.07   0.03  -
0.04
  28   1     0.04   0.01  -0.12     0.13  -0.04   0.03     0.13   0.02  -
0.11
                     19                    20                    21
                     ?A                    ?A                    ?A
 Frequencies --   676.4039              686.6313              704.1821
 Red. masses --     4.9639                5.9900                7.1440
 Frc consts  --     1.3381                1.6639                2.0872
 IR Inten    --     7.6918                5.4469               65.5584
 Raman Activ --     2.4787                7.8124                6.5898
 Depolar     --     0.5697                0.3752                0.4956
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01   0.01  -0.11    -0.13  -0.08  -0.11    -0.07   0.02  -
0.03
   2   6     0.05  -0.03  -0.06     0.14   0.08  -0.11    -0.09  -0.13  -
0.03
   3   6     0.01   0.01   0.09     0.12   0.14   0.10    -0.13  -0.04  -
0.06
   4   6    -0.01   0.07   0.03    -0.04  -0.07   0.08    -0.02   0.11
0.05
   5   6     0.00   0.00   0.13    -0.02  -0.01   0.09    -0.02   0.05
0.03
   6   6     0.10   0.06   0.03     0.09   0.15  -0.12     0.09   0.02
0.05
   7   6    -0.07  -0.07   0.09    -0.08  -0.07  -0.13    -0.02   0.08
0.09
   8   6    -0.11  -0.02  -0.11    -0.02  -0.02   0.12    -0.03   0.03
0.00
   9   6    -0.05   0.02  -0.08     0.06   0.00   0.13     0.11  -0.07  -
0.06
  10   6     0.06   0.07  -0.11     0.19   0.11   0.15     0.00   0.06  -
0.13
  11   6    -0.05  -0.04  -0.04    -0.21  -0.16  -0.16     0.01   0.04
0.03
  12   8     0.04  -0.04  -0.04     0.01   0.00  -0.02     0.09  -0.11
0.00
  13   6     0.11  -0.14   0.38    -0.09   0.10  -0.06    -0.18   0.41
0.10
  14   7    -0.08   0.00  -0.11     0.01  -0.04   0.03     0.08  -0.08  -
0.04
```

15	8	-0.03	-0.01	-0.04	-0.04	-0.02	0.03	0.06	0.05	-0.05
16	1	-0.02	0.00	-0.05	-0.11	-0.03	-0.09	-0.10	-0.02	0.01
17	1	0.01	-0.12	-0.11	0.25	-0.06	0.01	-0.11	-0.20	-0.05
18	1	-0.02	-0.13	0.20	-0.03	0.16	0.08	-0.17	-0.17	0.03
19	1	0.10	0.33	0.12	0.15	-0.01	0.08	0.04	0.18	0.07
20	1	0.19	0.17	0.18	-0.08	0.24	-0.05	0.28	0.03	0.10
21	1	-0.04	-0.06	0.10	-0.05	-0.07	-0.07	-0.03	0.08	0.04
22	1	-0.26	-0.10	-0.15	0.11	0.17	0.13	-0.23	-0.04	-0.07
23	1	0.22	0.07	-0.22	0.13	-0.04	0.18	-0.02	0.24	-0.10
24	1	0.12	-0.11	-0.05	-0.22	-0.15	-0.16	0.09	-0.08	0.04
25	1	-0.20	0.06	-0.12	-0.17	-0.20	-0.15	-0.02	0.08	0.04
26	1	0.06	-0.03	0.06	0.07	-0.02	0.01	-0.09	-0.04	0.04
27	8	0.01	0.09	0.00	0.02	-0.09	-0.01	0.08	-0.32	0.04
28	1	0.15	0.01	-0.01	-0.13	0.02	-0.05	-0.15	-0.20	0.08

	22			23			24		
	?A			?A			?A		
Frequencies --	800.2069			823.8986			835.1738		
Red. masses --	3.9631			5.0754			4.2247		
Frc consts --	1.4952			2.0299			1.7362		
IR Inten --	1.0231			2.2869			44.1472		
Raman Activ --	9.4528			17.0634			0.5929		
Depolar --	0.1081			0.0043			0.6695		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.01	-0.04	-0.03	0.08	-0.09	-0.07	-0.21	0.02	-0.07
2 6	-0.05	0.02	0.04	-0.07	-0.02	0.25	-0.12	-0.11	0.05
3 6	0.09	-0.04	-0.20	0.01	0.02	0.08	0.02	-0.13	0.03
4 6	0.11	0.01	0.20	0.12	0.04	-0.15	0.07	-0.10	-0.04
5 6	-0.07	0.03	0.02	0.01	-0.02	-0.02	0.07	-0.04	-0.02
6 6	-0.02	-0.07	0.03	-0.04	-0.06	0.26	0.08	0.12	-0.07
7 6	-0.04	0.00	-0.01	-0.09	0.10	-0.07	-0.01	0.24	0.11
8 6	0.04	0.13	0.22	0.07	0.12	-0.18	0.11	-0.06	0.05

9	6	0.04	-0.01	0.01	-0.02	0.00	-0.03	0.05	0.01	0.00
10	6	-0.02	0.05	-0.23	0.03	0.02	0.09	0.10	-0.06	-0.04
11	6	-0.07	-0.06	-0.05	-0.16	-0.15	-0.14	-0.06	0.02	-0.01
12	8	0.03	-0.03	0.00	-0.02	0.02	0.01	-0.08	0.07	0.00
13	6	0.00	-0.05	-0.01	-0.01	0.02	-0.02	-0.02	-0.04	0.01
14	7	-0.03	-0.01	0.01	0.01	0.00	0.00	-0.04	-0.02	0.01
15	8	-0.02	-0.03	0.00	0.01	0.00	-0.01	0.06	0.05	-0.02
16	1	0.09	0.05	-0.12	0.17	0.05	-0.05	-0.12	0.13	-0.16
17	1	-0.01	0.27	0.09	-0.21	0.23	0.11	0.00	-0.30	0.19
18	1	0.34	-0.16	-0.10	0.14	0.16	-0.01	0.09	-0.17	0.07
19	1	0.28	-0.07	0.15	0.03	0.20	-0.08	0.18	-0.17	-0.08
20	1	0.21	-0.05	0.09	0.20	-0.24	0.12	0.23	-0.01	-0.19
21	1	0.05	0.05	-0.11	0.09	0.16	-0.06	-0.06	0.19	0.29
22	1	-0.04	0.30	0.15	0.18	0.02	-0.11	0.12	-0.25	0.10
23	1	-0.13	0.29	-0.13	0.19	0.16	0.01	0.12	-0.19	-0.07
24	1	-0.16	-0.15	-0.03	-0.20	-0.20	-0.14	0.09	-0.13	-0.01
25	1	-0.03	0.00	0.08	-0.13	-0.12	-0.06	0.08	-0.14	-0.02
26	1	0.02	-0.03	0.00	0.01	0.01	0.01	-0.01	0.04	-0.01
27	8	-0.03	0.06	0.00	0.03	-0.04	0.01	-0.05	0.08	0.00
28	1	-0.03	0.07	-0.01	0.06	-0.06	0.00	-0.08	0.09	0.00

	25	26	27
	?A	?A	?A
Frequencies --	882.5784	889.8771	904.0917
Red. masses --	3.1985	2.4194	2.8046
Frc consts --	1.4679	1.1288	1.3507
IR Inten --	2.9001	10.7533	42.5334
Raman Activ --	12.7903	1.6515	3.5885
Depolar --	0.0845	0.6375	0.1632

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.16	-0.07	0.12	0.04	0.04	-0.07	-0.07	-0.02	0.01
2	6	0.14	-0.13	-0.06	-0.01	-0.05	0.13	-0.02	0.01	0.00

3	6	-0.04	0.00	-0.02	0.05	0.13	0.07	0.02	-0.06	0.01
4	6	0.06	0.01	-0.01	0.00	0.07	-0.07	-0.07	0.13	-0.08
5	6	-0.04	0.03	-0.03	-0.05	0.03	-0.06	-0.06	0.07	0.06
6	6	-0.12	0.15	-0.07	0.08	-0.01	-0.10	0.00	0.04	0.01
7	6	-0.07	0.10	0.11	-0.04	-0.03	0.04	-0.02	-0.14	0.05
8	6	0.02	0.12	0.00	-0.07	-0.01	0.07	0.23	0.03	-0.07
9	6	0.01	0.00	-0.02	-0.01	0.02	0.05	0.06	0.03	0.07
10	6	-0.02	-0.06	-0.04	-0.12	-0.04	-0.05	-0.01	-0.02	-0.05
11	6	-0.09	-0.09	-0.02	0.03	-0.03	-0.01	-0.04	0.02	0.04
12	8	0.02	-0.02	0.01	0.03	-0.03	0.01	0.04	-0.04	-0.02
13	6	-0.01	-0.01	-0.01	0.01	-0.01	-0.03	-0.02	-0.03	-0.06
14	7	-0.01	0.00	0.00	0.01	0.01	0.01	-0.03	-0.02	0.02
15	8	-0.01	-0.01	0.00	-0.01	-0.02	0.02	0.00	-0.01	-0.01
16	1	0.23	0.12	0.36	-0.01	-0.02	-0.07	-0.18	-0.17	0.06
17	1	0.09	-0.34	-0.14	-0.07	-0.36	0.05	0.01	0.01	0.03
18	1	-0.11	-0.02	-0.01	0.38	0.34	-0.07	0.09	-0.21	0.13
19	1	-0.11	-0.06	-0.01	0.10	0.04	-0.10	-0.10	0.26	-0.03
20	1	-0.34	0.21	-0.05	0.38	-0.01	-0.05	0.07	0.17	0.17
21	1	0.11	0.13	0.38	0.00	-0.01	0.02	-0.23	-0.26	0.23
22	1	-0.03	0.04	0.00	-0.07	-0.08	0.09	0.51	0.10	0.02
23	1	-0.07	-0.22	-0.03	-0.32	-0.34	0.05	-0.11	-0.06	0.01
24	1	0.01	0.01	-0.04	0.12	-0.18	0.00	0.04	0.11	0.02
25	1	-0.15	-0.08	-0.11	-0.05	0.08	0.02	-0.15	0.04	-0.09
26	1	-0.03	0.00	0.00	-0.05	0.00	-0.01	-0.10	0.02	-0.01
27	8	0.00	0.00	0.01	0.02	-0.01	0.00	0.00	0.02	0.00
28	1	0.01	-0.02	0.04	-0.02	0.00	0.01	-0.16	0.14	-0.05
		28			29			30		
		?A			?A			?A		

Frequencies --		932.5034			954.2093			974.7538		
Red. masses --		2.2005			3.2135			2.1486		
Frc consts --		1.1274			1.7239			1.2028		
IR Inten --		18.3541			145.1521			63.3074		
Raman Activ --		2.5636			6.5801			4.3464		
Depolar --		0.5593			0.6866			0.4631		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.08	0.02	0.04	-0.02	0.00	-0.04	0.04	-0.03	0.01
2	6	0.13	0.01	0.04	0.06	-0.02	0.07	0.04	0.15	-0.04
3	6	-0.03	0.01	-0.07	-0.03	0.06	0.07	-0.05	-0.05	0.05
4	6	0.10	0.12	-0.03	-0.01	-0.01	-0.06	0.01	-0.09	-0.06
5	6	0.03	-0.03	0.07	-0.19	0.21	-0.02	-0.05	0.09	0.04
6	6	-0.02	-0.06	-0.06	-0.12	-0.07	0.00	0.11	-0.04	-0.03
7	6	-0.03	0.06	0.01	0.00	0.06	-0.04	-0.01	0.08	0.03
8	6	0.00	-0.10	-0.03	0.04	-0.10	0.08	-0.03	0.02	0.02
9	6	0.00	-0.03	0.03	0.01	-0.03	-0.05	-0.03	0.06	0.02
10	6	-0.09	0.06	0.01	0.12	0.02	-0.02	-0.06	-0.04	-0.03
11	6	0.01	-0.07	0.01	0.05	0.03	-0.03	-0.06	-0.03	0.04
12	8	-0.01	0.01	-0.01	0.11	-0.08	0.01	0.04	-0.02	0.00
13	6	0.01	0.01	-0.01	0.01	0.00	0.04	0.01	-0.01	-0.01
14	7	0.01	0.01	0.00	0.00	0.00	-0.01	0.00	0.00	0.00
15	8	-0.03	-0.02	-0.02	0.01	-0.03	0.00	0.00	-0.01	-0.01
16	1	-0.14	-0.02	0.20	-0.07	-0.06	-0.02	0.09	0.05	-0.02
17	1	0.31	0.13	0.26	0.07	-0.07	0.10	0.01	0.47	-0.06
18	1	-0.14	-0.04	-0.05	-0.05	-0.06	0.16	-0.20	-0.31	0.24
19	1	0.31	0.40	0.06	0.06	-0.23	-0.17	-0.04	-0.20	-0.10
20	1	-0.08	-0.17	-0.19	-0.38	-0.17	-0.15	0.38	-0.13	-0.08
21	1	-0.02	0.06	0.04	-0.04	0.05	-0.05	0.06	0.12	-0.05
22	1	-0.01	-0.30	0.01	0.01	-0.25	0.09	0.02	-0.09	0.06
23	1	-0.21	0.23	0.11	0.33	0.09	-0.14	-0.13	-0.15	0.00

24	1	0.11	-0.04	0.00	-0.15	-0.11	0.00	0.16	0.19	-0.01
25	1	0.10	-0.23	-0.07	0.21	0.01	0.18	-0.11	-0.16	-0.22
26	1	0.08	-0.03	0.02	-0.34	0.10	0.02	-0.15	0.06	0.02
27	8	-0.01	0.02	-0.02	-0.03	0.03	0.00	0.02	-0.03	0.00
28	1	-0.01	0.02	-0.03	0.03	0.00	-0.01	-0.02	-0.01	0.00

	31			32			33		
	?A			?A			?A		
Frequencies --	1001.9306			1010.2601			1024.0598		
Red. masses --	2.4485			3.5355			2.0891		
Frc consts --	1.4482			2.1260			1.2908		
IR Inten --	7.2258			20.2589			4.3462		
Raman Activ --	7.1485			4.0716			2.1093		
Depolar --	0.2839			0.4118			0.1269		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.10	-0.05	-0.01	0.03	0.09	-0.02	0.06	-0.08	-0.10
2	6	0.01	-0.06	-0.03	-0.01	0.01	0.08	0.04	0.00	0.05
3	6	0.13	-0.08	0.01	0.03	-0.10	0.06	-0.02	0.03	-0.07
4	6	-0.13	-0.01	-0.01	-0.02	-0.06	-0.04	-0.06	-0.04	0.13
5	6	0.01	0.01	0.08	0.05	-0.05	-0.01	-0.02	0.02	0.00
6	6	-0.03	0.06	0.04	-0.12	-0.10	-0.16	0.03	-0.03	-0.05
7	6	0.01	0.11	-0.04	-0.04	-0.07	0.07	-0.08	0.05	0.06
8	6	-0.03	-0.12	0.00	-0.02	0.07	0.00	0.03	0.00	-0.11
9	6	-0.01	0.00	0.09	-0.04	0.21	0.01	0.05	-0.05	0.01
10	6	-0.08	0.09	-0.01	0.06	0.18	-0.03	0.01	-0.02	0.07
11	6	0.01	0.04	-0.08	0.04	-0.05	0.02	0.02	0.05	-0.01
12	8	-0.01	0.00	-0.02	-0.03	0.02	0.00	0.01	-0.01	0.00
13	6	0.01	0.00	-0.02	-0.01	-0.03	0.01	-0.01	0.00	-0.01
14	7	0.01	0.01	0.00	-0.04	-0.01	0.01	-0.01	-0.01	0.00
15	8	0.01	0.00	-0.01	0.02	0.02	-0.01	0.01	0.01	0.00
16	1	0.07	-0.06	0.15	0.12	0.19	-0.15	0.08	-0.12	-0.29
17	1	-0.14	0.02	-0.20	0.05	-0.04	0.15	0.14	0.17	0.18

18	1	0.34	-0.29	0.17	0.15	-0.13	0.08	-0.16	0.09	-0.12
19	1	-0.28	0.02	0.02	-0.13	-0.12	-0.05	-0.25	0.00	0.17
20	1	0.12	0.01	-0.01	-0.26	-0.21	-0.31	0.07	-0.27	-0.30
21	1	0.02	0.09	0.07	-0.05	-0.10	0.23	-0.25	-0.06	0.29
22	1	0.03	-0.29	0.06	0.08	0.14	0.04	-0.06	0.11	-0.18
23	1	-0.26	0.31	0.12	0.14	0.39	-0.06	-0.09	-0.02	0.14
24	1	-0.26	-0.11	-0.04	0.21	-0.15	0.02	0.13	-0.19	0.01
25	1	0.13	0.14	0.23	-0.08	0.04	-0.04	-0.14	0.31	0.09
26	1	-0.01	0.01	-0.01	0.07	-0.02	-0.01	-0.03	0.01	0.01
27	8	0.01	-0.01	-0.02	0.08	-0.12	0.01	-0.01	0.04	0.00
28	1	-0.06	0.05	-0.05	-0.18	0.08	-0.08	-0.06	0.07	0.00

	34			35			36		
	?A			?A			?A		
Frequencies --	1029.4377			1031.1737			1041.0778		
Red. masses --	2.9454			3.4378			2.3363		
Frc consts --	1.8391			2.1537			1.4919		
IR Inten --	0.6522			8.2242			3.0874		
Raman Activ --	3.0607			3.4168			7.2476		
Depolar --	0.7451			0.1873			0.3321		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.08	0.16	0.05	-0.12	0.16	-0.06	-0.03	-0.08	-0.07
2 6	-0.03	0.06	0.11	0.11	-0.03	-0.03	0.13	-0.02	0.09
3 6	-0.12	-0.14	-0.04	0.03	0.07	0.00	-0.06	-0.05	0.00
4 6	-0.05	0.09	0.00	-0.07	-0.09	0.08	0.02	-0.04	-0.02
5 6	0.01	0.01	-0.05	-0.01	0.02	0.01	0.02	-0.03	0.01
6 6	0.03	0.11	-0.03	0.02	-0.07	0.09	-0.03	0.10	0.06
7 6	0.03	-0.08	-0.04	0.19	0.00	0.10	-0.06	-0.02	-0.06
8 6	-0.05	-0.06	0.03	0.11	0.00	-0.06	-0.02	0.03	0.04
9 6	0.05	-0.04	0.03	-0.07	0.05	-0.07	-0.10	0.09	-0.01
10 6	0.08	-0.03	0.01	-0.16	-0.05	0.00	-0.06	-0.03	-0.05
11 6	0.03	-0.10	-0.13	-0.09	-0.01	-0.12	0.08	0.09	-0.03

12	8	0.01	-0.01	0.00	0.01	-0.01	0.00	-0.02	0.01	0.00
13	6	-0.01	0.00	0.00	0.01	0.00	-0.01	0.02	-0.01	0.00
14	7	0.00	0.00	0.00	0.01	0.01	0.00	0.01	0.01	0.00
15	8	-0.01	0.00	0.00	-0.01	0.00	0.01	0.02	0.02	-0.01
16	1	0.16	0.32	0.09	0.07	0.54	0.12	-0.13	-0.28	-0.13
17	1	0.05	0.27	0.22	0.25	-0.05	0.14	0.36	0.07	0.35
18	1	-0.32	-0.16	-0.03	0.02	0.06	0.01	-0.23	-0.15	0.06
19	1	-0.18	-0.02	-0.03	-0.10	-0.13	0.07	0.16	-0.06	-0.04
20	1	0.23	0.13	0.02	-0.09	-0.01	0.13	0.03	0.28	0.26
21	1	0.13	-0.09	0.21	0.26	0.00	0.20	-0.15	-0.04	-0.09
22	1	-0.07	0.01	0.01	0.09	0.08	-0.08	0.08	0.12	0.07
23	1	-0.01	-0.18	0.06	-0.09	-0.01	-0.05	-0.04	-0.19	-0.09
24	1	-0.19	-0.36	-0.08	-0.13	-0.36	-0.08	-0.16	-0.07	0.01
25	1	0.10	0.03	0.17	-0.01	0.06	0.10	0.14	0.21	0.22
26	1	-0.05	0.01	-0.02	-0.05	0.02	0.01	0.08	-0.02	0.00
27	8	-0.03	0.03	0.00	0.01	-0.04	0.00	0.04	-0.05	0.01
28	1	-0.04	0.04	0.01	0.08	-0.11	0.05	0.04	-0.06	0.00

	37			38			39		
	?A			?A			?A		
Frequencies --	1061.6044			1082.2830			1092.3286		
Red. masses --	2.7222			2.2504			2.5199		
Frc consts --	1.8076			1.5531			1.7715		
IR Inten --	34.1734			25.6908			69.1152		
Raman Activ --	8.4812			6.4221			7.9377		
Depolar --	0.7411			0.6588			0.7433		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	-0.06	0.02	0.02	-0.09	0.03	-0.02	0.03	0.06
2 6	0.04	0.05	-0.03	-0.07	0.01	0.01	-0.05	-0.03	-0.08
3 6	-0.08	0.11	0.08	0.02	-0.01	-0.07	0.04	0.03	-0.07
4 6	-0.11	0.05	-0.02	0.04	0.09	0.03	0.04	0.03	0.09
5 6	0.10	-0.12	0.00	-0.03	0.02	0.00	-0.03	0.04	-0.02

6	6	-0.04	-0.12	-0.01	0.02	0.02	-0.06	0.03	0.00	0.05
7	6	-0.01	0.04	0.05	0.13	-0.03	0.04	-0.13	0.05	-0.04
8	6	0.09	0.00	0.12	-0.02	-0.07	0.03	0.03	-0.07	-0.04
9	6	0.10	0.04	-0.05	-0.11	0.13	-0.03	-0.10	0.18	0.01
10	6	0.02	0.00	-0.11	0.04	-0.03	0.06	0.04	-0.07	0.03
11	6	-0.01	0.02	-0.08	-0.09	0.05	-0.04	0.08	-0.04	-0.02
12	8	-0.03	0.01	0.00	0.00	0.00	0.00	0.02	0.00	0.00
13	6	-0.02	-0.02	0.01	0.01	-0.01	0.01	0.02	-0.03	0.00
14	7	-0.04	-0.02	0.00	0.00	0.01	0.00	-0.01	0.00	0.00
15	8	0.00	0.03	0.00	0.00	-0.01	0.00	-0.03	-0.02	0.01
16	1	-0.09	-0.16	0.26	-0.09	-0.30	-0.06	0.04	0.19	0.22
17	1	-0.12	0.26	-0.22	-0.04	0.09	0.07	-0.16	0.07	-0.21
18	1	-0.25	0.26	-0.03	0.01	0.10	-0.16	-0.02	0.13	-0.15
19	1	-0.13	0.10	0.01	0.16	0.19	0.06	-0.01	0.07	0.12
20	1	0.16	-0.16	-0.02	0.05	-0.13	-0.22	0.17	-0.02	0.05
21	1	-0.03	0.04	0.03	0.34	0.01	0.34	-0.43	-0.06	-0.06
22	1	0.02	-0.21	0.13	0.01	-0.18	0.06	0.12	-0.05	0.00
23	1	0.12	-0.26	-0.20	0.15	-0.09	-0.02	0.16	-0.20	-0.06
24	1	-0.24	-0.11	-0.04	-0.35	0.27	-0.04	0.12	-0.27	0.00
25	1	0.08	0.10	0.17	-0.21	0.23	0.02	0.33	-0.24	0.10
26	1	0.22	-0.09	0.00	-0.01	0.00	0.00	-0.08	0.03	0.00
27	8	0.00	0.00	0.01	0.01	-0.05	0.00	0.05	-0.06	0.02
28	1	-0.17	0.13	-0.05	0.04	-0.10	0.05	-0.20	0.13	-0.08

	40	41	42
	?A	?A	?A
Frequencies --	1118.2493	1159.6807	1177.6174
Red. masses --	1.8847	1.5952	2.1938
Frc consts --	1.3885	1.2640	1.7925
IR Inten --	63.5988	3.1111	55.4886
Raman Activ --	4.6682	2.7165	1.9913
Depolar --	0.6490	0.6823	0.6306

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	0.01	0.00	-0.06	-0.01	0.05	0.00	-0.02	0.00
2	6	0.00	0.01	-0.01	0.00	-0.01	-0.04	-0.03	-0.01	0.00
3	6	0.00	0.00	0.01	0.05	-0.02	0.05	0.00	0.00	-0.01
4	6	-0.05	0.03	0.00	0.07	-0.02	-0.03	0.00	0.01	0.01
5	6	0.02	-0.03	0.00	0.03	0.02	-0.05	0.23	0.03	0.00
6	6	0.03	0.01	-0.04	0.00	-0.01	-0.02	0.00	-0.01	-0.01
7	6	-0.07	0.01	0.00	-0.02	-0.04	0.04	-0.01	0.01	0.01
8	6	0.07	0.00	0.07	-0.02	0.06	-0.02	0.01	0.02	0.02
9	6	-0.18	-0.11	-0.02	0.03	-0.03	-0.04	-0.01	0.00	0.00
10	6	0.00	0.02	0.00	-0.03	0.05	0.05	0.00	0.01	-0.02
11	6	0.02	-0.02	0.01	0.04	0.04	-0.07	-0.01	0.00	0.00
12	8	-0.01	0.00	0.00	0.02	0.01	0.00	0.07	0.03	-0.01
13	6	0.02	0.04	0.01	-0.01	0.01	0.01	0.00	0.01	0.00
14	7	0.06	0.04	-0.02	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	-0.04	-0.02	0.01	-0.16	-0.07	0.02
16	1	0.00	0.01	0.07	-0.21	-0.15	0.33	0.01	-0.08	-0.19
17	1	-0.06	0.04	-0.08	-0.10	0.18	-0.14	0.10	-0.13	0.16
18	1	-0.01	0.00	0.01	-0.02	-0.08	0.10	-0.05	0.02	-0.03
19	1	-0.08	-0.03	-0.02	0.29	-0.20	-0.13	-0.20	-0.02	0.02
20	1	0.13	-0.13	-0.18	0.22	-0.12	-0.10	-0.05	0.06	0.07
21	1	-0.10	-0.03	0.17	-0.13	-0.14	0.38	0.06	0.07	-0.14
22	1	0.41	0.17	0.18	-0.19	0.30	-0.15	0.08	-0.14	0.08
23	1	0.19	0.13	-0.12	-0.09	0.01	0.09	0.05	0.00	-0.05
24	1	0.13	-0.09	0.01	-0.20	-0.09	-0.03	0.00	-0.01	0.00
25	1	-0.03	0.01	-0.02	0.15	0.08	0.17	-0.07	0.07	0.00
26	1	0.07	-0.03	-0.01	-0.16	0.07	0.00	-0.75	0.35	0.03

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  27   8    -0.03   0.00  -0.02     0.00   0.01   0.00     0.00   0.00
0.00
  28   1     0.50  -0.42   0.17     0.03  -0.03   0.03     0.01  -0.01
0.00
                     43                    44                    45
                     ?A                    ?A                    ?A
 Frequencies --  1202.3179             1222.3806             1234.2257
 Red. masses --     2.5842                2.8870                1.7935
 Frc consts  --     2.2009                2.5416                1.6097
 IR Inten    --    12.4331               24.1581                4.7216
 Raman Activ --     2.4734                3.4538                2.0769
 Depolar     --     0.7193                0.5908                0.6700
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.01   0.03  -0.06    -0.05  -0.02   0.11     0.01  -0.01
0.03
   2   6     0.03  -0.07   0.04    -0.10   0.01  -0.06     0.01   0.12
0.00
   3   6    -0.07   0.11  -0.07     0.01   0.11  -0.06    -0.10   0.00
0.02
   4   6    -0.04  -0.10  -0.05     0.10  -0.07  -0.09     0.02   0.01
0.01
   5   6     0.05   0.00   0.10    -0.02   0.03   0.14     0.02  -0.02  -
0.04
   6   6    -0.07   0.03   0.05     0.02  -0.07  -0.05     0.13  -0.01
0.03
   7   6     0.07  -0.01  -0.04    -0.03  -0.05   0.09    -0.02   0.02
0.01
   8   6    -0.11  -0.01  -0.04    -0.07   0.11  -0.07    -0.02   0.00  -
0.01
   9   6    -0.03  -0.02   0.15    -0.03  -0.03   0.11    -0.02  -0.01
0.04
  10   6     0.10  -0.07  -0.11     0.09  -0.02  -0.03    -0.03  -0.11  -
0.04
  11   6     0.01   0.02   0.04     0.06   0.05  -0.10     0.00  -0.01  -
0.06
  12   8     0.02   0.01   0.00    -0.02  -0.01   0.00     0.00   0.00
0.01
  13   6     0.00   0.00  -0.03     0.00   0.01  -0.02     0.01   0.00  -
0.01
  14   7     0.02   0.01   0.00     0.01   0.01   0.00     0.01   0.01
0.00
  15   8    -0.02   0.00  -0.01     0.01  -0.01  -0.02     0.00   0.00
0.00
  16   1    -0.02   0.11   0.20     0.05   0.09  -0.03    -0.09  -0.18  -
0.03
  17   1    -0.16   0.13  -0.18     0.16  -0.05   0.26    -0.01  -0.38  -
0.06
  18   1     0.01   0.02   0.01    -0.04  -0.09   0.09     0.35  -0.10
0.11
  19   1     0.30   0.16   0.02    -0.36   0.02   0.00     0.02  -0.03  -
0.01
  20   1     0.17  -0.25  -0.20    -0.02   0.11   0.15    -0.41  -0.05  -
0.12
```

21	1	0.07	-0.08	0.39	0.11	0.05	-0.09	-0.10	-0.04	0.18
22	1	0.19	0.39	0.00	0.15	-0.38	0.13	-0.02	0.12	-0.03
23	1	0.10	0.00	-0.11	0.00	-0.03	0.03	0.15	0.49	-0.09
24	1	0.02	0.18	0.03	-0.19	-0.23	-0.04	-0.15	-0.04	-0.04
25	1	0.01	-0.06	-0.06	0.14	0.20	0.25	0.03	0.04	0.06
26	1	-0.16	0.08	0.03	0.23	-0.10	0.03	0.02	-0.01	0.00
27	8	0.01	0.01	0.00	-0.01	0.00	-0.01	0.02	0.00	0.01
28	1	-0.15	0.12	-0.03	0.18	-0.15	0.06	-0.18	0.15	-0.06

	46			47			48		
	?A			?A			?A		
Frequencies --	1245.2077			1258.1018			1274.4165		
Red. masses --	1.5225			1.7545			1.5734		
Frc consts --	1.3909			1.6362			1.5056		
IR Inten --	5.1435			8.4486			4.2840		
Raman Activ --	7.1934			13.9093			4.4483		
Depolar --	0.7338			0.7388			0.7131		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	0.00	-0.01	0.02	-0.02	0.00	-0.01	-0.03	-0.03
2 6	0.00	-0.01	0.00	-0.03	0.01	0.05	0.06	0.07	0.04
3 6	0.01	0.01	-0.04	-0.03	0.00	-0.06	-0.07	-0.08	0.01
4 6	-0.04	0.00	-0.07	-0.03	-0.05	-0.06	-0.02	-0.08	0.03
5 6	0.01	0.01	0.12	0.01	0.00	0.14	-0.04	-0.02	-0.03
6 6	0.03	0.00	0.01	0.04	0.06	-0.02	-0.01	-0.04	-0.05
7 6	-0.02	-0.02	-0.01	0.01	-0.02	-0.01	-0.01	-0.01	0.05
8 6	0.00	0.04	0.07	0.02	0.01	0.04	0.01	0.03	-0.04
9 6	0.03	0.01	-0.10	0.04	0.04	-0.11	0.00	0.01	0.03
10 6	-0.02	-0.03	0.04	0.00	-0.06	0.05	0.05	0.03	0.00
11 6	0.01	0.00	0.00	-0.01	0.02	-0.01	0.00	0.03	-0.02
12 8	0.00	0.00	-0.01	0.01	0.00	-0.01	0.02	0.02	0.00
13 6	0.00	0.00	0.02	0.00	-0.01	0.02	0.00	0.00	0.00
14 7	-0.01	-0.01	0.00	-0.02	-0.01	0.00	0.00	0.00	0.00

15	8	0.00	0.00	-0.01	0.00	0.01	-0.02	0.03	0.03	0.00
16	1	0.21	0.19	-0.31	-0.08	-0.01	0.49	0.02	0.08	0.11
17	1	0.07	-0.15	0.08	-0.11	0.08	-0.03	-0.17	-0.07	-0.24
18	1	-0.02	0.13	-0.13	0.15	0.12	-0.14	0.27	0.16	-0.16
19	1	-0.06	-0.03	-0.08	0.20	-0.08	-0.09	0.14	0.42	0.22
20	1	0.03	-0.05	-0.04	-0.21	0.00	-0.13	0.01	0.18	0.19
21	1	-0.24	-0.16	0.30	-0.06	0.00	-0.30	-0.03	0.01	-0.05
22	1	-0.07	0.02	0.04	0.03	0.00	0.05	0.00	-0.15	0.00
23	1	-0.09	0.11	0.10	-0.12	0.17	0.16	-0.15	-0.06	0.12
24	1	-0.30	0.33	-0.01	0.31	-0.35	0.01	-0.13	0.07	-0.01
25	1	0.36	-0.39	0.02	-0.19	0.23	0.00	0.22	-0.16	0.06
26	1	-0.01	0.00	0.01	-0.10	0.05	0.03	-0.31	0.14	0.01
27	8	0.00	0.00	0.01	-0.01	0.00	0.01	-0.02	0.00	-0.01
28	1	0.02	-0.02	0.03	0.05	-0.05	0.02	0.25	-0.22	0.08

	49			50			51		
	?A			?A			?A		
Frequencies --	1311.1154			1319.6762			1338.6808		
Red. masses --	1.6634			1.6399			1.4806		
Frc consts --	1.6847			1.6827			1.5633		
IR Inten --	4.2589			26.9642			33.9990		
Raman Activ --	0.6601			2.0102			1.4587		
Depolar --	0.7499			0.6691			0.6258		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.14	0.02	0.01	-0.02	0.00	-0.03	0.00	-0.02
2	6	0.05	0.02	-0.01	0.00	0.02	-0.02	0.03	-0.07	-0.01
3	6	-0.01	-0.03	-0.03	-0.02	-0.10	0.02	-0.10	0.03	0.01
4	6	0.00	-0.04	0.03	0.02	0.04	-0.01	0.06	0.07	0.02
5	6	0.00	0.02	0.07	-0.02	0.01	0.11	0.04	0.01	0.00
6	6	-0.04	-0.03	0.02	0.02	-0.04	-0.02	0.03	0.00	0.03
7	6	-0.09	0.03	-0.03	0.04	0.04	0.03	0.00	0.00	-0.02
8	6	0.03	0.00	-0.03	-0.01	-0.03	-0.03	-0.03	-0.04	-0.01

9	6	0.02	0.04	-0.02	-0.06	-0.07	0.06	0.03	0.06	-0.01
10	6	0.03	-0.02	0.01	-0.02	0.07	-0.02	0.06	0.02	-0.02
11	6	0.06	-0.08	0.00	-0.03	0.02	-0.01	-0.01	0.01	0.02
12	8	-0.01	0.00	-0.01	0.00	0.00	-0.02	-0.01	-0.01	0.00
13	6	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00
14	7	-0.01	-0.01	0.00	0.02	0.01	0.00	-0.01	-0.01	0.00
15	8	0.00	0.00	-0.01	0.01	0.01	-0.02	-0.02	-0.01	0.00
16	1	-0.31	-0.40	-0.11	-0.02	-0.06	0.06	-0.04	-0.03	-0.09
17	1	-0.06	-0.26	-0.16	0.06	0.05	0.06	-0.03	0.37	-0.06
18	1	-0.02	0.16	-0.17	0.11	0.50	-0.41	0.49	-0.04	0.09
19	1	0.00	-0.27	-0.06	-0.04	-0.37	-0.17	-0.30	-0.29	-0.08
20	1	0.25	0.02	0.13	-0.11	0.14	0.16	-0.25	-0.01	-0.03
21	1	0.35	0.17	0.14	-0.08	0.00	0.01	-0.01	-0.02	0.09
22	1	0.09	-0.07	0.00	-0.05	0.22	-0.09	0.06	0.06	0.01
23	1	-0.13	0.07	0.12	0.18	-0.25	-0.19	-0.30	-0.19	0.20
24	1	-0.16	0.18	-0.01	0.03	-0.07	-0.01	0.01	0.01	0.01
25	1	-0.20	0.19	-0.02	0.04	-0.06	0.00	0.05	-0.10	-0.03
26	1	0.04	-0.02	0.01	-0.06	0.03	0.02	0.11	-0.05	0.00
27	8	-0.01	0.00	0.00	0.02	0.00	0.00	-0.02	-0.01	-0.01
28	1	0.05	-0.05	0.03	-0.17	0.15	-0.07	0.22	-0.20	0.08

	52	53	54
	?A	?A	?A
Frequencies --	1345.8547	1348.5440	1375.1411
Red. masses --	1.5017	1.6620	1.6414
Frc consts --	1.6026	1.7808	1.8288
IR Inten --	0.5930	22.6584	7.6800
Raman Activ --	3.1678	1.3076	1.5965
Depolar --	0.7255	0.6471	0.6711

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.04	-0.03	-0.05	-0.02	0.05	0.02	-0.05	-0.05	0.02
2	6	0.05	-0.01	-0.01	-0.01	-0.11	-0.06	0.03	0.07	-0.08

3	6	-0.05	0.00	0.02	0.00	-0.02	0.06	-0.02	-0.06	0.04
4	6	0.04	0.04	0.03	0.00	-0.05	-0.01	0.07	0.01	-0.01
5	6	0.01	0.00	0.00	-0.06	-0.04	-0.01	-0.04	-0.02	-0.01
6	6	-0.09	0.05	-0.05	0.07	0.04	0.01	-0.06	0.03	0.08
7	6	0.03	-0.04	-0.01	-0.06	-0.02	-0.05	0.01	-0.02	-0.01
8	6	0.03	0.05	0.00	0.00	0.05	0.02	-0.07	-0.03	0.03
9	6	-0.02	-0.01	0.02	0.02	-0.02	0.00	0.03	-0.01	-0.07
10	6	0.00	-0.08	0.04	-0.06	-0.01	0.00	0.01	0.02	-0.01
11	6	-0.01	0.03	0.03	0.06	-0.04	0.01	0.02	0.02	0.00
12	8	0.00	0.00	0.00	0.02	0.01	0.00	0.01	0.01	0.00
13	6	0.00	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.02
14	7	0.01	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00
15	8	0.00	0.00	0.00	0.03	0.02	0.00	0.02	0.01	0.00
16	1	0.00	0.10	0.11	0.00	0.05	-0.07	0.08	0.16	0.02
17	1	0.02	0.09	-0.05	0.11	0.56	0.11	0.19	-0.29	0.09
18	1	0.21	0.10	-0.04	0.18	0.26	-0.13	0.14	0.16	-0.11
19	1	-0.26	-0.22	-0.05	-0.01	0.23	0.11	-0.33	0.18	0.11
20	1	0.51	0.04	0.03	-0.22	-0.01	-0.10	0.28	-0.32	-0.24
21	1	0.00	-0.05	-0.05	0.15	0.02	0.17	0.08	0.01	-0.03
22	1	-0.26	-0.32	-0.04	0.01	-0.28	0.10	0.39	0.18	0.18
23	1	0.24	0.47	-0.06	0.19	0.09	-0.16	-0.15	-0.08	0.08
24	1	0.06	-0.02	0.02	-0.10	0.14	0.01	0.07	-0.09	0.01
25	1	0.03	-0.06	-0.03	-0.12	0.18	0.02	-0.07	0.14	0.03
26	1	0.04	-0.02	0.00	-0.22	0.10	0.01	-0.11	0.06	0.00
27	8	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.00	0.01
28	1	-0.05	0.04	-0.02	-0.08	0.07	-0.02	-0.10	0.09	-0.03
			55			56			57	
			?A			?A			?A	

Frequencies --	1383.6418			1385.8125			1396.4618		
Red. masses --	1.4645			1.6382			1.5538		
Frc consts --	1.6520			1.8537			1.7852		
IR Inten --	2.6237			7.1343			30.7706		
Raman Activ --	0.8996			3.0126			2.6919		
Depolar --	0.6561			0.6744			0.7493		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	0.01	-0.02	0.06	-0.01	0.03	-0.01	-0.01	-0.03
2 6	-0.02	0.01	-0.04	-0.06	0.00	-0.09	0.00	0.05	0.00
3 6	-0.08	0.02	-0.06	-0.01	0.03	0.05	0.02	-0.04	-0.02
4 6	-0.05	-0.02	0.00	-0.03	0.01	-0.03	0.02	0.00	0.00
5 6	0.02	0.01	0.01	-0.03	-0.04	-0.01	0.00	0.01	0.03
6 6	-0.02	0.00	0.01	-0.04	-0.05	-0.01	0.02	0.04	0.08
7 6	-0.02	0.00	0.02	0.00	0.06	-0.02	0.00	-0.03	-0.04
8 6	0.06	0.02	0.00	0.01	-0.08	0.00	0.02	0.03	0.00
9 6	-0.05	-0.04	-0.02	0.06	0.08	0.04	0.07	0.07	0.10
10 6	0.01	0.06	0.07	0.02	-0.05	-0.01	-0.05	0.03	-0.04
11 6	0.03	-0.04	0.00	0.00	-0.02	0.00	0.02	-0.01	0.01
12 8	0.00	-0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00
13 6	0.00	0.00	0.00	0.00	0.00	-0.01	-0.01	0.00	-0.02
14 7	0.01	0.01	0.00	-0.02	-0.01	0.01	-0.01	-0.01	0.01
15 8	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00
16 1	0.02	0.06	0.16	0.07	0.00	0.04	-0.02	0.06	0.18
17 1	0.22	-0.10	0.23	0.36	0.01	0.42	0.00	-0.26	-0.01
18 1	0.55	-0.24	0.15	0.11	0.08	0.02	-0.14	0.05	-0.09
19 1	0.19	0.03	-0.01	0.16	0.08	-0.03	-0.10	-0.08	-0.02
20 1	0.15	-0.11	-0.08	0.20	0.14	0.24	-0.11	-0.31	-0.32
21 1	-0.01	0.03	-0.15	-0.08	0.02	0.08	-0.13	-0.11	0.04
22 1	-0.18	-0.05	-0.08	-0.18	0.37	-0.17	-0.36	-0.23	-0.11
23 1	0.12	-0.40	-0.04	0.04	0.25	0.01	0.18	-0.24	-0.23

```
  24   1    -0.15   0.19  -0.01     0.09  -0.02   0.00    -0.02   0.02
0.01
  25   1    -0.06   0.08   0.01    -0.07   0.08   0.01    -0.06   0.03  -
0.04
  26   1     0.07  -0.04  -0.01    -0.13   0.06   0.00     0.01   0.00
0.00
  27   8     0.02   0.00   0.01    -0.03   0.00  -0.02    -0.03  -0.01  -
0.03
  28   1    -0.13   0.12  -0.05     0.28  -0.25   0.11     0.34  -0.30
0.11
                     58                    59                    60
                     ?A                    ?A                    ?A
 Frequencies --  1415.6062             1417.3585             1430.5209
 Red. masses --     1.5105                1.4528                1.5266
 Frc consts  --     1.7835                1.7196                1.8406
 IR Inten    --     1.3116                1.8239                5.4154
 Raman Activ --     1.6247                5.2736                3.5567
 Depolar     --     0.6905                0.6997                0.7415
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.04   0.05  -0.04    -0.05  -0.10  -0.02    -0.04   0.00
0.15
   2   6    -0.02  -0.03  -0.01    -0.01   0.02   0.00     0.07  -0.02  -
0.01
   3   6     0.02   0.00   0.04     0.01  -0.01   0.04    -0.02   0.00
0.00
   4   6     0.00   0.01   0.02    -0.05   0.07   0.04    -0.03   0.02  -
0.04
   5   6    -0.01  -0.01  -0.01     0.01  -0.01  -0.01    -0.02  -0.05
0.03
   6   6     0.00   0.07   0.01     0.01  -0.01   0.01    -0.03   0.04
0.02
   7   6    -0.02  -0.04   0.14    -0.03   0.00  -0.01     0.02  -0.01
0.03
   8   6     0.01  -0.02  -0.04     0.00   0.01  -0.05     0.05  -0.01
0.00
   9   6    -0.01   0.01   0.02    -0.03   0.00   0.01    -0.04   0.00
0.03
  10   6     0.02  -0.03  -0.04     0.05  -0.01  -0.04     0.02   0.00  -
0.01
  11   6     0.00  -0.02  -0.02     0.07  -0.03   0.02     0.00  -0.01  -
0.04
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.01
0.00
  13   6     0.00   0.00  -0.01     0.00   0.00   0.00     0.00   0.00  -
0.01
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.01  -
0.01
  16   1    -0.12  -0.15   0.13     0.28   0.50   0.10     0.15   0.02  -
0.67
  17   1     0.09   0.12   0.13     0.00  -0.03   0.02    -0.13   0.05  -
0.26
```

18	1	-0.13	0.12	-0.05	-0.13	0.08	-0.03	0.07	0.00	0.00
19	1	-0.02	-0.09	-0.02	0.40	-0.33	-0.18	0.21	0.00	-0.08
20	1	-0.01	-0.20	-0.31	-0.08	0.00	0.01	0.09	-0.15	-0.17
21	1	0.01	0.10	-0.59	0.11	0.05	0.04	-0.10	-0.01	-0.26
22	1	0.08	0.17	-0.05	0.10	-0.17	0.03	-0.27	0.06	-0.14
23	1	-0.12	0.19	0.07	-0.25	0.10	0.16	-0.06	-0.03	0.03
24	1	-0.30	0.23	-0.03	-0.13	0.21	0.01	0.03	-0.21	-0.02
25	1	0.19	-0.21	0.02	-0.14	0.24	0.04	-0.11	0.14	0.02
26	1	-0.04	0.02	0.00	0.01	-0.01	0.00	-0.13	0.06	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.03	-0.02	0.00	-0.02	0.02	-0.01	0.03	-0.02	0.01

	61	62	63
	?A	?A	?A
Frequencies --	1438.1263	1455.8968	1463.5678
Red. masses --	1.4983	1.7112	1.4722
Frc consts --	1.8258	2.1371	1.8580
IR Inten --	3.3708	57.0738	5.5462
Raman Activ --	4.4549	3.0600	2.6040
Depolar --	0.6654	0.7047	0.5309

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.06	-0.05	-0.03	0.00	-0.03	0.03	0.04	0.00	0.01
2	6	0.02	0.00	0.05	0.03	-0.01	0.01	-0.02	0.01	-0.03
3	6	0.01	0.02	-0.04	-0.02	-0.02	-0.02	0.00	0.00	0.01
4	6	0.04	0.01	-0.05	-0.05	0.01	0.03	-0.04	0.01	0.02
5	6	-0.01	-0.02	0.03	0.04	0.07	0.00	-0.01	-0.04	0.00
6	6	0.03	-0.01	-0.03	-0.01	0.02	-0.02	0.01	0.01	0.04
7	6	-0.09	-0.02	0.02	-0.04	-0.02	0.04	-0.08	-0.07	-0.04
8	6	0.06	-0.08	0.04	-0.08	-0.02	-0.06	0.04	0.02	-0.02
9	6	0.00	0.01	0.01	0.14	0.03	0.00	-0.03	0.00	0.01
10	6	-0.03	0.00	0.03	-0.10	0.00	0.06	0.02	0.01	-0.02
11	6	0.05	0.01	0.01	0.00	0.03	-0.02	-0.06	0.11	0.01

12	8	0.00	0.00	0.00	-0.01	-0.01	0.00	0.01	0.00	0.00
13	6	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	-0.02	-0.01	0.01	0.00	0.00	0.00
15	8	0.00	0.00	0.00	-0.02	-0.02	0.00	0.01	0.01	0.00
16	1	0.10	0.26	0.08	0.11	0.07	-0.19	0.00	-0.10	-0.03
17	1	-0.16	0.02	-0.16	-0.03	0.03	-0.07	0.12	-0.06	0.13
18	1	-0.03	-0.10	0.05	0.18	-0.01	-0.03	0.02	0.00	0.01
19	1	-0.33	0.11	0.03	0.35	-0.10	-0.07	0.19	-0.10	-0.06
20	1	-0.07	0.07	0.03	0.10	0.01	-0.01	-0.01	-0.13	-0.11
21	1	0.50	0.23	-0.05	0.17	0.10	-0.12	0.58	0.15	0.18
22	1	-0.23	0.46	-0.20	0.47	0.06	0.15	-0.09	-0.14	-0.04
23	1	0.15	-0.02	-0.09	0.46	-0.01	-0.30	-0.12	-0.05	0.07
24	1	-0.09	0.12	0.02	0.01	-0.04	0.00	0.28	-0.30	0.03
25	1	0.03	0.07	0.05	0.13	-0.07	0.06	0.33	-0.33	0.01
26	1	-0.05	0.02	0.00	0.18	-0.08	-0.01	-0.08	0.03	0.00
27	8	0.00	0.00	-0.01	-0.02	0.00	-0.01	0.00	0.00	0.00
28	1	-0.03	0.02	0.00	0.13	-0.11	0.05	-0.06	0.05	-0.01

	64			65			66		
	?A			?A			?A		
Frequencies --	1491.7223			1635.0007			2539.7087		
Red. masses --	2.2608			1.1045			12.6892		
Frc consts --	2.9640			1.7396			48.2227		
IR Inten --	119.7513			2.4366			39.1444		
Raman Activ --	4.2947			9.2794			120.3509		
Depolar --	0.7239			0.6679			0.1673		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.01	-0.02	0.03	-0.01	0.01	0.00	0.00	0.00	0.00
2 6	-0.01	-0.01	-0.02	0.00	0.00	0.00	0.00	0.00	0.00
3 6	-0.02	-0.08	0.06	0.00	0.00	0.00	0.00	0.00	0.00
4 6	-0.03	-0.08	-0.04	0.00	0.00	0.00	0.00	0.00	0.00
5 6	0.11	0.24	-0.04	0.00	0.00	0.00	0.00	0.00	0.00

```
   6   6     0.00   0.02   0.02     0.00   0.00   0.00     0.00   0.00
0.00
   7   6    -0.02   0.00  -0.01     0.00  -0.01   0.00     0.00   0.00
0.00
   8   6     0.05  -0.01   0.04     0.00   0.00   0.00     0.00   0.00
0.00
   9   6    -0.03   0.00   0.01     0.00   0.00   0.00    -0.08  -0.07
0.02
  10   6     0.03  -0.01  -0.04     0.00   0.00   0.00     0.00   0.00
0.00
  11   6     0.00   0.01   0.00    -0.06  -0.05  -0.04     0.00   0.00
0.00
  12   8    -0.04  -0.04   0.01     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.68   0.40  -
0.13
  14   7     0.01   0.00   0.00     0.00   0.00   0.00    -0.51  -0.28
0.10
  15   8    -0.05  -0.06   0.01     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.05   0.05  -0.06    -0.02  -0.01  -0.01     0.00   0.00
0.00
  17   1     0.04   0.06   0.04    -0.01  -0.01  -0.02     0.00   0.00
0.00
  18   1     0.01   0.35  -0.23     0.00   0.00   0.00     0.00   0.00
0.00
  19   1     0.06   0.40   0.13    -0.02  -0.02  -0.01     0.00   0.00
0.00
  20   1    -0.03  -0.04  -0.05    -0.01  -0.02  -0.02     0.00   0.00
0.00
  21   1     0.10   0.04   0.00    -0.01  -0.02  -0.01     0.00   0.00
0.00
  22   1    -0.24   0.11  -0.11    -0.02  -0.02  -0.01     0.01   0.00
0.01
  23   1    -0.18   0.12   0.10     0.00  -0.01   0.00     0.01   0.00  -
0.01
  24   1     0.07  -0.05   0.00     0.53   0.45  -0.12     0.00   0.00
0.00
  25   1    -0.01   0.05   0.03     0.22   0.19   0.64     0.00   0.00
0.00
  26   1     0.54  -0.25  -0.02    -0.01   0.00   0.00     0.00   0.00
0.00
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1    -0.01   0.01   0.00     0.00   0.00   0.00    -0.02   0.02  -
0.01
                     67                     68                     69
                     ?A                     ?A                     ?A
 Frequencies --  3177.3431              3214.0542              3218.3349
 Red. masses --     1.0589                 1.0882                 1.1022
 Frc consts  --     6.2985                 6.6232                 6.7260
 IR Inten    --    73.3153                59.6495                48.5133
 Raman Activ --   145.9826               102.5182               101.0339
 Depolar     --     0.2592                 0.3876                 0.6823
```

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.01	-0.01	0.00	0.00	0.00
7	6	-0.01	0.02	0.00	0.03	-0.07	-0.01	0.01	-0.02	0.00
8	6	0.00	0.00	0.00	-0.01	0.00	0.02	0.00	0.00	0.01
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	-0.05	-0.04	-0.02	-0.02	-0.02	0.02	0.02	0.02	-0.08
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	-0.04	0.02	-0.01	-0.03	0.02	-0.01	-0.02	0.01	0.00
17	1	-0.02	0.00	0.01	0.01	0.00	-0.01	0.01	0.00	-0.01
18	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	1	0.00	0.01	-0.01	0.00	-0.01	0.02	0.00	0.00	-0.01
20	1	0.00	0.00	0.00	-0.02	-0.15	0.13	-0.01	-0.05	0.04
21	1	0.08	-0.22	-0.04	-0.32	0.80	0.14	-0.10	0.24	0.04
22	1	0.00	0.00	0.00	0.08	-0.04	-0.19	0.04	-0.02	-0.10
23	1	0.00	0.00	0.00	-0.01	0.00	-0.01	0.00	0.00	0.00
24	1	0.03	0.04	0.57	-0.01	-0.01	-0.10	0.07	0.08	0.80
25	1	0.51	0.45	-0.37	0.24	0.21	-0.16	-0.34	-0.30	0.22
26	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     70                     71                     72
                     ?A                     ?A                     ?A
 Frequencies --  3246.4102              3250.1937              3266.4858
 Red. masses --     1.0870                 1.0884                 1.0891
 Frc consts  --     6.7498                 6.7740                 6.8468
 IR Inten    --    23.1201                59.2293                96.6906
 Raman Activ --    96.9432                59.1226               184.6118
 Depolar     --     0.5550                 0.5626                 0.2906
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.00
0.00
   2   6    -0.02   0.00   0.01    -0.04   0.00   0.04    -0.04   0.00
0.04
   3   6     0.00   0.00   0.00     0.00  -0.01  -0.01     0.00  -0.01  -
0.01
   4   6     0.00  -0.01   0.02     0.00   0.00  -0.01     0.00   0.00
0.01
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.02  -0.02     0.01   0.03  -0.03    -0.01  -0.04
0.04
   7   6     0.00  -0.01   0.00    -0.01   0.02   0.00     0.00  -0.01
0.00
   8   6     0.03  -0.01  -0.06    -0.01   0.01   0.03     0.00   0.00  -
0.01
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00     0.01   0.00   0.01    -0.01   0.00  -
0.01
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1    -0.01   0.01   0.00    -0.06   0.04  -0.01    -0.10   0.06  -
0.02
  17   1     0.18   0.01  -0.15     0.51   0.02  -0.42     0.51   0.02  -
0.42
  18   1     0.00   0.02   0.03    -0.01   0.07   0.10    -0.01   0.09
0.12
  19   1    -0.03   0.09  -0.23     0.02  -0.06   0.14    -0.01   0.03  -
0.07
  20   1    -0.04  -0.28   0.25    -0.06  -0.40   0.37     0.07   0.49  -
0.45
```

```
  21   1    -0.04   0.11   0.02     0.08  -0.21  -0.04    -0.05   0.14
0.03
  22   1    -0.32   0.16   0.76     0.14  -0.07  -0.34    -0.03   0.01
0.06
  23   1    -0.02   0.00  -0.04    -0.07   0.01  -0.11     0.11  -0.02
0.17
  24   1     0.00   0.00   0.04     0.00   0.00  -0.04     0.00   0.00
0.02
  25   1     0.00   0.00   0.00    -0.02  -0.01   0.01     0.03   0.02  -
0.02
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     73                     74                     75
                     ?A                     ?A                     ?A
 Frequencies --  3280.3283              3289.2971              3308.0046
 Red. masses --     1.0872                 1.0882                 1.0899
 Frc consts  --     6.8925                 6.9366                 7.0273
 IR Inten    --    52.2482                27.7875                66.8642
 Raman Activ --   108.7049                79.1772               190.7291
 Depolar     --     0.3203                 0.6297                 0.1686
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01  -0.01   0.00     0.00   0.00   0.00    -0.02   0.01
0.00
   2   6     0.00   0.00   0.00    -0.01   0.00   0.00     0.01   0.00  -
0.01
   3   6     0.00   0.00   0.00     0.00   0.03   0.04     0.00  -0.04  -
0.05
   4   6    -0.01   0.03  -0.07     0.00   0.00   0.00     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00     0.00   0.01  -0.01     0.00   0.01  -
0.01
   7   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   8   6     0.01  -0.01  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00    -0.04   0.01  -0.06    -0.03   0.00  -
0.04
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

```
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1    -0.15   0.10  -0.04    -0.02   0.01   0.00     0.21  -0.13
0.05
  17   1    -0.02   0.00   0.02     0.06   0.01  -0.05    -0.11  -0.01
0.09
  18   1     0.00   0.04   0.05     0.02  -0.34  -0.47    -0.03   0.45
0.62
  19   1     0.10  -0.35   0.85     0.00   0.00   0.00     0.00   0.01  -
0.03
  20   1     0.00   0.02  -0.02    -0.02  -0.13   0.12    -0.02  -0.10
0.09
  21   1    -0.02   0.05   0.01     0.01  -0.03  -0.01     0.01  -0.02
0.00
  22   1    -0.11   0.06   0.26     0.01   0.00  -0.02     0.01  -0.01  -
0.03
  23   1     0.03  -0.01   0.05     0.43  -0.07   0.66     0.30  -0.05
0.46
  24   1     0.00   0.00   0.03     0.00   0.00  -0.01     0.00   0.00
0.01
  25   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     76                     77                     78
                     ?A                     ?A                     ?A
 Frequencies --  3320.7786              3872.2191              3944.8433
 Red. masses --     1.0899                 1.0653                 1.0662
 Frc consts  --     7.0814                 9.4110                 9.7757
 IR Inten    --    34.9767                48.3850                26.8993
 Raman Activ --   238.8063               109.0679                51.0456
 Depolar     --     0.0854                 0.2398                 0.1683
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.07   0.04  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
   2   6    -0.01   0.00   0.01     0.00   0.00   0.00     0.00   0.00
0.00
   3   6     0.00   0.01   0.01     0.00   0.00   0.00     0.00   0.00
0.00
   4   6     0.00   0.01  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   7   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   8   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

```
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.01   0.00   0.01     0.00   0.00   0.00     0.00   0.00
0.00
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.02   0.06  -0.01     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.78  -0.48   0.18     0.00   0.00   0.00     0.00   0.00
0.00
  17   1     0.13   0.01  -0.11     0.00   0.00   0.00     0.00   0.00
0.00
  18   1     0.00  -0.11  -0.15     0.00   0.00   0.00     0.00   0.00
0.00
  19   1     0.02  -0.07   0.17     0.00   0.00   0.00     0.00   0.00
0.00
  20   1     0.01   0.05  -0.05     0.00   0.00   0.00     0.00   0.00
0.00
  21   1    -0.01   0.04   0.01     0.00   0.00   0.00     0.01   0.00
0.00
  22   1    -0.02   0.01   0.04     0.00   0.00   0.00     0.00   0.00
0.00
  23   1    -0.06   0.01  -0.09     0.00   0.00   0.00     0.00   0.00
0.00
  24   1     0.00   0.01   0.05     0.00   0.00   0.00     0.00   0.00
0.00
  25   1     0.03   0.03  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
  26   1     0.00   0.00   0.00    -0.35  -0.93   0.12     0.00   0.00
0.00
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.03   0.05
0.02
  28   1     0.00   0.00   0.00     0.00   0.00   0.00    -0.48  -0.79  -
0.39

 --------------------
 - Thermochemistry -
 --------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Atom  1 has atomic number  6 and mass  12.00000
 Atom  2 has atomic number  6 and mass  12.00000
 Atom  3 has atomic number  6 and mass  12.00000
 Atom  4 has atomic number  6 and mass  12.00000
 Atom  5 has atomic number  6 and mass  12.00000
 Atom  6 has atomic number  6 and mass  12.00000
 Atom  7 has atomic number  6 and mass  12.00000
 Atom  8 has atomic number  6 and mass  12.00000
 Atom  9 has atomic number  6 and mass  12.00000
```

```
Atom 10 has atomic number  6 and mass  12.00000
Atom 11 has atomic number  6 and mass  12.00000
Atom 12 has atomic number  8 and mass  15.99491
Atom 13 has atomic number  6 and mass  12.00000
Atom 14 has atomic number  7 and mass  14.00307
Atom 15 has atomic number  8 and mass  15.99491
Atom 16 has atomic number  1 and mass   1.00783
Atom 17 has atomic number  1 and mass   1.00783
Atom 18 has atomic number  1 and mass   1.00783
Atom 19 has atomic number  1 and mass   1.00783
Atom 20 has atomic number  1 and mass   1.00783
Atom 21 has atomic number  1 and mass   1.00783
Atom 22 has atomic number  1 and mass   1.00783
Atom 23 has atomic number  1 and mass   1.00783
Atom 24 has atomic number  1 and mass   1.00783
Atom 25 has atomic number  1 and mass   1.00783
Atom 26 has atomic number  1 and mass   1.00783
Atom 27 has atomic number  8 and mass  15.99491
Atom 28 has atomic number  1 and mass   1.00783
Molecular mass:   218.08172 amu.
Principal axes and moments of inertia in atomic units:
                          1         2         3
    EIGENVALUES --  2083.26790 2574.49153 3644.51087
          X            0.99996   0.00433   0.00764
          Y           -0.00441   0.99992   0.01152
          Z           -0.00759  -0.01155   0.99990
THIS MOLECULE IS AN ASYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER  1.
WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
          MAY CAUSE SIGNIFICANT ERROR
ROTATIONAL TEMPERATURES (KELVIN)      0.04158     0.03364     0.02377
ROTATIONAL CONSTANTS (GHZ)            0.86630     0.70101     0.49519
   1 IMAGINARY FREQUENCIES IGNORED.
Zero-point vibrational energy     622237.7 (Joules/Mol)
                                 148.71838 (Kcal/Mol)
WARNING-- EXPLICIT CONSIDERATION OF  15 DEGREES OF FREEDOM AS
          VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
VIBRATIONAL TEMPERATURES:    167.19   219.07   277.25   349.14   446.64
         (KELVIN)            482.02   500.97   529.66   581.42   606.49
                             622.83   717.47   777.41   815.84   879.51
                             910.14   927.06   973.19   987.90  1013.16
                            1151.31  1185.40  1201.62  1269.83  1280.33
                            1300.78  1341.66  1372.89  1402.45  1441.55
                            1453.53  1473.39  1481.12  1483.62  1497.87
                            1527.40  1557.15  1571.61  1608.90  1668.51
                            1694.32  1729.86  1758.72  1775.77  1791.57
                            1810.12  1833.59  1886.39  1898.71  1926.05
                            1936.37  1940.24  1978.51  1990.74  1993.86
                            2009.19  2036.73  2039.25  2058.19  2069.13
                            2094.70  2105.74  2146.24  2352.39  3654.05
                            4571.46  4624.28  4630.44  4670.83  4676.28
                            4699.72  4719.63  4732.54  4759.45  4777.83
                            5571.23  5675.72
```

Zero-point correction=	0.236998
(Hartree/Particle)	
Thermal correction to Energy=	0.247069
Thermal correction to Enthalpy=	0.248013
Thermal correction to Gibbs Free Energy=	0.201754
Sum of electronic and zero-point Energies=	-736.169238
Sum of electronic and thermal Energies=	-736.159167
Sum of electronic and thermal Enthalpies=	-736.158223
Sum of electronic and thermal Free Energies=	-736.204482

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	155.038	44.357	97.360
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	42.042
ROTATIONAL	0.889	2.981	31.348
VIBRATIONAL	153.260	38.395	23.970
VIBRATION 1	0.608	1.936	3.163
VIBRATION 2	0.619	1.900	2.644
VIBRATION 3	0.635	1.850	2.202
VIBRATION 4	0.659	1.775	1.783
VIBRATION 5	0.699	1.654	1.360
VIBRATION 6	0.716	1.606	1.236
VIBRATION 7	0.726	1.579	1.174
VIBRATION 8	0.741	1.538	1.088
VIBRATION 9	0.769	1.461	0.948
VIBRATION 10	0.784	1.423	0.887
VIBRATION 11	0.794	1.399	0.849
VIBRATION 12	0.854	1.253	0.661
VIBRATION 13	0.895	1.161	0.565
VIBRATION 14	0.923	1.103	0.510
VIBRATION 15	0.970	1.008	0.431

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.158544D-92	-92.799849	-213.679549
TOTAL V=0	0.162497D+17	16.210845	37.326850
VIB (BOT)	0.791360-107	-107.101626	-246.610607
VIB (BOT) 1	0.176014D+01	0.245546	0.565391
VIB (BOT) 2	0.133085D+01	0.124129	0.285817
VIB (BOT) 3	0.103760D+01	0.016030	0.036910
VIB (BOT) 4	0.807035D+00	-0.093107	-0.214388
VIB (BOT) 5	0.608980D+00	-0.215397	-0.495970
VIB (BOT) 6	0.555985D+00	-0.254937	-0.587014
VIB (BOT) 7	0.530500D+00	-0.275314	-0.633934
VIB (BOT) 8	0.495182D+00	-0.305236	-0.702831
VIB (BOT) 9	0.439732D+00	-0.356812	-0.821590
VIB (BOT) 10	0.416064D+00	-0.380840	-0.876916
VIB (BOT) 11	0.401590D+00	-0.396218	-0.912325
VIB (BOT) 12	0.329972D+00	-0.481523	-1.108749
VIB (BOT) 13	0.293128D+00	-0.532943	-1.227146
VIB (BOT) 14	0.272211D+00	-0.565094	-1.301176
VIB (BOT) 15	0.241427D+00	-0.617214	-1.421189
VIB (V=0)	0.811089D+02	1.909068	4.395792
VIB (V=0) 1	0.232978D+01	0.367314	0.845772
VIB (V=0) 2	0.192167D+01	0.283680	0.653197

VIB (V=0)	3	0.165179D+01	0.217954	0.501857
VIB (V=0)	4	0.144937D+01	0.161180	0.371130
VIB (V=0)	5	0.128794D+01	0.109897	0.253047
VIB (V=0)	6	0.124774D+01	0.096125	0.221336
VIB (V=0)	7	0.122899D+01	0.089549	0.206195
VIB (V=0)	8	0.120371D+01	0.080521	0.185407
VIB (V=0)	9	0.116586D+01	0.066645	0.153455
VIB (V=0)	10	0.115047D+01	0.060875	0.140169
VIB (V=0)	11	0.114131D+01	0.057402	0.132174
VIB (V=0)	12	0.109907D+01	0.041024	0.094462
VIB (V=0)	13	0.107959D+01	0.033259	0.076581
VIB (V=0)	14	0.106930D+01	0.029098	0.067001
VIB (V=0)	15	0.105524D+01	0.023350	0.053764
ELECTRONIC		0.100000D+01	0.000000	0.000000
TRANSLATIONAL		0.126587D+09	8.102389	18.656441
ROTATIONAL		0.158266D+07	6.199387	14.274617

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000002680	0.000005865	0.000004929
2	6	0.000001910	-0.000001351	-0.000000186
3	6	-0.000001996	-0.000001639	-0.000001266
4	6	0.000003261	0.000000196	0.000003557
5	6	-0.000002148	0.000016833	-0.000006007
6	6	0.000001039	-0.000000800	-0.000003944
7	6	0.000004731	-0.000008563	-0.000007307
8	6	-0.000013313	0.000004124	0.000007587
9	6	0.000051408	-0.000032101	-0.000002954
10	6	-0.000010545	0.000001419	-0.000002252
11	6	-0.000000622	0.000002455	-0.000001100
12	8	0.000002211	-0.000013891	0.000000461
13	6	0.000005700	0.000001424	-0.000002319
14	7	0.000008158	-0.000012512	0.000001974
15	8	-0.000012884	-0.000015895	0.000004326
16	1	-0.000002199	0.000003150	-0.000001290
17	1	0.000000876	-0.000002738	0.000001649
18	1	-0.000004129	-0.000000007	-0.000001373
19	1	-0.000004560	0.000000798	0.000001728
20	1	0.000000314	-0.000000402	0.000001434
21	1	0.000002780	0.000005680	0.000005729
22	1	0.000000500	0.000004770	-0.000001042
23	1	0.000000354	0.000003774	0.000000548
24	1	-0.000000651	0.000000597	0.000000181
25	1	0.000000156	-0.000000275	-0.000000174
26	1	0.000000253	0.000000510	-0.000002265
27	8	-0.000020689	0.000033414	-0.000004854
28	1	-0.000012595	0.000005165	0.000004228

Cartesian Forces: Max 0.000051408 RMS 0.000009460

Internal Coordinate Forces (Hartree/Bohr or radian)

Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J

1	C	0.000003(	1)	0.000006(	29)	0.000005(	57)
2	C	0.000002(	2)	-0.000001(	30)	0.000000(	58)
3	C	-0.000002(	3)	-0.000002(	31)	-0.000001(	59)
4	C	0.000003(	4)	0.000000(	32)	0.000004(	60)
5	C	-0.000002(	5)	0.000017(	33)	-0.000006(	61)
6	C	0.000001(	6)	-0.000001(	34)	-0.000004(	62)
7	C	0.000005(	7)	-0.000009(	35)	-0.000007(	63)
8	C	-0.000013(	8)	0.000004(	36)	0.000008(	64)
9	C	0.000051(	9)	-0.000032(	37)	-0.000003(	65)
10	C	-0.000011(	10)	0.000001(	38)	-0.000002(	66)
11	C	-0.000001(	11)	0.000002(	39)	-0.000001(	67)
12	O	0.000002(	12)	-0.000014(	40)	0.000000(	68)
13	C	0.000006(	13)	0.000001(	41)	-0.000002(	69)
14	N	0.000008(	14)	-0.000013(	42)	0.000002(	70)
15	O	-0.000013(	15)	-0.000016(	43)	0.000004(	71)
16	H	-0.000002(	16)	0.000003(	44)	-0.000001(	72)
17	H	0.000001(	17)	-0.000003(	45)	0.000002(	73)
18	H	-0.000004(	18)	0.000000(	46)	-0.000001(	74)
19	H	-0.000005(	19)	0.000001(	47)	0.000002(	75)
20	H	0.000000(	20)	0.000000(	48)	0.000001(	76)
21	H	0.000003(	21)	0.000006(	49)	0.000006(	77)
22	H	0.000001(	22)	0.000005(	50)	-0.000001(	78)
23	H	0.000000(	23)	0.000004(	51)	0.000001(	79)
24	H	-0.000001(	24)	0.000001(	52)	0.000000(	80)
25	H	0.000000(	25)	0.000000(	53)	0.000000(	81)
26	H	0.000000(	26)	0.000001(	54)	-0.000002(	82)
27	O	-0.000021(	27)	0.000033(	55)	-0.000005(	83)
28	H	-0.000013(	28)	0.000005(	56)	0.000004(	84)

Internal Forces: Max 0.000051408 RMS 0.000009460

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number 1 out of a maximum of 94
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.

Eigenvalues ---	-0.00474	0.00515	0.00627	0.00750	0.01127
Eigenvalues ---	0.01237	0.02043	0.02409	0.02610	0.03448
Eigenvalues ---	0.03944	0.04243	0.04306	0.04364	0.04452
Eigenvalues ---	0.04756	0.04831	0.04872	0.04940	0.05107
Eigenvalues ---	0.05189	0.05226	0.05301	0.05408	0.05536
Eigenvalues ---	0.06031	0.06110	0.07308	0.08225	0.09411
Eigenvalues ---	0.09839	0.10682	0.13061	0.14270	0.14739
Eigenvalues ---	0.15711	0.16607	0.18789	0.19287	0.19873
Eigenvalues ---	0.21875	0.25609	0.26331	0.27929	0.29380
Eigenvalues ---	0.34805	0.35143	0.36585	0.38474	0.40084
Eigenvalues ---	0.45398	0.48687	0.49256	0.49461	0.50752
Eigenvalues ---	0.52924	0.55727	0.57613	0.59127	0.64253
Eigenvalues ---	0.64769	0.67127	0.71149	0.77106	0.86423
Eigenvalues ---	0.89092	0.92557	0.93805	0.94188	0.96476
Eigenvalues ---	0.97531	1.00808	1.04295	1.05680	1.07770
Eigenvalues ---	1.10436	1.15282	3.11839		

Eigenvalue 1 out of range, new value = 0.004738 Eigenvector:

	1
X1	0.00146
Y1	-0.00264
Z1	0.00037
X2	-0.01221
Y2	0.00691
Z2	0.00389
X3	-0.01768
Y3	0.01322
Z3	0.00600
X4	0.00571
Y4	-0.00383
Z4	0.00633
X5	-0.00266
Y5	0.00312
Z5	0.00273
X6	-0.00700
Y6	0.01450
Z6	0.01642
X7	0.00252
Y7	-0.00298
Z7	0.02733
X8	0.00433
Y8	-0.00885
Z8	0.02317
X9	-0.01091
Y9	-0.00192
Z9	0.03482
X10	-0.02177
Y10	0.01742
Z10	0.01962
X11	0.00915
Y11	-0.00468
Z11	0.00846
X12	-0.00003
Y12	0.00627
Z12	-0.02003
X13	-0.00034
Y13	-0.01752
Z13	-0.00410
X14	0.00874
Y14	-0.03843
Z14	-0.04184
X15	0.00455
Y15	-0.00262
Z15	0.00553
X16	0.00396
Y16	-0.00317
Z16	-0.01238
X17	-0.01776
Y17	0.00791
Z17	-0.00274
X18	-0.02631

Y18	0.01764
Z18	0.00146
X19	0.01516
Y19	-0.00876
Z19	0.00279
X20	0.00632
Y20	0.01646
Z20	0.01610
X21	0.01542
Y21	0.00047
Z21	0.06894
X22	0.00588
Y22	-0.00070
Z22	0.01795
X23	-0.02229
Y23	0.01336
Z23	0.01863
X24	0.01706
Y24	-0.00643
Z24	0.00731
X25	0.00341
Y25	-0.00322
Z25	0.00275
X26	0.00296
Y26	0.00678
Z26	-0.00845
X27	-0.10959
Y27	-0.06341
Z27	0.19154
X28	0.39124
Y28	0.19915
Z28	-0.85767

Angle between quadratic step and forces= 73.42 degrees.
Linear search not attempted -- first point.
TrRot= 0.000032 -0.000009 -0.000025 -0.000002 0.000006 -0.000002

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
X1	-3.78865	0.00000	0.00000	-0.00004	-0.00002	-3.78866
Y1	-0.85293	0.00001	0.00000	-0.00004	-0.00003	-0.85297
Z1	-0.89262	0.00000	0.00000	0.00008	0.00008	-0.89254
X2	-3.06753	0.00000	0.00000	0.00002	0.00006	-3.06747
Y2	-0.88243	0.00000	0.00000	-0.00010	-0.00009	-0.88252
Z2	1.96529	0.00000	0.00000	0.00004	0.00004	1.96532
X3	-1.17501	0.00000	0.00000	-0.00011	-0.00006	-1.17507
Y3	1.33893	0.00000	0.00000	0.00001	0.00001	1.33893
Z3	2.38824	0.00000	0.00000	0.00001	-0.00001	2.38823
X4	-1.55516	0.00000	0.00000	-0.00012	-0.00010	-1.55526
Y4	0.66604	0.00000	0.00000	0.00005	0.00004	0.66609
Z4	-2.01383	0.00000	0.00000	0.00006	0.00004	-2.01379
X5	-1.17495	0.00000	0.00000	-0.00016	-0.00012	-1.17507
Y5	2.83186	0.00002	0.00000	0.00002	0.00001	2.83188
Z5	-0.09829	-0.00001	0.00000	0.00002	0.00000	-0.09829
X6	-0.81882	0.00000	0.00000	0.00013	0.00016	-0.81866
Y6	-2.82620	0.00000	0.00000	0.00003	0.00003	-2.82617

Z6	2.05732	0.00000	0.00000	-0.00006	-0.00008	2.05724
X7	-0.57507	0.00000	0.00000	0.00010	0.00011	-0.57497
Y7	-3.67733	-0.00001	0.00000	0.00010	0.00009	-3.67724
Z7	-0.75245	-0.00001	0.00000	-0.00011	-0.00013	-0.75257
X8	0.70973	-0.00001	0.00000	-0.00004	-0.00002	0.70971
Y8	-1.28432	0.00000	0.00000	0.00021	0.00020	-1.28412
Z8	-1.93364	0.00001	0.00000	-0.00005	-0.00008	-1.93372
X9	2.70978	0.00005	0.00000	0.00011	0.00014	2.70993
Y9	-0.64351	-0.00003	0.00000	0.00010	0.00008	-0.64343
Z9	0.10389	0.00000	0.00000	-0.00007	-0.00011	0.10377
X10	1.08364	-0.00001	0.00000	0.00002	0.00006	1.08370
Y10	-0.57224	0.00000	0.00000	0.00015	0.00014	-0.57211
Z10	2.49493	0.00000	0.00000	-0.00006	-0.00009	2.49485
X11	-3.30273	0.00000	0.00000	0.00005	0.00006	-3.30267
Y11	-3.58017	0.00000	0.00000	0.00000	0.00001	-3.58016
Z11	-1.73520	0.00000	0.00000	-0.00002	-0.00002	-1.73523
X12	-3.66857	0.00000	0.00000	-0.00017	-0.00012	-3.66869
Y12	4.21143	-0.00001	0.00000	-0.00008	-0.00007	4.21135
Z12	-0.10803	0.00000	0.00000	-0.00001	-0.00002	-0.10804
X13	4.54660	0.00001	0.00000	0.00034	0.00038	4.54698
Y13	1.37140	0.00000	0.00000	-0.00010	-0.00013	1.37127
Z13	-0.38750	0.00000	0.00000	0.00000	-0.00005	-0.38755
X14	6.26255	0.00001	0.00000	0.00064	0.00068	6.26323
Y14	2.63021	-0.00001	0.00000	-0.00047	-0.00051	2.62970
Z14	-0.74877	0.00000	0.00000	0.00012	0.00006	-0.74870
X15	0.73534	-0.00001	0.00000	-0.00013	-0.00008	0.73526
Y15	4.44763	-0.00002	0.00000	-0.00007	-0.00008	4.44754
Z15	-0.49547	0.00000	0.00000	0.00004	0.00001	-0.49546
X16	-5.60866	0.00000	0.00000	-0.00007	-0.00004	-5.60870
Y16	-0.03881	0.00000	0.00000	-0.00007	-0.00005	-0.03886
Z16	-1.30145	0.00000	0.00000	0.00012	0.00013	-1.30133
X17	-4.62860	0.00000	0.00000	0.00010	0.00014	-4.62846
Y17	-1.13449	0.00000	0.00000	-0.00026	-0.00025	-1.13474
Z17	3.25692	0.00000	0.00000	0.00011	0.00011	3.25703
X18	-1.40389	0.00000	0.00000	-0.00020	-0.00014	-1.40402
Y18	2.53600	0.00000	0.00000	0.00000	0.00000	2.53599
Z18	4.02002	0.00000	0.00000	0.00000	-0.00002	4.02000
X19	-1.87346	0.00000	0.00000	-0.00028	-0.00027	-1.87373
Y19	1.38666	0.00000	0.00000	0.00005	0.00005	1.38671
Z19	-3.89663	0.00000	0.00000	0.00009	0.00007	-3.89656
X20	-0.86176	0.00000	0.00000	0.00023	0.00026	-0.86150
Y20	-4.33399	0.00000	0.00000	0.00002	0.00001	-4.33398
Z20	3.43419	0.00000	0.00000	-0.00007	-0.00009	3.43410
X21	0.38409	0.00000	0.00000	0.00017	0.00017	0.38426
Y21	-5.45991	0.00001	0.00000	0.00015	0.00014	-5.45977
Z21	-1.06221	0.00001	0.00000	-0.00013	-0.00016	-1.06237
X22	1.55394	0.00000	0.00000	-0.00006	-0.00006	1.55388
Y22	-1.60328	0.00000	0.00000	0.00034	0.00032	-1.60296
Z22	-3.76998	0.00000	0.00000	-0.00008	-0.00011	-3.77010
X23	2.20769	0.00000	0.00000	-0.00002	0.00004	2.20773
Y23	-0.60041	0.00000	0.00000	0.00025	0.00023	-0.60018
Z23	4.19488	0.00000	0.00000	-0.00002	-0.00006	4.19481
X24	-3.42816	0.00000	0.00000	0.00001	0.00000	-3.42816
Y24	-3.82952	0.00000	0.00000	0.00007	0.00007	-3.82944

```
  Z24       -3.76894   0.00000   0.00000  -0.00002  -0.00003  -3.76896
  X25       -4.51545   0.00000   0.00000   0.00015   0.00016  -4.51529
  Y25       -4.95122   0.00000   0.00000  -0.00009  -0.00008  -4.95130
  Z25       -0.80255   0.00000   0.00000  -0.00003  -0.00002  -0.80258
  X26       -3.19258   0.00000   0.00000  -0.00030  -0.00024  -3.19282
  Y26        5.96145   0.00000   0.00000  -0.00009  -0.00008   5.96137
  Z26       -0.34136   0.00000   0.00000  -0.00035  -0.00035  -0.34171
  X27        4.45747  -0.00002   0.00000  -0.00006  -0.00004   4.45743
  Y27       -2.82424   0.00003   0.00000   0.00014   0.00011  -2.82413
  Z27        0.40437   0.00000   0.00000  -0.00035  -0.00040   0.40397
  X28        3.78410  -0.00001   0.00000  -0.00114  -0.00112   3.78297
  Y28       -4.35697   0.00001   0.00000  -0.00015  -0.00017  -4.35715
  Z28       -0.30538   0.00000   0.00000   0.00134   0.00129  -0.30409
       Item               Value     Threshold  Converged?
Maximum Force            0.000051     0.000450     YES
RMS     Force            0.000009     0.000300     YES
Maximum Displacement     0.001290     0.001800     YES
RMS     Displacement     0.000245     0.001200     YES
Predicted change in Energy=-1.451325D-08
Optimization completed.
   -- Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1\1\GINC-PELICAN\Freq\RHF\3-21+G*\C12H12N1O3(1-)\SINGH\20-Mar-2002\0\\
#N RHF/3-21+G* FREQ\\Freq calc of output str of mech1s8ts2\\-1,1\C,-2.
0048650087,-0.4513530261,-0.4723539739\C,-1.6232680087,-0.4669600261,1
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C,-0.4333020087,-1.4955620261,1.0886870261\C,-0.3043160087,-1.94596102
61,-0.3981769739\C,0.3755739913,-0.6796340261,-1.0232389739\C,1.433954
9913,-0.3405320261,0.0549750261\C,0.5734379913,-0.3028180261,1.3202620
261\C,-1.7477300087,-1.8945460261,-0.9182299739\O,-1.9413220087,2.2285
909739,-0.0571649739\C,2.4059579913,0.7257149739,-0.2050549739\N,3.314
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,-0.6996613,-2.2216272,-3.9716239,-1.1148914,-1.3134672,-3.092967,1.32
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2938,-1.0467977,-2.5413731,0.3339324,2.9370664,1.2407443,3.0482901,1.6
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5917,-0.01810271,-0.02310261,-0.01253022,0.00051314,-0.00118294,-0.000
09187,-0.00014881,-0.00013538,-0.00003022,-0.00013291,0.00035304,0.000
16981,0.00311528,-0.00600878,-0.00020150,-0.00014182,0.00054981,0.0001
3638,0.00029666,0.00020929,0.00013847,-0.00017531,-0.00006745,0.000119
70,-0.00003103,-0.00000692,0.00005805,-0.00002224,0.00001531,0.0000694
9,-0.00030797,0.00016752,-0.00004266,-0.00009141,-0.00005297,0.0002827
7,-0.00312313,-0.00001650,-0.00085074,0.00048587,-0.00003277,0.0008522
1,-0.00005192,-0.00003070,0.00018369,-0.00005505,0.00005136,-0.0000640
1,-0.00019861,-0.00006540,0.00002774,-0.00001672,-0.00002363,-0.000000
58,-0.12934010,-0.38968932,-0.16202455,0.15106783,0.41506775,-0.000194
77,0.00006270,0.00012885,0.00020184,-0.00017242,-0.00021594,0.00011279
,0.00036709,-0.00045180,-0.00024028,-0.00012649,-0.00077059,0.00058806
,0.00031574,0.00079477,0.00141834,-0.00011845,-0.00016081,-0.00162921,
-0.00028420,0.00115477,-0.00080949,0.00182031,0.00209694,0.00213289,0.
01083131,0.00033014,0.00112479,-0.00324322,-0.00089207,0.00015839,0.00
026681,-0.00052819,-0.00007129,-0.00008914,-0.00031326,-0.00394775,0.0
0386700,-0.00109276,0.00209864,0.00053828,-0.00019991,-0.00030269,0.00
018009,-0.00026542,0.00005529,0.00006116,-0.00012781,-0.00006592,0.000
06392,-0.00003842,0.00000517,0.00001431,-0.00002749,0.00003317,0.00001
124,-0.00003224,0.00047839,0.00027190,-0.00064504,-0.00185547,-0.00072
218,0.00150192,0.00021943,0.00056502,-0.00130065,-0.00014054,-0.000317
31,0.00003916,-0.00024811,0.00003962,-0.00018287,0.00021727,0.00000064
,0.00000571,0.00003174,-0.00003002,-0.00000391,-0.09157053,-0.18931531
,-0.08381964,0.09219986,0.17514162,0.08501656\\-0.00000268,-0.00000587
,-0.00000493,-0.00000191,0.00000135,0.00000019,0.00000200,0.00000164,0
.00000127,-0.00000326,-0.00000020,-0.00000356,0.00000215,-0.00001683,0
.00000601,-0.00000104,0.00000080,0.00000394,-0.00000473,0.00000856,0.0
0000731,0.00001331,-0.00000412,-0.00000759,-0.00005141,0.00003210,0.00
000295,0.00001054,-0.00000142,0.00000225,0.00000062,-0.00000246,0.0000
0110,-0.00000221,0.00001389,-0.00000046,-0.00000570,-0.00000142,0.0000
0232,-0.00000816,0.00001251,-0.00000197,0.00001288,0.00001590,-0.00000
433,0.00000220,-0.00000315,0.00000129,-0.00000088,0.00000274,-0.000001

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 65,0.00000413,0.,0.00000137,0.00000456,-0.00000080,-0.00000173,-0.0000
 0031,0.00000040,-0.00000143,-0.00000278,-0.00000568,-0.00000573,-0.000
 00050,-0.00000477,0.00000104,-0.00000035,-0.00000377,-0.00000055,0.000
 00065,-0.00000060,-0.00000018,-0.00000016,0.00000028,0.00000017,-0.000
 00025,-0.00000051,0.00000226,0.00002069,-0.00003341,0.00000485,0.00001
 260,-0.00000517,-0.00000423\\\@


 YOU CAN WIPE THE SLATE CLEAN, BUT YOU'LL STILL
 HAVE TO EAT A LITTLE CHALK DUST.
 Job cpu time:  0 days  3 hours 15 minutes 13.0 seconds.
 File lengths (MBytes):  RWF=  309 Int=    0 D2E=    0 Chk=    7 Scr=
1
 Normal termination of Gaussian 98.
```

Entering Link 1 = C:\G98W\l1.exe PID=   156.

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Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

****
Gaussian 98: x86-Win32-G98RevA.7 11-Apr-1999
11-Mar-2002
****
%chk=mech1s10ts3F
Default route: MaxDisk=2000MB

#N RHF/3-21+G* FREQ

1/10=4,30=1,38=1/1,3;
2/17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11,27=262144000/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Freq calc of output str of mech1s10ts3

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C -1.96629 0.7571 -0.47983

C	-1.69973	0.49411	1.03217
C	-0.20401	0.86397	1.30755
C	-0.52215	0.73447	-1.04888
C	0.28174	1.49002	0.00314
C	-1.32488	-1.03328	1.06793
C	-1.42966	-1.45595	-0.42153
C	-0.15052	-0.80227	-1.00829
C	0.91641	-1.09562	0.07268
C	0.17411	-0.66163	1.34265
C	-2.56746	-0.57338	-0.96209
C	2.16141	-0.33412	-0.18459
N	3.32413	-0.25868	-0.5092
O	1.17366	-2.50988	0.1519
O	1.69552	1.18146	-0.1091
O	0.05632	2.87647	-0.12466
H	-2.51196	1.66115	-0.6999
H	-2.45442	0.8614	1.70913
H	0.04422	1.43279	2.19115
H	-0.41451	1.1709	-2.03047
H	-1.8262	-1.67602	1.77341
H	-1.49695	-2.51806	-0.59118
H	0.13931	-1.18445	-1.97687
H	0.63847	-1.02392	2.24502
H	-2.67088	-0.62627	-2.04039
H	-3.52385	-0.79218	-0.50003
H	2.85411	1.18811	-0.49144
H	2.02013	-2.76935	-0.24021
H	0.51585	3.40184	0.54557

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 97 maximum allowed number of steps= 174.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C	0	-1.966293		0.757101		-0.479828	
2	2	C	0	-1.699725		0.494105		1.032165	
3	3	C	0	-0.204011		0.863970		1.307550	
4	4	C	0	-0.522153		0.734471		-1.048881	
5	5	C	0	0.281742		1.490024		0.003142	
6	6	C	0	-1.324883		-1.033284		1.067932	
7	7	C	0	-1.429656		-1.455954		-0.421532	
8	8	C	0	-0.150520		-0.802271		-1.008294	
9	9	C	0	0.916407		-1.095621		0.072683	
10	10	C	0	0.174112		-0.661633		1.342653	
11	11	C	0	-2.567463		-0.573376		-0.962093	
12	12	C	0	2.161405		-0.334120		-0.184592	
13	13	N	0	3.324133		-0.258682		-0.509199	
14	14	O	0	1.173658		-2.509883		0.151901	

15	15	O	0	1.695517	1.181463	-0.109098
16	16	O	0	0.056320	2.876467	-0.124658
17	17	H	0	-2.511962	1.661153	-0.699904
18	18	H	0	-2.454416	0.861399	1.709132
19	19	H	0	0.044224	1.432786	2.191148
20	20	H	0	-0.414510	1.170895	-2.030466
21	21	H	0	-1.826195	-1.676023	1.773410
22	22	H	0	-1.496949	-2.518061	-0.591185
23	23	H	0	0.139314	-1.184446	-1.976870
24	24	H	0	0.638471	-1.023921	2.245024
25	25	H	0	-2.670875	-0.626268	-2.040393
26	26	H	0	-3.523852	-0.792179	-0.500030
27	27	H	0	2.854112	1.188112	-0.491437
28	28	H	0	2.020130	-2.769349	-0.240211
29	29	H	0	0.515853	3.401835	0.545570

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.966293	0.757101	-0.479828
2	6	0	-1.699725	0.494105	1.032165
3	6	0	-0.204011	0.863970	1.307550
4	6	0	-0.522153	0.734471	-1.048881
5	6	0	0.281742	1.490024	0.003142
6	6	0	-1.324883	-1.033284	1.067932
7	6	0	-1.429656	-1.455954	-0.421532
8	6	0	-0.150520	-0.802271	-1.008294
9	6	0	0.916407	-1.095621	0.072683
10	6	0	0.174112	-0.661633	1.342653
11	6	0	-2.567463	-0.573376	-0.962093
12	6	0	2.161405	-0.334120	-0.184592
13	7	0	3.324133	-0.258682	-0.509199
14	8	0	1.173658	-2.509883	0.151901
15	8	0	1.695517	1.181463	-0.109098
16	8	0	0.056320	2.876467	-0.124658
17	1	0	-2.511962	1.661153	-0.699904
18	1	0	-2.454416	0.861399	1.709132
19	1	0	0.044224	1.432786	2.191148
20	1	0	-0.414510	1.170895	-2.030466
21	1	0	-1.826195	-1.676023	1.773410
22	1	0	-1.496949	-2.518061	-0.591185
23	1	0	0.139314	-1.184446	-1.976870
24	1	0	0.638471	-1.023921	2.245024
25	1	0	-2.670875	-0.626268	-2.040393
26	1	0	-3.523852	-0.792179	-0.500030
27	1	0	2.854112	1.188112	-0.491437
28	1	0	2.020130	-2.769349	-0.240211
29	1	0	0.515853	3.401835	0.545570

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				

2	C	1.557674	0.000000			
3	C	2.512325	1.565183	0.000000		
4	C	1.552377	2.403165	2.381334	0.000000	
5	C	2.413317	2.444781	1.526231	1.524421	0.000000
6	C	2.452029	1.573119	2.216606	2.872321	3.175233
7	C	2.277935	2.447223	3.142289	2.452568	3.433368
8	C	2.451112	2.871254	2.853481	1.581561	2.542532
9	C	3.470995	3.208112	2.572981	2.583911	2.663305
10	C	3.148901	2.223375	1.572156	2.855403	2.536829
11	C	1.537581	2.422715	3.578149	2.429257	3.647913
12	C	4.279698	4.132164	3.042548	3.015023	2.626000
13	N	5.387141	5.308638	4.124163	4.008931	3.546352
14	O	4.575102	4.249134	3.823138	3.852724	4.100841
15	O	3.704912	3.647274	2.390795	2.449705	1.451402
16	O	2.951071	3.177669	2.483775	2.403532	1.410451
17	H	1.078656	2.240936	3.161014	2.222581	2.885886
18	H	2.245148	1.078308	2.285957	3.369924	3.285138
19	H	3.410695	2.294716	1.079777	3.362472	2.201604
20	H	2.232428	3.389621	3.358700	1.079612	2.173056
21	H	3.319157	2.296714	3.049602	3.933997	4.195367
22	H	3.310494	3.427758	4.088400	3.426175	4.425123
23	H	3.231767	3.905623	3.886038	2.231803	3.330694
24	H	4.169131	3.040163	2.269970	3.910090	3.387213
25	H	2.201252	3.411595	4.417573	2.729783	4.168054
26	H	2.196968	2.707321	4.126926	3.412051	4.465891
27	H	4.839650	4.851849	3.562799	3.451912	2.636825
28	H	5.327742	5.109442	4.532480	4.403851	4.606894
29	H	3.769232	3.687879	2.745829	3.276364	2.001014

		6	7	8	9	10
6	C	0.000000				
7	C	1.551815	0.000000			
8	C	2.396500	1.551702	0.000000		
9	C	2.453118	2.424479	1.546900	0.000000	
10	C	1.568624	2.513039	2.377418	1.533679	0.000000
11	C	2.424154	1.538101	2.428197	3.671628	3.582719
12	C	3.769861	3.769665	2.498529	1.481922	2.527662
13	N	4.969980	4.903025	3.552154	2.614612	3.676188
14	O	3.043380	2.866502	2.452639	1.439649	2.415163
15	O	3.925980	4.101255	2.855102	2.413539	2.796293
16	O	4.314643	4.589785	3.789025	4.068928	3.832105
17	H	3.434296	3.311379	3.426364	4.466588	4.096629
18	H	2.297130	3.310587	3.931938	4.227333	3.059917
19	H	3.036045	4.164521	3.907664	3.411955	2.263494
20	H	3.909892	3.243382	2.237836	3.366255	3.883628
21	H	1.078020	2.241304	3.362916	3.278903	2.283805
22	H	2.233123	1.077674	2.220537	2.878948	3.158876
23	H	3.381944	2.225862	1.080833	2.193725	3.360622
24	H	2.289190	3.402106	3.354954	2.191222	1.077569
25	H	3.411604	2.202207	2.729175	4.189746	4.420430
26	H	2.711476	2.198276	3.411422	4.487313	4.133698
27	H	4.982994	5.034545	3.640959	3.047682	3.737358
28	H	3.989270	3.695796	3.028377	2.029156	3.218029
29	H	4.830264	5.321504	4.531341	4.539953	4.154985

		11	12	13	14	15

11	C	0.000000				
12	C	4.798327	0.000000			
13	N	5.917351	1.209544	0.000000		
14	O	4.357411	2.413051	3.182688	0.000000	
15	O	4.688290	1.587370	2.210540	3.737177	0.000000
16	O	4.414403	3.839641	4.544847	5.507967	2.358018
17	H	2.250543	5.107545	6.146718	5.630889	4.275749
18	H	3.034271	5.130425	6.290247	5.191669	4.542064
19	H	4.559443	3.639856	4.572826	4.580261	2.842721
20	H	2.969698	3.508227	4.281985	4.564332	2.853766
21	H	3.041099	4.640628	5.809048	3.510517	4.910348
22	H	2.250638	4.280008	5.324880	2.772072	4.910267
23	H	2.954627	2.832696	3.626868	2.712622	3.392324
24	H	4.557039	2.949269	3.922259	2.622150	3.394548
25	H	1.084538	5.184619	6.198370	4.809843	5.105210
26	H	1.084462	5.712396	6.868741	5.044018	5.593738
27	H	5.719950	1.700349	1.521331	4.112539	1.220070
28	H	5.137063	2.439957	2.841870	0.968292	3.966293
29	H	5.251875	4.147088	4.732690	5.961216	2.598124

		16	17	18	19	20
16	O	0.000000				
17	H	2.898960	0.000000			
18	H	3.705007	2.538971	0.000000		
19	H	2.728978	3.865801	2.608069	0.000000	
20	H	2.600531	2.531808	4.271018	4.254533	0.000000
21	H	5.279365	4.210024	2.614824	3.652077	4.956538
22	H	5.633048	4.302081	4.198684	5.072059	4.105070
23	H	4.464145	4.093573	4.949700	4.922532	2.420170
24	H	4.600795	5.080103	3.661634	2.528130	4.919939
25	H	4.834955	2.656023	4.039671	5.432992	2.884628
26	H	5.139796	2.661336	2.959461	4.992402	3.982951
27	H	3.288268	5.390916	5.755842	3.892505	3.612865
28	H	5.978724	6.354567	6.083077	5.241531	4.965683
29	H	0.967671	3.707943	4.078013	2.609121	3.532510

		21	22	23	24	25
21	H	0.000000				
22	H	2.531549	0.000000			
23	H	4.262567	2.525076	0.000000		
24	H	2.592727	3.851825	4.254329	0.000000	
25	H	4.044819	2.656537	2.865791	5.429060	0.000000
26	H	2.971826	2.663703	3.969095	4.991388	1.768563
27	H	5.936167	5.716415	3.899445	4.158170	6.018033
28	H	4.477080	3.543469	3.010875	3.336449	5.462507
29	H	5.725157	6.355215	5.247710	4.742414	5.750483

		26	27	28	29
26	H	0.000000			
27	H	6.678327	0.000000		
28	H	5.891727	4.052177	0.000000	
29	H	5.916270	3.382811	6.400298	0.000000

Interatomic angles:

C1-C2-C3=107.1229	C2-C1-C4=101.1955	C1-C4-C3= 76.158
C2-C3-C4= 71.6619	C2-C1-C5= 72.3986	C1-C5-C3= 75.522
C2-C3-C5=104.5192	C1-C4-C5=103.3193	C2-C4-C5= 73.164
C3-C5-C4=102.6308	C1-C2-C6=103.1074	C1-C6-C3= 64.8837

C3-C2-C6= 89.8702 C4-C1-C6= 88.7047 C4-C2-C6= 90.0025
C4-C3-C6= 77.2279 C5-C1-C6= 81.475 C5-C2-C6=102.2379
C5-C3-C6=114.8124 C5-C4-C6= 86.7794 C2-C1-C7= 76.7508
C3-C1-C7= 81.8289 C3-C2-C7=100.7985 C4-C1-C7= 77.0597
C4-C2-C7= 60.7401 C3-C4-C7= 81.0765 C5-C1-C7= 94.0417
C5-C2-C7= 89.1484 C5-C4-C7=117.4684 C1-C7-C6= 77.0474
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C2-C1-C8= 88.5727 C3-C1-C8= 70.1729 C2-C3-C8= 74.7597
C1-C4-C8=102.906 C2-C4-C8= 89.7555 C3-C4-C8= 89.7738
C5-C1-C8= 63.0185 C2-C5-C8= 70.2677 C3-C5-C8= 85.1846
C5-C4-C8=109.8746 C1-C8-C6= 60.7595 C2-C6-C8= 90.199
C3-C6-C8= 76.3112 C4-C8-C6= 90.043 C5-C8-C6= 79.9549
C1-C7-C8= 77.012 C2-C7-C8= 88.8488 C3-C8-C7= 85.621
C4-C8-C7=103.0224 C5-C8-C7=111.6866 C6-C7-C8=101.1016
C1-C3-C9= 86.0783 C2-C3-C9= 98.7262 C1-C4-C9=111.6622
C2-C4-C9= 79.9847 C4-C3-C9= 62.7317 C1-C5-C9= 86.1216
C2-C5-C9= 77.682 C5-C3-C9= 76.3277 C5-C4-C9= 75.9894
C1-C6-C9= 90.0837 C2-C6-C9=103.4827 C3-C6-C9= 66.6468
C4-C9-C6= 69.4784 C5-C9-C6= 76.597 C1-C7-C9= 95.0939
C2-C7-C9= 82.3727 C3-C9-C7= 77.8573 C4-C7-C9= 63.9823
C5-C9-C7= 84.7429 C6-C7-C9= 72.4543 C1-C8-C9=118.7457
C2-C8-C9= 87.7741 C3-C9-C8= 83.7199 C4-C8-C9=111.3624
C5-C8-C9= 77.0397 C6-C8-C9= 73.3988 C7-C8-C9=102.9695
C1-C2-C10=111.5643 C1-C3-C10= 98.2397 C2-C3-C10= 90.2553
C1-C4-C10= 85.8107 C4-C2-C10= 76.1103 C4-C3-C10= 90.0834
C1-C5-C10= 78.9633 C5-C2-C10= 65.6356 C5-C3-C10=109.9125
C4-C5-C10= 85.5059 C1-C6-C10=100.8083 C2-C6-C10= 90.0942
C3-C10-C6= 89.7803 C4-C10-C6= 74.7008 C5-C10-C6= 98.5703
C1-C7-C10= 82.0234 C7-C2-C10= 64.8958 C3-C10-C7= 97.9065
C4-C7-C10= 70.1922 C5-C10-C7= 85.6691 C7-C6-C10=107.2865
C1-C8-C10= 81.3915 C2-C10-C8= 77.1486 C3-C10-C8= 90.1423
C4-C8-C10= 89.999 C5-C10-C8= 62.2134 C6-C10-C8= 71.4769
C7-C8-C10= 76.323 C2-C10-C9=116.0633 C3-C10-C9=111.8706
C4-C9-C10= 83.6585 C5-C10-C9= 77.4224 C6-C10-C9=104.504
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C3-C1-C11=122.2905 C3-C2-C11=126.2436 C4-C1-C11=103.6585
C4-C2-C11= 60.4463 C3-C4-C11= 96.1083 C5-C1-C11=133.6119
C5-C2-C11= 97.0833 C5-C4-C11=133.3283 C1-C11-C6= 72.6082
C6-C2-C11= 71.1104 C3-C6-C11=100.7975 C4-C11-C6= 72.5717
C1-C11-C7= 95.5699 C2-C11-C7= 72.4572 C4-C11-C7= 72.4613
C6-C7-C11=103.3549 C1-C11-C8= 72.4441 C2-C11-C8= 72.5838
C3-C8-C11= 84.8855 C4-C8-C11= 71.0347 C5-C8-C11= 94.397
C8-C6-C11= 60.4879 C8-C7-C11=103.6024 C9-C4-C11= 94.1247
C9-C6-C11= 97.6659 C9-C7-C11=134.6022 C9-C8-C11=133.7175
C10-C2-C11=100.8229 C10-C4-C11= 84.9601 C10-C6-C11=126.2664
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C2-C4-C12= 98.769 C3-C4-C12= 67.4618 C1-C5-C12=116.1993
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C6-C4-C12= 79.5929 C7-C4-C12= 86.5302 C1-C8-C12=119.6821
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C2-C10-C12=120.7229 C3-C10-C12= 92.8585 C4-C10-C12= 67.809

C5-C10-C12= 62.4647 C6-C10-C12=132.5473 C7-C10-C12= 96.8077
C10-C8-C12= 62.3908 C10-C9-C12=113.889 C11-C4-C12=123.2528
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C5-C9-N13= 84.4259 C6-C9-N13=157.4449 C7-C9-N13=153.2906
C8-C9-N13=114.7666 C10-C9-N13=122.643 C4-C12-N13=139.1632
C5-C12-N13=131.6015 C8-C12-N13=144.3616 C9-C12-N13=152.4053
C10-C12-N13=157.8229 C1-C7-O14=125.1885 C2-C7-O14=105.9245
C4-C7-O14= 92.4928 C6-C7-O14= 81.1886 C1-C8-O14=137.8085
C2-C8-O14=105.634 C3-C8-O14= 91.8775 C4-C8-O14=144.6377
C5-C8-O14=110.3493 C6-C8-O14= 77.7389 C7-C8-O14= 88.4463
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C6-C9-O14= 99.5495 C7-C9-O14= 92.1849 C8-C9-O14=110.3645
C2-C10-O14=132.6677 C3-C10-O14=146.216 C4-C10-O14= 93.563
C5-C10-O14=111.7887 C6-C10-O14= 97.3443 C7-C10-O14= 71.1021
C8-C10-O14= 61.556 C10-C9-O14=108.5966 C11-C7-O14=162.3841
C11-C8-O14=126.4433 C4-C12-O14= 89.7256 C5-C12-O14=108.867
C7-O14-C12= 90.7071 C8-O14-C12= 61.7881 C12-C9-O14=111.3602
C10-O14-C12= 63.1372 N13-C9-O14= 99.3318 N13-C12-O14=119.1535
C1-C3-O15= 98.1292 C2-C3-O15=133.3443 C1-C4-O15=134.3367
C2-C4-O15= 97.4486 C4-C3-O15= 61.7722 C1-C5-O15=145.8247
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C6-C3-O15=116.8319 C6-C4-O15= 94.7365 C7-C4-O15=113.5662
C1-C8-O15= 88.2264 C2-C8-O15= 79.1257 C8-C3-O15= 65.276
C8-C4-O15= 87.4054 C8-C5-O15= 86.7421 C6-C8-O15= 96.371
C7-C8-O15=134.9594 C3-O15-C9= 64.761 C4-O15-C9= 64.1836
C5-O15-C9= 83.1259 C6-C9-O15=107.5487 C7-C9-O15=115.9276
C8-C9-O15= 89.49 C2-C10-O15= 92.4888 C10-C3-O15= 87.1917
C4-O15-C10= 65.5661 C10-C5-O15= 84.367 C6-C10-O15=125.8148
C7-C10-O15=101.0165 C8-C10-O15= 66.4152 C10-C9-O15= 87.2276
C11-C4-O15=147.8578 C11-C8-O15=124.8961 C3-O15-C12= 97.7341
C4-O15-C12= 94.1999 C5-O15-C12=119.5081 C8-C12-O15= 85.5838
C9-C12-O15=103.6383 C10-C12-O15= 82.1965 C3-O15-N13=127.3075
C4-O15-N13=118.5975 C5-O15-N13=150.4762 C8-O15-N13= 88.0919
C9-O15-N13= 68.7034 C10-O15-N13= 93.7503 N13-C12-O15=103.6124
O14-C8-O15= 89.1795 O14-C9-O15=150.8429 O14-C10-O15= 91.333
O14-C12-O15=137.2327 C2-C1-O16= 83.5198 C1-C3-O16= 72.4073
C2-C3-O16=100.9631 C1-C4-O16= 94.011 C2-C4-O16= 82.7664
C3-C4-O16= 62.5404 C1-C5-O16= 97.5574 C2-C5-O16=108.0011
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C6-C3-O16=133.1718 C6-C4-O16=109.4117 C7-C1-O16=122.2199
C7-C4-O16=141.8715 C8-C1-O16= 88.5738 C8-C3-O16= 90.1828
C8-C4-O16=143.0834 C8-C5-O16=145.3879 C9-C3-O16=107.1402
C9-C4-O16=109.2867 C9-C5-O16=174.1359 C10-C3-O16=140.7082
C10-C4-O16= 93.152 C10-C5-O16=151.0206 C11-C1-O16=157.996
C11-C4-O16=131.9661 C12-C4-O16= 89.5079 C12-C5-O16=142.2552
C1-O16-O15= 87.7652 C3-O15-O16= 63.0671 C4-O16-O15= 61.9162
O15-C5-O16=110.9559 C8-O15-O16= 92.7451 C9-O15-O16=117.0186
C10-O15-O16= 95.6815 C12-O15-O16=152.8771 N13-O15-O16=168.3139
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C4-C1-H17=114.0814 C2-H17-C4= 65.1483 C3-C4-H17= 86.6498
C5-C1-H17=104.9232 C5-C2-H17= 75.8942 C3-C5-H17= 85.666
C5-C4-H17= 99.0391 C6-C1-H17=150.8194 C6-C2-H17=127.5596
C6-C4-H17= 83.7243 C7-C1-H17=159.8266 C7-C2-H17= 89.7625
C7-C4-H17= 90.054 C8-C1-H17=149.7656 C8-C2-H17= 83.19

C8-C4-H17=127.6954 C8-C5-H17= 77.993 C9-C4-H17=136.5172
C9-C5-H17=107.1347 C10-C2-H17=133.1664 C10-C4-H17=106.897
C10-C5-H17= 97.9239 C11-C1-H17=117.6101 C2-H17-C11= 65.2856
C4-H17-C11= 65.7834 C5-H17-C11= 89.6206 C6-C11-H17= 94.4833
C7-C11-H17=120.6998 C8-C11-H17= 94.0866 C12-C4-H17=154.1066
C12-C5-H17=135.7827 O15-C4-H17=132.3887 O15-C5-H17=159.5092
C1-H17-O16= 82.1086 C2-H17-O16= 75.1579 C3-O16-H17= 71.451
O16-C4-H17= 77.4978 O16-C5-H17= 76.4036 C11-H17-O16=117.465
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C8-C2-H18=167.8414 C8-C3-H18= 99.2285 C8-C6-H18=113.7831
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C11-C2-H18=114.5939 C11-C6-H18= 79.9343 O15-C3-H18=152.4248
O16-C1-H18= 89.903 O16-C3-H18=101.8524 H17-C1-H18= 92.8661
H17-C2-H18= 93.1057 C3-H18-H17= 81.6787 C4-H17-H18= 89.8485
C5-H17-H18= 74.2305 C6-H18-H17= 90.3498 C11-H17-H18= 78.3664
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C2-C3-H19=119.2193 C4-C2-H19= 91.3783 C4-C3-H19=150.3564
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C4-C5-H19=128.0299 C6-C2-H19=101.806 C6-C3-H19=130.9656
C7-C2-H19=122.8273 C8-C2-H19= 97.6755 C8-C3-H19=165.3375
C8-C5-H19=110.7057 C9-C3-H19=133.9345 C9-C5-H19= 88.5399
C2-C10-H19= 61.5105 C10-C3-H19=115.9526 C4-C10-H19= 81.2316
C5-H19-C10= 69.2262 C6-C10-H19=103.2997 C7-C10-H19=121.2656
C8-C10-H19=114.6824 C9-C10-H19=126.8709 C11-C2-H19=150.2484
C12-C5-H19= 97.4818 C12-C10-H19= 98.7265 O14-C10-H19=156.4445
C2-H19-O15= 89.806 O15-C3-H19=103.431 C4-O15-H19= 78.5035
O15-C5-H19=100.161 C8-O15-H19= 86.5995 C9-O15-H19= 80.5
O15-C10-H19= 67.4153 C12-O15-H19=107.0606 N13-O15-H19=129.1995
C1-O16-H19= 73.6902 C2-H19-O16= 77.9463 O16-C3-H19= 91.1993
C4-O16-H19= 81.5925 O16-C5-H19= 95.6449 C10-H19-O16= 99.8543
O15-O16-H19= 67.4933 H17-C2-H19=116.9236 H17-C5-H19= 98.0024
H17-O16-H19= 86.7143 C1-H18-H19= 88.9732 H18-C2-H19= 94.329
H18-C3-H19= 94.77 C5-H19-H18= 85.7205 C6-H18-H19= 76.1846
C10-H19-H18= 77.4657 O15-H19-H18=112.8049 O16-H19-H18= 87.8974
H17-H18-H19= 97.3577 C2-C1-H20=125.9138 C3-C1-H20= 89.9252
C1-C4-H20=114.8438 C2-C4-H20=151.2375 C3-C4-H20=149.8131
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C5-C4-H20=111.9945 C6-C1-H20=113.076 C6-C4-H20=161.2102
C7-C1-H20= 91.9541 C7-C4-H20=129.0866 C1-H20-C8= 66.5028
C2-C8-H20= 82.1171 C3-C8-H20= 81.583 C8-C4-H20=113.122
C5-H20-C8= 70.3809 C6-C8-H20=115.0186 C7-C8-H20=116.5464
C9-C4-H20=128.7149 C9-C5-H20= 87.605 C9-C8-H20=124.5944
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C11-C1-H20=102.3748 C2-C11-H20= 77.1544 C11-C4-H20=109.5155
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C11-C8-H20= 78.9395 C12-C4-H20=108.3705 C12-C5-H20= 93.4641
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C3-O15-H20= 79.1055 O15-C4-H20=100.6481 O15-C5-H20=102.0348

C8-H20-O15= 66.9529 C9-O15-H20= 78.9618 C10-O15-H20= 86.8368
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O15-O16-H20= 70.0774 H17-C1-H20= 93.1283 C2-H17-H20= 90.2913
H17-C4-H20= 93.6394 C5-H20-H17= 75.2373 C8-H20-H17= 91.6284
C11-H17-H20= 76.5229 O15-H20-H17=104.9506 O16-H20-H17= 68.7676
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C1-C6-H21=136.6168 C2-C6-H21=118.879 C3-C6-H21=132.4333
C4-C6-H21=168.2913 C1-C7-H21= 94.5181 C2-H21-C7= 65.2548
C4-C7-H21=113.8072 C7-C6-H21=115.743 C8-C2-H21= 80.3547
C8-C6-H21=148.4644 C8-C7-H21=123.885 C9-C6-H21=132.4718
C9-C7-H21= 89.2074 C2-C10-H21= 61.2527 C3-C10-H21=102.9775
C4-C10-H21= 99.298 C5-C10-H21=120.896 C10-C6-H21=118.1017
C7-H21-C10= 67.4627 C8-C10-H21= 92.3292 C9-C10-H21=117.0271
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C12-C10-H21=149.3318 O14-C7-H21= 85.9096 O14-C10-H21= 96.6367
O15-C10-H21=150.1375 H17-C2-H21=136.1849 C1-H18-H21= 85.7938
H18-C2-H21= 94.6282 C3-H18-H21= 76.6377 H18-C6-H21= 94.6136
C7-H21-H18= 85.5926 C10-H21-H18= 76.9839 H17-H18-H21=109.5383
H19-C2-H21=105.3883 H19-C10-H21=106.8594 H19-H18-H21= 88.7327
C1-C6-H22= 89.7912 C2-C6-H22=127.6118 C3-C6-H22=133.5015
C4-C6-H22= 83.2924 C1-C7-H22=159.8419 C2-C7-H22=150.6869
C4-C7-H22=149.6609 C6-C7-H22=115.0717 C1-C8-H22= 90.1086
C2-C8-H22= 83.5821 C3-C8-H22=106.7014 C4-C8-H22=127.8165
C5-C8-H22=136.4693 C6-H22-C8= 65.1076 C8-C7-H22=114.0246
C3-C9-H22= 97.0037 C4-C9-H22= 77.4759 C5-C9-H22=105.8961
C9-C6-H22= 75.6455 C9-C7-H22=103.8269 C9-C8-H22= 98.072
C10-C6-H22=111.1788 C10-C7-H22=117.5084 C10-C8-H22= 86.7183
C10-C9-H22= 85.7007 C1-C11-H22=120.6647 C2-C11-H22= 94.2839
C4-C11-H22= 94.0486 C6-H22-C11= 65.4547 C11-C7-H22=117.6457
C8-H22-C11= 65.7828 C9-H22-C11= 90.5621 C12-C8-H22=130.0848
C12-C9-H22=156.6517 N13-C9-H22=151.4961 C6-H22-O14= 74.017
C7-H22-O14= 83.9576 O14-C8-H22= 72.5747 C9-O14-H22= 79.3971
C10-O14-H22= 74.675 C11-H22-O14=119.9912 C12-O14-H22=111.0776
O15-C8-H22=150.4309 O15-C9-H22=136.0037 H17-C11-H22=145.7899
H18-C6-H22=135.8812 H20-C8-H22=134.0731 H20-C11-H22=102.8245
C2-H21-H22= 90.3247 H21-C6-H22= 93.0929 H21-C7-H22= 92.6567
C8-H22-H21= 89.8455 C9-H22-H21= 74.2939 C10-H21-H22= 81.8162
C11-H22-H21= 78.736 O14-H22-H21= 82.7576 H18-H21-H22=109.333
C1-C4-H23=116.1467 C2-C4-H23=114.7904 C3-C4-H23=114.7472
C5-C4-H23=123.835 C6-C4-H23= 81.958 C1-C7-H23= 91.7002
C2-C7-H23=113.3075 C4-H23-C7= 66.7601 C6-C7-H23=126.1476
C1-C8-H23=128.0837 C2-C8-H23=160.2499 C3-C8-H23=159.85
C4-C8-H23=112.556 C5-C8-H23=129.0274 C6-C8-H23=150.8912
C7-C8-H23=114.2654 C3-C9-H23=108.9643 C4-H23-C9= 71.4398
C5-C9-H23= 86.0148 C6-C9-H23= 93.2348 C7-H23-C9= 66.5341
C9-C8-H23=111.9758 C10-C4-H23= 81.6972 C10-C7-H23= 90.1227
C10-C8-H23=150.5122 C10-C9-H23=127.8535 C1-C11-H23= 85.8998
C2-C11-H23= 92.6204 C11-C4-H23= 78.5506 C6-C11-H23= 77.22
C11-C7-H23=101.8802 C11-C8-H23=108.4996 C9-H23-C11= 89.7286
C4-H23-C12= 71.9642 C5-C12-H23= 75.0957 C7-H23-C12= 95.6054

C12-C8-H23= 96.5204 C12-C9-H23= 98.9869 C10-C12-H23= 77.418
C11-H23-C12=111.9977 N13-C9-H23= 97.5414 N13-C12-H23=122.3528
C4-H23-O14=101.9362 C7-H23-O14= 70.1728 O14-C8-H23= 91.8881
O14-C9-H23= 94.2973 C10-O14-H23= 81.6732 C11-H23-O14=100.4191
C12-O14-H23= 66.8013 O15-C4-H23= 92.7566 O15-C8-H23=110.7644
O15-C9-H23= 94.7141 O15-C12-H23= 96.1533 O16-C4-H23=148.7379
H17-C4-H23=133.5602 H17-C11-H23=102.8716 C1-H20-H23= 87.8964
H20-C4-H23= 86.5585 C5-H20-H23= 92.8017 C7-H23-H20= 88.4461
H20-C8-H23= 86.2203 C9-H23-H20= 93.5745 C11-H23-H20= 66.2146
C12-H23-H20= 83.4092 O14-H23-H20=125.4622 O15-H20-H23= 79.6009
O16-H20-H23=125.4946 H17-H20-H23=111.4933 H21-C7-H23=145.1841
C4-H23-H22= 91.9409 C6-H22-H23= 90.3795 H22-C7-H23= 93.1087
H22-C8-H23= 93.3085 C9-H23-H22= 74.8247 C11-H22-H23= 76.1981
C12-H23-H22=105.8965 O14-H23-H22= 63.7921 H20-H23-H22=112.2016
H21-H22-H23=114.9094 C1-C3-H24=121.2505 C2-C3-H24=103.3442
C4-C3-H24=114.3951 C5-C3-H24=125.1693 C1-C6-H24=123.0884
C2-C6-H24=102.2445 C6-C3-H24= 61.3448 C4-C6-H24= 97.8591
C7-C6-H24=123.5425 C8-C3-H24= 80.9424 C8-C6-H24= 91.4211
C3-H24-C9= 70.4189 C4-C9-H24=109.6652 C5-C9-H24= 87.9307
C6-H24-C9= 66.3523 C7-C9-H24= 94.8307 C8-C9-H24=126.8048
C2-C10-H24=130.9115 C3-C10-H24=116.6536 C4-C10-H24=166.1285
C5-C10-H24=135.158 C6-C10-H24=118.6075 C7-C10-H24=139.1669
C8-C10-H24=150.1169 C9-C10-H24=112.9369 C11-C6-H24=150.394
C3-H24-C12= 69.9345 C4-C12-H24= 81.9197 C5-C12-H24= 74.5712
C6-H24-C12= 91.1596 C8-C12-H24= 75.5197 C12-C9-H24=105.1805
C12-C10-H24=102.1653 N13-C9-H24=109.0845 N13-C12-H24=137.0596
C3-H24-O14=102.556 C6-H24-O14= 76.2479 C7-O14-H24= 76.4653
C8-O14-H24= 82.6953 O14-C9-H24= 90.0148 O14-C10-H24= 88.6955
C12-O14-H24= 71.5721 O15-C3-H24= 93.4559 O15-C9-H24= 94.8612
O15-C10-H24=114.9547 O15-C12-H24= 91.8669 O16-C3-H24=150.8227
H18-C3-H24=106.9708 H18-C6-H24=105.9515 C2-H19-H24= 77.9887
H19-C3-H24= 90.8504 C5-H19-H24= 91.2081 C6-H24-H19= 77.9608
C9-H24-H19= 92.3202 H19-C10-H24= 91.2555 C12-H24-H19= 82.9081
O14-H24-H19=125.5667 O15-H19-H24= 78.1584 O16-H19-H24=122.0809
H18-H19-H24= 90.9303 C2-H21-H24= 76.627 C3-H24-H21= 77.3641
H21-C6-H24= 93.7141 C7-H21-H24= 89.1552 C9-H24-H21= 86.1017
H21-C10-H24= 94.0231 C12-H24-H21=113.5687 O14-H24-H21= 84.6229
H18-H21-H24= 89.3578 H19-H24-H21= 90.979 H22-C6-H24=116.7969
H22-C9-H24= 97.958 H22-O14-H24= 91.0898 H22-H21-H24= 97.4654
H23-C9-H24=151.9604 H23-C12-H24= 94.7271 H23-O14-H24=105.7662
C2-C1-H25=129.5554 C3-C1-H25=139.0805 C4-C1-H25= 91.6462
C2-C4-H25= 83.0485 C3-C4-H25=119.4517 C5-C1-H25=129.1165
C5-C4-H25=155.8979 C6-C1-H25= 94.1493 C6-C4-H25= 74.9841
C1-H25-C7= 62.3034 C2-C7-H25= 94.2584 C4-C7-H25= 71.5809
C6-C7-H25=129.8672 C8-C1-H25= 71.6062 C2-C8-H25= 75.0105
C3-C8-H25=104.593 C4-C8-H25= 73.18 C5-C8-H25=104.4362
C6-C8-H25= 83.1835 C8-C7-H25= 91.6006 C9-C4-H25=104.0539
C9-C7-H25=129.7358 C9-C8-H25=155.9857 C10-C4-H25=104.6212
C10-C7-H25=139.1711 C10-C8-H25=119.752 C1-C11-H25=113.0372
C2-C11-H25=150.9334 C4-C11-H25= 94.0724 C6-C11-H25=150.7179
C7-C11-H25=113.0776 C8-C11-H25= 94.0941 C12-C4-H25=128.9066
C12-C8-H25=165.2634 O14-C7-H25=142.8875 O14-C8-H25=136.2513
O15-C4-H25=160.5413 O15-C8-H25=132.1751 O16-C1-H25=139.1157
O16-C4-H25=140.6558 H17-C1-H25=102.7179 C2-H17-H25= 87.8949

C4-H17-H25= 67.3714 C5-H17-H25= 97.4582 C7-H25-H17= 85.3963
C8-H25-H17= 79.0136 H17-C11-H25= 99.5904 O16-H17-H25=120.9439
H18-C1-H25=130.6024 H18-H17-H25=102.0607 H20-C1-H25= 81.173
H20-C4-H25= 87.1195 C5-H20-H25=110.2022 C7-H25-H20= 77.9551
H20-C8-H25= 70.2121 C11-H25-H20= 83.7775 O15-H20-H25=125.6599
O16-H20-H25=123.5557 H20-H17-H25= 67.5152 H21-C7-H25=131.0849
C1-H25-H22= 85.3736 C4-H25-H22= 78.9887 C6-H22-H25= 88.0439
H22-C7-H25=102.732 C8-H22-H25= 67.37 C9-H22-H25= 98.3014
H22-C11-H25= 99.6174 O14-H22-H25=124.7404 H17-H25-H22=108.1517
H20-H25-H22= 95.5165 H21-H22-H25=102.4278 C1-H25-H23= 78.0427
H23-C4-H25= 69.7371 H23-C7-H25= 80.6579 H23-C8-H25= 86.0749
C9-H23-H25=111.1115 C11-H25-H23= 83.9129 C12-H23-H25=130.9611
O14-H23-H25=119.1091 H17-H25-H23= 95.6174 H20-H23-H25= 65.5158
H23-H22-H25= 67.1001 C2-C1-H26= 90.641 C3-C1-H26=122.2654
C3-C2-H26=148.8392 C4-C1-H26=130.2315 C4-C2-H26= 83.5458
C5-C1-H26=151.2123 C5-C2-H26=120.0941 C6-C1-H26= 71.1163
C6-C2-H26= 73.2685 C3-C6-H26=113.3592 C4-C6-H26= 75.2711
C1-H26-C7= 62.4329 C2-C7-H26= 71.0629 C4-C7-H26= 94.226
C6-C7-H26= 90.9369 C8-C1-H26= 94.2769 C8-C2-H26= 75.3352
C8-C6-H26= 83.5608 C8-C7-H26=130.1363 C9-C6-H26=120.5712
C9-C7-H26=152.1586 C10-C2-H26=113.5728 C10-C6-H26=148.7813
C10-C7-H26=122.5198 C1-C11-H26=112.6907 C2-C11-H26= 93.098
C4-C11-H26=150.0386 C6-C11-H26= 93.2657 C7-C11-H26=112.7598
C8-C11-H26=150.1007 O14-C7-H26=169.5294 O16-C1-H26=173.4436
H17-C1-H26=103.3275 C2-H17-H26= 66.4019 C4-H17-H26= 88.1569
C5-H17-H26=107.1643 C6-H26-H17= 79.4582 C7-H26-H17= 85.3435
H17-C11-H26= 99.9295 O16-H17-H26=135.1052 H18-C1-H26= 83.5456
H18-C2-H26= 92.612 C3-H18-H26=103.0167 H18-C6-H26= 71.8984
C7-H26-H18= 78.3347 C11-H26-H18= 83.4907 H18-H17-H26= 69.3282
H19-C2-H26=172.8619 H19-H18-H26=127.3421 H20-C1-H26=128.1067
H20-C11-H26=155.6642 H20-H17-H26=100.1341 C1-H26-H21= 78.3286
H21-C2-H26= 72.3396 H21-C6-H26= 93.1135 H21-C7-H26= 84.0346
C10-H21-H26=102.9412 C11-H26-H21= 83.2329 H17-H26-H21= 96.57
H21-H18-H26= 64.0851 C1-H26-H22= 85.2824 C2-H26-H22= 79.3101
C6-H22-H26= 66.5723 H22-C7-H26=103.4433 C8-H22-H26= 88.119
C9-H22-H26=108.0504 H22-C11-H26=100.0742 O14-H22-H26=136.2196
H17-H26-H22=107.7819 H18-H26-H22= 96.465 H21-H22-H26= 69.7302
H23-C7-H26=127.5696 H23-C11-H26=155.8577 H23-H22-H26= 99.7685
H24-C6-H26=172.9936 H24-H21-H26=127.4007 C1-H26-H25= 66.4171
C2-H26-H25= 97.0877 C4-H25-H26= 96.318 C6-H26-H25= 96.9416
C7-H26-H25= 66.4195 C8-H25-H26= 96.3136 H25-C11-H26=109.2503
H17-H25-H26= 70.7356 H18-H26-H25=115.0529 H20-H25-H26=115.6393
H21-H26-H25=114.751 H22-H25-H26= 70.8033 H23-H25-H26=115.8085
C1-C5-H27=146.7653 C2-C5-H27=145.3844 C3-C5-H27=115.0765
C4-C5-H27=109.1634 C8-C5-H27= 89.3131 C9-C5-H27= 70.2001
C10-C5-H27= 92.4826 C4-C12-H27= 89.632 C5-C12-H27= 71.4958
C8-C12-H27=119.0265 C9-C12-H27=146.4724 C10-C12-H27=123.0474
C5-H27-N13=114.3607 C9-N13-H27= 90.9919 C12-N13-H27= 76.0653
O14-C12-H27=177.6188 C3-O15-H27=160.2026 C4-O15-H27=137.769
C5-O15-H27=161.4544 C8-O15-H27=121.2711 C9-O15-H27=109.59
C10-O15-H27=133.0747 C12-O15-H27= 73.2373 N13-H27-O15=106.9695
O16-C5-H27=104.5645 O16-O15-H27=130.855 H17-C5-H27=154.8893
H19-C5-H27=106.7788 H19-O15-H27=143.5821 H20-C5-H27= 96.9051
H20-O15-H27=119.417 H23-C12-H27=116.447 H24-C12-H27=124.64

C3-C9-H28=159.8951 C4-C9-H28=145.0949 C5-C9-H28=157.8774
C6-C9-H28=125.4846 C7-C9-H28=111.8586 C8-C9-H28=115.0764
C10-C9-H28=128.6347 C4-C12-H28=107.1975 C5-C12-H28=130.805
C8-C12-H28= 75.635 C12-C9-H28= 86.5666 C10-C12-H28= 80.731
N13-C9-H28= 74.2656 N13-C12-H28= 96.4185 C7-O14-H28=144.2368
C8-O14-H28=117.8385 C9-O14-H28=113.401 C10-O14-H28=140.0418
C12-O14-H28= 80.0555 N13-H28-O14=101.6962 O15-C9-H28=126.2284
O15-C12-H28=159.5564 O15-N13-H28=102.7308 H22-C9-H28= 90.7374
H22-O14-H28=137.1259 C4-H23-H28=113.4473 C7-H23-H28= 88.457
C8-H23-H28= 80.6045 H23-C9-H28= 90.8719 C11-H23-H28=118.884
H23-C12-H28= 69.1848 N13-H28-H23= 76.5259 H23-O14-H28= 98.4227
H20-H23-H28=131.914 H22-H23-H28= 79.0619 H24-C9-H28=104.4097
H24-C12-H28= 75.8444 H24-O14-H28=130.8082 H25-H23-H28=136.7078
H27-C12-H28=155.9214 H27-N13-H28=134.2109 C1-C3-H29= 91.4775
C2-C3-H29=114.8419 C4-C3-H29= 79.0872 C1-C5-H29=116.9617
C2-C5-H29=111.7114 C3-C5-H29=101.3889 C4-C5-H29=136.2454
C6-C3-H29=153.3384 C8-C3-H29=108.0335 C8-C5-H29=171.5385
C9-C3-H29=117.1663 C9-C5-H29=153.2022 C10-C3-H29=147.1439
C10-C5-H29=132.236 C12-C5-H29=126.8209 C3-O15-H29= 66.6365
C4-O15-H29= 80.884 O15-C5-H29= 96.3221 C8-O15-H29=112.3069
C9-O15-H29=129.8471 C10-O15-H29=100.6864 C12-O15-H29=163.9876
N13-O15-H29=159.5359 C1-O16-H29=143.0104 C3-O16-H29= 95.1807
C4-O16-H29=149.822 C5-O16-H29=113.2674 O15-O16-H29= 93.1858
H17-C5-H29= 97.0446 H17-O16-H29=141.791 H18-C3-H29=107.9314
C2-H19-H29= 97.3275 C3-H19-H29= 85.5839 H19-C5-H29= 76.5886
C10-H19-H29=116.8405 O15-H29-H19= 66.1742 O16-H29-H19= 86.6328
H18-H19-H29=102.8236 H20-C5-H29=115.5614 H20-O15-H29= 80.6248
H20-O16-H29=161.74 H24-C3-H29=141.8129 H24-H19-H29=134.7738
H27-C5-H29= 92.6424 H27-O15-H29=120.3628

Stoichiometry C12H13NO3
Framework group C1[X(C12H13NO3)]
Deg. of freedom 81
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.006135	0.630251	-0.497947
2	6	0	-1.737173	0.384175	1.016468
3	6	0	-0.270701	0.848641	1.305481
4	6	0	-0.558348	0.700082	-1.053743
5	6	0	0.186019	1.504967	0.005473
6	6	0	-1.265946	-1.116188	1.055924
7	6	0	-1.329889	-1.544063	-0.434366
8	6	0	-0.089769	-0.809822	-1.009496
9	6	0	0.983768	-1.034924	0.081259
10	6	0	0.203693	-0.649730	1.344303
11	6	0	-2.516715	-0.735684	-0.985476
12	6	0	2.179923	-0.195402	-0.164728
13	7	0	3.338387	-0.045767	-0.478683
14	8	0	1.330031	-2.429915	0.163068

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   15          8             0        1.617574    1.287322   -0.093760
   16          8             0       -0.126261    2.874248   -0.124620
   17          1             0       -2.606360    1.497722   -0.723165
   18          1             0       -2.519934    0.702267    1.686432
   19          1             0       -0.067378    1.431773    2.191221
   20          1             0       -0.469802    1.142896   -2.034375
   21          1             0       -1.731645   -1.789909    1.756888
   22          1             0       -1.327695   -2.608228   -0.604450
   23          1             0        0.232721   -1.172314   -1.975312
   24          1             0        0.681951   -0.982016    2.250951
   25          1             0       -2.606667   -0.794619   -2.064669
   26          1             0       -3.461377   -1.015279   -0.532156
   27          1             0        2.776833    1.368069   -0.465470
   28          1             0        2.194892   -2.634659   -0.221230
   29          1             0        0.292647    3.427597    0.549701
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.8970808      0.7253537      0.5207456
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,N-
14,O-16,
 O-16,O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1
 Standard basis: 3-21+G* (6D, 7F)
 There are   234 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    262144 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
   234 basis functions      343 primitive gaussians
    58 alpha electrons       58 beta electrons
       nuclear repulsion energy      1241.9243303594 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   234 RedAO= T  NBF=   234
 NBsUse=   234 1.00D-04 NBFU=   234
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -736.874056621     A.U. after   18 cycles
             Convg  =    0.5917D-08             -V/T =  2.0022
             S**2   =   0.0000
 Range of M.O.s used for correlation:     1   234
 NBasis=   234 NAE=    58 NBE=    58 NFC=     0 NFV=     0
 NROrb=    234 NOA=    58 NOB=    58 NVA=   176 NVB=   176

 **** Warning!!: The largest alpha MO coefficient is  0.10925165D+03

          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
```

```
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   3 vectors were produced by pass 12.
   1 vectors were produced by pass 13.
 Inv2:  IOpt= 1 Iter= 1 AM= 6.60D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  40 with in-core refinement.
 G2DrvN: will do   29 atoms at a time, making    1 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  90 IRICut=      82 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
          There are  90 degrees of freedom in the 1st order CPHF.
  87 vectors were produced by pass  0.
 AX will form  87 AO Fock derivatives at one time.
  87 vectors were produced by pass  1.
  87 vectors were produced by pass  2.
  87 vectors were produced by pass  3.
  87 vectors were produced by pass  4.
  87 vectors were produced by pass  5.
  87 vectors were produced by pass  6.
  44 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
 Inv2:  IOpt= 1 Iter= 1 AM= 5.10D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 656 with in-core refinement.

 ********************************************************************

            Population analysis using the SCF density.

 ********************************************************************

 Alpha  occ. eigenvalues --  -20.52610 -20.51637 -20.49667 -15.48429 -
11.32992
 Alpha  occ. eigenvalues --  -11.28677 -11.27840 -11.20279 -11.20147 -
11.20109
 Alpha  occ. eigenvalues --  -11.19944 -11.19405 -11.19123 -11.19055 -
11.18660
 Alpha  occ. eigenvalues --  -11.17884  -1.45444  -1.39554  -1.38273  -
1.25012
 Alpha  occ. eigenvalues --   -1.22109  -1.10723  -1.08251  -1.06553  -
0.96149
```

```
 Alpha  occ. eigenvalues --   -0.93422  -0.90006  -0.87398  -0.81389  -
0.79666
 Alpha  occ. eigenvalues --   -0.77663  -0.74684  -0.73207  -0.72884  -
0.69731
 Alpha  occ. eigenvalues --   -0.67277  -0.64882  -0.63719  -0.63084  -
0.61224
 Alpha  occ. eigenvalues --   -0.59118  -0.57178  -0.56246  -0.55541  -
0.53800
 Alpha  occ. eigenvalues --   -0.52073  -0.51799  -0.50142  -0.48727  -
0.48691
 Alpha  occ. eigenvalues --   -0.48075  -0.46682  -0.46529  -0.45885  -
0.44477
 Alpha  occ. eigenvalues --   -0.42820  -0.39593  -0.38338
 Alpha virt. eigenvalues --    0.06036   0.06442   0.07390   0.07606
0.08598
 Alpha virt. eigenvalues --    0.09110   0.09349   0.09732   0.10798
0.11811
 Alpha virt. eigenvalues --    0.12127   0.12906   0.13562   0.14046
0.14932
 Alpha virt. eigenvalues --    0.16012   0.16565   0.16920   0.17571
0.18368
 Alpha virt. eigenvalues --    0.18594   0.18981   0.19095   0.19828
0.19926
 Alpha virt. eigenvalues --    0.20326   0.21650   0.22148   0.23386
0.23702
 Alpha virt. eigenvalues --    0.23764   0.24017   0.24219   0.24905
0.25102
 Alpha virt. eigenvalues --    0.25356   0.25734   0.26923   0.27443
0.28185
 Alpha virt. eigenvalues --    0.28617   0.28726   0.28932   0.29465
0.29766
 Alpha virt. eigenvalues --    0.29876   0.30644   0.31648   0.32525
0.33247
 Alpha virt. eigenvalues --    0.33820   0.34354   0.35550   0.36031
0.37149
 Alpha virt. eigenvalues --    0.38027   0.38309   0.38906   0.39354
0.39701
 Alpha virt. eigenvalues --    0.40766   0.41608   0.42290   0.43177
0.43854
 Alpha virt. eigenvalues --    0.44718   0.45221   0.45639   0.46215
0.46763
 Alpha virt. eigenvalues --    0.47283   0.48051   0.48679   0.49306
0.49634
 Alpha virt. eigenvalues --    0.49959   0.51745   0.53381   0.53948
0.54106
 Alpha virt. eigenvalues --    0.54812   0.55904   0.56253   0.57456
0.57728
 Alpha virt. eigenvalues --    0.58598   0.59652   0.60337   0.61087
0.61760
 Alpha virt. eigenvalues --    0.62847   0.64455   0.65306   0.65552
0.66597
 Alpha virt. eigenvalues --    0.68516   0.72267   0.72486   0.87718
1.08197
```

```
 Alpha virt. eigenvalues --    1.10057   1.11494   1.13320   1.13583
1.14478
 Alpha virt. eigenvalues --    1.15260   1.16473   1.16749   1.17443
1.18174
 Alpha virt. eigenvalues --    1.18411   1.19600   1.20100   1.20652
1.22406
 Alpha virt. eigenvalues --    1.22861   1.24477   1.25770   1.27123
1.27815
 Alpha virt. eigenvalues --    1.31590   1.31918   1.32178   1.37717
1.39507
 Alpha virt. eigenvalues --    1.41242   1.42452   1.46811   1.49145
1.50456
 Alpha virt. eigenvalues --    1.51533   1.52417   1.53176   1.54027
1.56383
 Alpha virt. eigenvalues --    1.57509   1.59164   1.59543   1.62628
1.64214
 Alpha virt. eigenvalues --    1.65417   1.66398   1.71271   1.73295
1.75384
 Alpha virt. eigenvalues --    1.77502   1.81864   1.84287   1.86211
1.90866
 Alpha virt. eigenvalues --    2.01911   2.08703   2.14520   2.16263
2.18249
 Alpha virt. eigenvalues --    2.21203   2.24326   2.27161   2.30913
2.33050
 Alpha virt. eigenvalues --    2.35204   2.38315   2.43950   2.50974
2.53619
 Alpha virt. eigenvalues --    2.62540   2.79510   2.92683   3.10521
3.17068
 Alpha virt. eigenvalues --    3.28022   3.46898   3.68183   3.82432
3.83779
 Alpha virt. eigenvalues --    4.11494
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   14.119293  -6.128104   3.524841  -4.673323  -0.736671   4.171501
  2  C   -6.128104  18.432403 -10.694051   1.708322   4.102730 -10.486984
  3  C    3.524841 -10.694051  34.910231  10.458904 -30.509583   8.812082
  4  C   -4.673323   1.708322  10.458904  24.386589 -23.164599  -1.966533
  5  C   -0.736671   4.102730 -30.509583 -23.164599  59.805895  -2.813885
  6  C    4.171501 -10.486984   8.812082  -1.966533  -2.813885  20.571920
  7  C   -1.458317   4.467764  -3.858860   0.838253   2.584789  -7.266083
  8  C    1.709704  -1.913225  -2.837314  -7.133594   5.981168   1.957124
  9  C    1.244264  -2.546901   6.996563   3.194410  -9.249103   6.640187
 10  C   -3.119438   9.330138 -15.059289  -2.134819   9.982054 -12.786507
 11  C   -3.057022   0.500848   0.636085   1.322219  -1.431983  -0.232066
 12  C    0.194615  -1.207888   2.108644   0.809493  -3.435102  -0.978113
 13  N   -0.002257   0.054459  -0.433056  -0.283826   0.642041   0.110506
 14  O   -0.010490   0.011817   0.041402   0.044523  -0.030774  -0.113937
 15  O   -0.043443   0.101255   1.549738   1.370140  -3.927547  -0.002760
 16  O   -0.056835   0.043316   0.643829   0.644525  -1.506117   0.012507
 17  H    0.583076  -0.140943   0.049703  -0.187550  -0.001923   0.049418
 18  H   -0.098424   0.572747  -0.118834   0.036073  -0.031433  -0.110451
 19  H    0.051260  -0.141469   0.672503   0.036887  -0.204687   0.084173
 20  H   -0.031633  -0.002212   0.092402   0.639142  -0.273117   0.006429
 21  H   -0.008824  -0.102826   0.083359   0.014885  -0.017337   0.547482
```

22	H	-0.020814	0.031375	-0.003201	0.045972	0.006681	-0.088869
23	H	0.028815	-0.000621	0.010162	-0.116723	-0.013162	0.001750
24	H	-0.010137	0.066716	-0.061153	0.021061	-0.041786	-0.133824
25	H	-0.091614	0.018960	0.011774	0.047488	-0.031382	0.028605
26	H	-0.074328	0.006089	-0.005182	0.021978	0.003047	0.022096
27	H	-0.005166	0.012004	-0.210896	-0.175153	0.440099	-0.008327
28	H	0.002872	-0.005511	0.007464	-0.003932	-0.024062	0.014104
29	H	-0.010234	-0.014278	-0.078192	-0.005922	0.159334	0.010939
		7	8	9	10	11	12
1	C	-1.458317	1.709704	1.244264	-3.119438	-3.057022	0.194615
2	C	4.467764	-1.913225	-2.546901	9.330138	0.500848	-1.207888
3	C	-3.858860	-2.837314	6.996563	-15.059289	0.636085	2.108644
4	C	0.838253	-7.133594	3.194410	-2.134819	1.322219	0.809493
5	C	2.584789	5.981168	-9.249103	9.982054	-1.431983	-3.435102
6	C	-7.266083	1.957124	6.640187	-12.786507	-0.232066	-0.978113
7	C	16.592255	-5.661081	-0.424486	5.219721	-3.162443	-2.505616
8	C	-5.661081	22.495614	-19.623383	6.415760	0.617029	4.744658
9	C	-0.424486	-19.623383	66.555215	-23.877941	-0.486073	-27.077060
10	C	5.219721	6.415760	-23.877941	30.908870	0.411217	1.791065
11	C	-3.162443	0.617029	-0.486073	0.411217	12.425290	-0.733235
12	C	-2.505616	4.744658	-27.077060	1.791065	-0.733235	36.327624
13	N	0.086393	0.161212	0.985197	0.189798	0.003503	-2.275537
14	O	0.079090	0.257152	-1.162219	0.438847	0.010180	0.262587
15	O	0.073521	-0.618576	1.241290	-0.573606	0.023264	-1.099000
16	O	0.001699	-0.092327	0.163200	-0.136444	0.011874	-0.038037
17	H	-0.023330	0.053312	0.011255	-0.022035	-0.024324	0.003454
18	H	-0.008261	0.016431	-0.015686	0.087618	0.029737	0.001261
19	H	-0.016768	-0.000657	0.024706	-0.180280	0.001749	0.028205
20	H	0.005729	-0.158827	0.048840	-0.024839	0.030469	0.006996
21	H	-0.093702	0.040460	-0.051539	-0.086763	0.035839	0.000093
22	H	0.553391	-0.183780	0.015500	0.028330	-0.035909	0.000639
23	H	-0.043215	0.588381	-0.202074	0.079699	0.017724	-0.003295
24	H	0.037986	0.040085	-0.247904	0.630739	0.001930	0.050150
25	H	-0.142200	0.067386	-0.023348	0.004764	0.418313	0.007936
26	H	-0.117301	0.061181	-0.022048	0.005642	0.415917	0.001425
27	H	0.006650	0.075114	0.115586	0.091296	-0.000129	-0.161359
28	H	-0.009614	-0.090719	0.084401	-0.042616	-0.004865	0.108919
29	H	-0.005620	0.001484	-0.011346	-0.018129	-0.000636	0.010378
		13	14	15	16	17	18
1	C	-0.002257	-0.010490	-0.043443	-0.056835	0.583076	-0.098424
2	C	0.054459	0.011817	0.101255	0.043316	-0.140943	0.572747
3	C	-0.433056	0.041402	1.549738	0.643829	0.049703	-0.118834
4	C	-0.283826	0.044523	1.370140	0.644525	-0.187550	0.036073
5	C	0.642041	-0.030774	-3.927547	-1.506117	-0.001923	-0.031433
6	C	0.110506	-0.113937	-0.002760	0.012507	0.049418	-0.110451
7	C	0.086393	0.079090	0.073521	0.001699	-0.023330	-0.008261
8	C	0.161212	0.257152	-0.618576	-0.092327	0.053312	0.016431
9	C	0.985197	-1.162219	1.241290	0.163200	0.011255	-0.015686
10	C	0.189798	0.438847	-0.573606	-0.136444	-0.022035	0.087618
11	C	0.003503	0.010180	0.023264	0.011874	-0.024324	0.029737
12	C	-2.275537	0.262587	-1.099000	-0.038037	0.003454	0.001261
13	N	8.368744	0.020480	-0.233406	-0.000132	-0.000025	-0.000028
14	O	0.020480	8.677026	0.027696	0.001966	0.000008	0.000051
15	O	-0.233406	0.027696	10.284947	0.107126	-0.001033	-0.000152

16	O	-0.000132	0.001966	0.107126	8.546478	0.004248	0.002947
17	H	-0.000025	0.000008	-0.001033	0.004248	0.366124	-0.000134
18	H	-0.000028	0.000051	-0.000152	0.002947	-0.000134	0.371935
19	H	-0.000770	-0.000153	-0.001905	0.000328	-0.000031	0.000061
20	H	-0.001021	-0.000068	0.004865	0.008186	0.000161	-0.000014
21	H	-0.000091	0.003860	0.000257	0.000048	-0.000009	-0.000508
22	H	-0.000025	0.004817	-0.000012	0.000020	-0.000015	-0.000009
23	H	-0.000868	0.002014	0.003602	0.000150	-0.000019	0.000001
24	H	-0.002399	0.005542	0.003273	0.000159	0.000000	-0.000077
25	H	-0.000054	0.000014	0.000003	0.000104	-0.000242	-0.000027
26	H	-0.000007	0.000028	0.000058	-0.000058	-0.000479	0.000134
27	H	0.220629	-0.003074	-0.211132	-0.010783	0.000000	0.000000
28	H	-0.012207	0.189072	0.001705	0.000002	0.000000	0.000000
29	H	-0.001095	-0.000016	-0.004307	0.189534	-0.000016	0.000018

		19	20	21	22	23	24
1	C	0.051260	-0.031633	-0.008824	-0.020814	0.028815	-0.010137
2	C	-0.141469	-0.002212	-0.102826	0.031375	-0.000621	0.066716
3	C	0.672503	0.092402	0.083359	-0.003201	0.010162	-0.061153
4	C	0.036887	0.639142	0.014885	0.045972	-0.116723	0.021061
5	C	-0.204687	-0.273117	-0.017337	0.006681	-0.013162	-0.041786
6	C	0.084173	0.006429	0.547482	-0.088869	0.001750	-0.133824
7	C	-0.016768	0.005729	-0.093702	0.553391	-0.043215	0.037986
8	C	-0.000657	-0.158827	0.040460	-0.183780	0.588381	0.040085
9	C	0.024706	0.048840	-0.051539	0.015500	-0.202074	-0.247904
10	C	-0.180280	-0.024839	-0.086763	0.028330	0.079699	0.630739
11	C	0.001749	0.030469	0.035839	-0.035909	0.017724	0.001930
12	C	0.028205	0.006996	0.000093	0.000639	-0.003295	0.050150
13	N	-0.000770	-0.001021	-0.000091	-0.000025	-0.000868	-0.002399
14	O	-0.000153	-0.000068	0.003860	0.004817	0.002014	0.005542
15	O	-0.001905	0.004865	0.000257	-0.000012	0.003602	0.003273
16	O	0.000328	0.008186	0.000048	0.000020	0.000150	0.000159
17	H	-0.000031	0.000161	-0.000009	-0.000015	-0.000019	0.000000
18	H	0.000061	-0.000014	-0.000508	-0.000009	0.000001	-0.000077
19	H	0.369926	-0.000017	-0.000088	0.000000	0.000000	-0.000270
20	H	-0.000017	0.353234	0.000000	-0.000014	-0.000115	0.000000
21	H	-0.000088	0.000000	0.368713	-0.000305	-0.000012	-0.000062
22	H	0.000000	-0.000014	-0.000305	0.361298	0.000082	-0.000017
23	H	0.000000	-0.000115	-0.000012	0.000082	0.367467	-0.000014
24	H	-0.000270	0.000000	-0.000062	-0.000017	-0.000014	0.353796
25	H	0.000000	0.000062	-0.000029	-0.000281	0.000056	0.000000
26	H	0.000000	-0.000028	0.000079	-0.000431	-0.000034	0.000000
27	H	-0.000045	-0.000151	0.000000	0.000000	-0.000017	-0.000015
28	H	0.000000	0.000001	0.000000	0.000007	0.000543	0.000169
29	H	0.000587	-0.000040	0.000000	0.000000	0.000000	0.000002

		25	26	27	28	29
1	C	-0.091614	-0.074328	-0.005166	0.002872	-0.010234
2	C	0.018960	0.006089	0.012004	-0.005511	-0.014278
3	C	0.011774	-0.005182	-0.210896	0.007464	-0.078192
4	C	0.047488	0.021978	-0.175153	-0.003932	-0.005922
5	C	-0.031382	0.003047	0.440099	-0.024062	0.159334
6	C	0.028605	0.022096	-0.008327	0.014104	0.010939
7	C	-0.142200	-0.117301	0.006650	-0.009614	-0.005620
8	C	0.067386	0.061181	0.075114	-0.090719	0.001484
9	C	-0.023348	-0.022048	0.115586	0.084401	-0.011346

10	C	0.004764	0.005642	0.091296	-0.042616	-0.018129
11	C	0.418313	0.415917	-0.000129	-0.004865	-0.000636
12	C	0.007936	0.001425	-0.161359	0.108919	0.010378
13	N	-0.000054	-0.000007	0.220629	-0.012207	-0.001095
14	O	0.000014	0.000028	-0.003074	0.189072	-0.000016
15	O	0.000003	0.000058	-0.211132	0.001705	-0.004307
16	O	0.000104	-0.000058	-0.010783	0.000002	0.189534
17	H	-0.000242	-0.000479	0.000000	0.000000	-0.000016
18	H	-0.000027	0.000134	0.000000	0.000000	0.000018
19	H	0.000000	0.000000	-0.000045	0.000000	0.000587
20	H	0.000062	-0.000028	-0.000151	0.000001	-0.000040
21	H	-0.000029	0.000079	0.000000	0.000000	0.000000
22	H	-0.000281	-0.000431	0.000000	0.000007	0.000000
23	H	0.000056	-0.000034	-0.000017	0.000543	0.000000
24	H	0.000000	0.000000	-0.000015	0.000169	0.000002
25	H	0.434293	-0.016443	0.000000	0.000000	0.000000
26	H	-0.016443	0.432211	0.000000	0.000000	0.000000
27	H	0.000000	0.000000	0.371978	-0.000006	0.000000
28	H	0.000000	0.000000	-0.000006	0.311305	0.000000
29	H	0.000000	0.000000	0.000000	0.000000	0.320849

Total atomic charges:

		1
1	C	0.006835
2	C	-0.075928
3	C	-0.740073
4	C	0.205111
5	C	-0.263583
6	C	-0.052483
7	C	0.249659
8	C	-0.969773
9	C	3.700499
10	C	-1.552850
11	C	-1.744502
12	C	-0.943900
13	N	-0.596158
14	O	-0.757440
15	O	-0.075859
16	O	-0.541514
17	H	0.281349
18	H	0.265024
19	H	0.276753
20	H	0.295580
21	H	0.267020
22	H	0.285571
23	H	0.279723
24	H	0.286048
25	H	0.265863
26	H	0.266452
27	H	0.452898
28	H	0.472970
29	H	0.456707

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

		1

```
  1  C    0.288184
  2  C    0.189096
  3  C   -0.463320
  4  C    0.500691
  5  C   -0.263583
  6  C    0.214537
  7  C    0.535230
  8  C   -0.690050
  9  C    3.700499
 10  C   -1.266802
 11  C   -1.212186
 12  C   -0.943900
 13  N   -0.596158
 14  O   -0.284470
 15  O    0.377039
 16  O   -0.084807
 17  H    0.000000
 18  H    0.000000
 19  H    0.000000
 20  H    0.000000
 21  H    0.000000
 22  H    0.000000
 23  H    0.000000
 24  H    0.000000
 25  H    0.000000
 26  H    0.000000
 27  H    0.000000
 28  H    0.000000
 29  H    0.000000
 Sum of Mulliken charges=   0.00000
 Electronic spatial extent (au):  <R**2>=  2427.5537
 Charge=     0.0000 electrons
 Dipole moment (Debye):
    X=    -4.0421    Y=     1.1826    Z=     1.2856  Tot=     4.4034
 Quadrupole moment (Debye-Ang):
   XX=  -110.1487   YY=   -97.0435   ZZ=   -91.2499
   XY=     4.0956   XZ=     1.3911   YZ=     7.0378
 Octapole moment (Debye-Ang**2):
  XXX=   -74.3433  YYY=    27.7818  ZZZ=     2.4433  XYY=    20.5129
  XXY=     1.4561  XXZ=    10.3207  XZZ=    -2.1592  YZZ=     4.9184
  YYZ=    11.3146  XYZ=     3.4620
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -1921.6522 YYYY= -1086.5988 ZZZZ=  -500.4202 XXXY=     2.4947
 XXXZ=    38.8968 YYYX=    27.5253 YYYZ=    86.2314 ZZZX=     6.8909
 ZZZY=     0.6873 XXYY=  -404.9149 XXZZ=  -364.1422 YYZZ=  -264.0273
 XXYZ=    -3.6892 YYXZ=   -12.6905 ZZXY=     0.6623
 N-N= 1.241924330359D+03 E-N=-4.207547880302D+03  KE= 7.352406298316D+02
  Exact polarizability: 142.504  -2.309 123.468  -2.628   1.842 104.762
 Approx polarizability: 123.982  -3.327 115.457  -3.778   0.843 102.563
 Full mass-weighted force constant matrix:
 Low frequencies ----2070.7427   -0.2492   -0.1169    0.0004    0.0007
0.0010
 Low frequencies ---    0.4226   76.1530  144.9916
 ******    1 imaginary frequencies (negative Signs) ******
```

Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
Raman scattering activities (A**4/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1		2		3	
	?A		?A		?A	
Frequencies --	-2070.7427		76.1530		144.9916	
Red. masses --	1.0873		4.6251		1.5854	
Frc consts --	2.7468		0.0158		0.0196	
IR Inten --	901.2753		30.2922		120.3507	
Raman Activ --	5.2479		4.2138		0.3716	
Depolar --	0.6040		0.7201		0.7244	

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	-0.04	0.00	0.05	-0.01	0.00	0.02
2	6	0.00	0.00	0.00	0.03	0.00	0.04	0.02	-0.01	0.01
3	6	0.00	0.00	0.00	0.04	0.01	-0.02	0.02	-0.01	-0.01
4	6	0.00	0.00	0.00	-0.06	0.00	-0.01	-0.02	0.02	-0.01
5	6	0.01	-0.01	0.00	-0.02	0.00	-0.05	0.00	0.01	-0.02
6	6	0.00	0.00	0.00	0.03	0.00	0.02	0.03	-0.01	-0.01
7	6	0.00	0.00	0.00	-0.02	0.00	0.02	0.01	0.01	-0.02
8	6	0.00	0.00	0.00	-0.04	0.01	-0.03	0.00	0.02	-0.03
9	6	0.00	-0.01	0.00	-0.01	0.01	-0.07	0.01	0.00	-0.03
10	6	0.00	0.00	0.00	0.03	0.00	-0.03	0.02	-0.01	-0.02
11	6	0.00	0.00	0.00	-0.05	-0.01	0.07	-0.01	0.00	0.01
12	6	-0.05	0.04	0.01	-0.01	0.02	0.02	0.04	-0.04	0.01
13	7	0.00	0.04	0.00	0.10	-0.01	0.38	0.05	0.03	0.10
14	8	0.00	0.00	0.00	-0.01	-0.01	-0.20	-0.04	-0.01	0.09
15	8	-0.02	-0.02	0.00	-0.02	-0.04	-0.19	-0.02	0.00	-0.08
16	8	0.00	0.00	0.00	0.01	0.01	-0.04	-0.03	0.01	0.01
17	1	0.00	0.00	0.00	-0.05	-0.01	0.07	-0.02	0.00	0.04
18	1	0.00	0.00	0.00	0.06	0.00	0.08	0.03	-0.02	0.03
19	1	0.00	0.00	0.00	0.07	0.01	-0.03	0.04	-0.01	-0.01
20	1	0.00	0.00	0.00	-0.10	0.00	-0.01	-0.04	0.03	0.00

21	1	0.00	0.00	0.00	0.05	0.00	0.04	0.04	-0.02	-0.01
22	1	0.00	0.00	0.00	-0.02	0.00	0.02	0.00	0.01	-0.03
23	1	0.00	0.00	0.00	-0.08	0.01	-0.03	-0.02	0.04	-0.04
24	1	0.00	0.00	0.00	0.07	0.00	-0.05	0.04	-0.02	-0.04
25	1	0.00	0.00	0.00	-0.10	-0.01	0.08	-0.03	0.02	0.02
26	1	0.00	0.00	0.00	-0.03	-0.01	0.11	0.00	-0.01	0.03
27	1	0.81	-0.57	-0.12	0.09	0.05	0.25	0.02	-0.01	0.04
28	1	-0.01	-0.01	0.00	0.40	0.18	0.62	-0.49	-0.23	-0.80
29	1	0.01	0.00	-0.01	-0.02	0.00	-0.01	0.02	0.01	-0.02

		4			5			6		
		?A			?A			?A		
Frequencies --		243.7453			256.2110			261.3332		
Red. masses --		4.2126			5.8481			4.2480		
Frc consts --		0.1475			0.2262			0.1709		
IR Inten --		31.8924			5.3018			49.2059		
Raman Activ --		0.4714			0.3120			0.9588		
Depolar --		0.7499			0.6918			0.5745		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.07	0.09	-0.01	0.02	-0.01	0.05	-0.08	-0.03	0.02
2	6	0.04	0.08	0.00	0.01	-0.01	0.04	-0.07	-0.04	0.01
3	6	0.07	-0.05	0.00	-0.03	0.03	0.01	-0.07	-0.01	0.00
4	6	0.07	-0.06	-0.02	0.03	-0.04	0.01	-0.07	0.00	0.01
5	6	0.03	-0.06	-0.01	0.01	0.00	0.01	-0.02	0.00	0.00
6	6	-0.08	0.04	0.00	0.03	0.00	0.03	-0.05	-0.04	0.00
7	6	-0.12	0.03	0.02	0.00	-0.01	0.04	-0.04	-0.03	0.00
8	6	-0.04	-0.09	0.01	-0.02	0.00	-0.02	-0.05	-0.01	0.00
9	6	0.00	-0.05	-0.01	0.00	-0.01	-0.06	-0.01	0.02	0.00
10	6	-0.03	-0.08	-0.01	0.03	0.00	-0.02	-0.05	-0.03	-0.01
11	6	-0.06	0.15	0.01	-0.02	0.00	0.08	-0.06	-0.04	0.01
12	6	-0.04	0.05	0.02	0.03	-0.02	0.05	-0.07	0.10	0.02
13	7	-0.02	-0.04	0.05	0.01	0.09	0.05	-0.04	-0.02	0.03

14	8	0.28	0.02	0.00	-0.10	-0.05	-0.22	0.23	0.10	0.01
15	8	0.04	0.04	0.01	0.03	0.04	0.35	-0.02	-0.06	0.02
16	8	-0.17	-0.11	-0.03	-0.01	-0.03	-0.32	0.31	0.06	-0.05
17	1	0.16	0.16	-0.02	0.04	0.00	0.04	-0.10	-0.04	0.03
18	1	0.06	0.15	-0.01	-0.01	-0.03	0.03	-0.06	-0.05	0.02
19	1	0.13	-0.06	-0.01	0.00	0.02	0.02	-0.08	-0.03	0.01
20	1	0.11	-0.07	-0.02	0.00	-0.02	0.02	-0.09	0.00	0.00
21	1	-0.14	0.10	0.02	0.07	-0.01	0.05	-0.04	-0.04	-0.01
22	1	-0.24	0.03	0.03	-0.01	-0.01	0.04	-0.03	-0.03	-0.01
23	1	-0.08	-0.13	0.01	-0.05	-0.02	-0.02	-0.06	0.02	-0.01
24	1	-0.06	-0.12	-0.01	0.07	0.02	-0.03	-0.05	-0.02	0.00
25	1	-0.08	0.15	0.01	-0.08	-0.02	0.09	-0.08	-0.04	0.01
26	1	-0.08	0.24	0.02	0.00	0.02	0.14	-0.05	-0.05	0.02
27	1	0.02	0.03	0.03	0.02	0.01	0.24	-0.07	0.09	0.03
28	1	0.13	0.16	-0.42	-0.23	-0.11	-0.48	0.02	0.20	-0.54
29	1	-0.43	-0.04	0.07	-0.01	0.16	-0.48	0.58	-0.02	-0.14

	7			8			9		
	?A			?A			?A		
Frequencies --	322.2721			346.1992			351.9153		
Red. masses --	3.3338			1.8286			2.2291		
Frc consts --	0.2040			0.1291			0.1626		
IR Inten --	5.1209			90.5642			129.9249		
Raman Activ --	1.2732			1.0797			2.3699		
Depolar --	0.6630			0.7392			0.7464		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.04	0.10	0.00	-0.02	-0.04	0.01	0.00	-0.07
2 6	0.01	-0.07	0.07	0.00	0.02	-0.04	0.01	0.05	-0.05
3 6	0.00	-0.03	0.04	-0.01	0.01	-0.05	0.01	-0.01	-0.05
4 6	-0.02	0.00	0.04	0.01	-0.02	-0.05	0.02	-0.04	-0.05
5 6	-0.01	-0.02	0.03	0.01	0.00	-0.01	0.00	-0.02	-0.02
6 6	0.04	-0.07	-0.09	0.02	0.02	0.00	-0.03	0.04	0.01

7	6	-0.05	0.02	-0.12	-0.02	-0.02	0.02	-0.06	-0.02	0.04
8	6	-0.01	-0.02	-0.08	-0.03	-0.04	-0.05	-0.03	-0.07	-0.01
9	6	0.02	-0.02	-0.06	-0.01	0.01	-0.07	0.01	-0.05	-0.03
10	6	0.02	-0.01	-0.08	0.02	0.04	-0.06	0.00	0.00	-0.03
11	6	-0.07	0.13	0.00	-0.05	-0.05	0.07	-0.05	-0.01	0.04
12	6	0.02	0.00	-0.07	-0.01	0.03	-0.06	0.05	-0.03	-0.03
13	7	0.03	0.10	0.00	0.02	0.03	0.02	0.03	0.15	0.01
14	8	0.01	-0.01	0.23	-0.02	0.02	0.05	0.01	-0.06	0.00
15	8	-0.02	-0.02	0.03	0.02	-0.03	0.09	-0.03	0.04	0.05
16	8	0.02	-0.03	-0.12	0.08	0.01	0.05	-0.01	0.00	0.14
17	1	0.05	0.10	0.18	-0.01	-0.03	-0.07	0.03	0.01	-0.10
18	1	0.01	-0.16	0.11	0.00	0.03	-0.05	0.01	0.11	-0.07
19	1	0.03	-0.07	0.05	0.00	0.00	-0.04	0.02	0.01	-0.07
20	1	-0.07	0.05	0.06	0.01	-0.02	-0.05	0.06	-0.07	-0.06
21	1	0.10	-0.14	-0.11	0.05	0.04	0.04	-0.04	0.09	0.05
22	1	-0.14	0.03	-0.19	-0.02	-0.03	0.05	-0.09	-0.03	0.09
23	1	-0.02	0.06	-0.11	-0.08	-0.06	-0.06	-0.08	-0.12	-0.01
24	1	0.03	-0.07	-0.10	0.06	0.05	-0.08	0.00	0.00	-0.02
25	1	-0.13	0.24	0.00	-0.18	-0.13	0.08	-0.13	-0.09	0.05
26	1	-0.05	0.10	0.03	-0.01	0.00	0.20	-0.03	0.06	0.13
27	1	-0.01	0.06	0.11	0.03	0.05	0.16	-0.03	0.04	0.05
28	1	0.17	-0.06	0.63	-0.04	-0.03	0.03	0.06	-0.08	0.14
29	1	0.06	0.06	-0.21	-0.60	-0.16	0.61	0.78	0.00	-0.35

	10	11	12
	?A	?A	?A
Frequencies --	382.8570	432.5645	447.0548
Red. masses --	4.1386	2.8339	6.0931
Frc consts --	0.3574	0.3124	0.7175
IR Inten --	44.0241	4.7592	30.7172
Raman Activ --	0.8410	1.6910	4.4856
Depolar --	0.7310	0.6783	0.5263

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	0.03	0.00	0.01	0.02	-0.02	0.08	-0.02	-0.01
2	6	-0.03	0.03	0.03	0.03	-0.01	-0.04	0.04	-0.03	0.01
3	6	-0.01	-0.01	0.05	0.02	-0.06	-0.03	0.06	-0.08	0.07
4	6	0.02	-0.04	0.06	0.01	0.00	-0.06	0.06	-0.11	-0.01
5	6	-0.01	-0.04	0.02	0.02	-0.05	-0.06	0.04	-0.15	0.04
6	6	-0.08	0.02	0.05	-0.03	-0.04	-0.06	-0.01	-0.04	0.04
7	6	-0.05	0.01	0.06	0.03	0.03	-0.08	-0.05	-0.06	0.04
8	6	0.00	-0.05	0.09	0.07	0.06	0.00	-0.06	-0.06	0.00
9	6	0.04	-0.07	0.05	0.02	0.03	0.12	-0.09	0.18	-0.05
10	6	-0.02	-0.05	0.07	-0.06	-0.08	0.07	0.00	-0.01	0.01
11	6	0.06	0.07	-0.10	-0.10	0.02	0.14	0.05	0.01	-0.07
12	6	0.06	0.04	-0.03	0.04	0.07	0.18	-0.10	0.28	-0.08
13	7	0.04	0.30	-0.04	-0.01	0.07	-0.05	0.00	0.00	0.03
14	8	-0.04	-0.11	-0.07	-0.06	0.01	-0.03	-0.22	0.23	0.02
15	8	-0.10	-0.08	-0.11	0.01	0.02	-0.05	0.11	0.05	-0.05
16	8	0.13	-0.03	-0.07	0.04	-0.06	-0.02	0.04	-0.22	0.03
17	1	0.07	0.05	-0.02	0.03	0.04	0.00	0.13	0.01	-0.01
18	1	-0.03	0.06	0.01	0.04	0.00	-0.03	0.03	0.01	-0.03
19	1	0.00	-0.03	0.06	0.02	-0.02	-0.06	0.04	-0.02	0.04
20	1	0.07	-0.07	0.05	0.00	0.00	-0.06	0.12	-0.04	0.03
21	1	-0.11	0.05	0.06	-0.12	-0.06	-0.14	0.00	0.00	0.08
22	1	-0.09	0.01	0.08	0.04	0.04	-0.14	-0.08	-0.06	0.04
23	1	-0.03	-0.06	0.09	0.20	0.05	0.05	-0.05	-0.13	0.03
24	1	-0.08	-0.04	0.10	-0.14	-0.09	0.11	0.11	-0.11	-0.08
25	1	0.31	0.12	-0.13	-0.50	-0.06	0.19	0.23	0.03	-0.08
26	1	-0.05	0.07	-0.34	0.07	0.04	0.52	-0.05	0.07	-0.24

27	1	-0.15	0.18	-0.04	-0.09	0.05	-0.29	0.03	0.29	0.09
28	1	-0.05	-0.14	-0.08	-0.03	0.01	0.04	-0.28	0.10	-0.03
29	1	-0.43	-0.11	0.35	-0.05	-0.10	0.07	0.35	-0.15	-0.22

	13			14			15		
	?A			?A			?A		
Frequencies --	475.7643			505.5318			535.4939		
Red. masses --	6.8893			3.2567			7.0671		
Frc consts --	0.9188			0.4904			1.1940		
IR Inten --	5.9317			11.6454			14.0390		
Raman Activ --	5.2351			1.8214			13.3676		
Depolar --	0.6896			0.7028			0.0708		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.10	0.04	-0.05	0.14	0.00	-0.10	-0.06	-0.06	0.00
2	6	-0.17	0.09	-0.03	-0.01	-0.01	-0.07	-0.10	-0.09	-0.02
3	6	-0.15	0.07	0.12	-0.05	0.02	0.14	-0.06	-0.04	0.04
4	6	-0.03	0.01	0.08	0.15	-0.01	0.09	0.00	-0.01	0.08
5	6	-0.02	-0.15	0.13	0.00	0.07	0.15	0.11	0.13	0.04
6	6	-0.04	0.12	-0.04	0.01	-0.02	-0.04	-0.16	-0.11	0.02
7	6	0.05	0.08	-0.02	0.03	-0.03	-0.02	-0.17	-0.11	0.03
8	6	0.02	0.10	-0.01	0.04	-0.04	0.01	-0.08	-0.05	0.08
9	6	0.08	0.09	-0.02	-0.03	-0.03	-0.03	0.02	0.03	0.01
10	6	-0.05	0.13	0.05	-0.01	-0.01	0.01	-0.10	-0.08	0.02
11	6	-0.06	-0.03	0.04	0.01	-0.02	0.10	-0.14	-0.06	-0.04
12	6	0.21	-0.09	-0.13	-0.11	0.01	-0.14	0.23	-0.01	-0.05
13	7	0.24	-0.02	-0.06	-0.07	-0.01	0.03	0.24	-0.04	-0.05
14	8	0.06	0.11	-0.04	-0.01	-0.03	-0.01	-0.02	0.00	-0.01
15	8	0.02	-0.23	-0.01	-0.05	0.00	-0.10	0.25	0.25	-0.07
16	8	-0.07	-0.23	0.01	0.00	0.08	-0.05	0.00	0.16	-0.04
17	1	-0.10	0.01	-0.16	0.17	0.01	-0.15	-0.05	-0.05	0.02
18	1	-0.23	0.01	-0.06	-0.13	-0.05	-0.19	-0.11	-0.07	-0.04
19	1	-0.23	0.12	0.10	-0.18	-0.07	0.24	-0.19	-0.16	0.14

20	1	0.09	0.15	0.15	0.34	0.05	0.13	-0.01	-0.08	0.05
21	1	-0.04	0.09	-0.08	-0.02	0.00	-0.04	-0.15	-0.07	0.06
22	1	0.11	0.07	0.04	0.03	-0.03	-0.03	-0.17	-0.10	-0.01
23	1	0.01	0.14	-0.03	0.04	0.01	-0.01	-0.13	-0.04	0.06
24	1	-0.11	0.06	0.06	0.00	-0.09	-0.02	-0.15	-0.10	0.04
25	1	-0.23	-0.11	0.06	-0.31	-0.17	0.14	-0.11	-0.08	-0.04
26	1	0.04	-0.09	0.22	0.11	0.12	0.42	-0.17	0.02	-0.06
27	1	0.11	-0.05	0.14	-0.01	0.07	0.18	0.34	-0.03	-0.10
28	1	0.03	0.11	-0.09	-0.04	-0.03	-0.09	0.00	-0.06	0.08
29	1	0.06	-0.07	-0.21	-0.02	0.21	-0.14	-0.22	0.22	0.04

	16			17			18		
	?A			?A			?A		
Frequencies --	585.5964			630.6886			683.9290		
Red. masses --	3.4135			5.2343			4.0389		
Frc consts --	0.6897			1.2267			1.1131		
IR Inten --	3.0038			1.9240			4.9145		
Raman Activ --	0.4069			2.4864			0.5117		
Depolar --	0.4091			0.7375			0.7500		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.09	-0.02	0.00	0.00	0.07	-0.17	0.01	-0.02	-0.10
2	6	0.02	0.16	0.03	0.09	-0.10	-0.12	0.04	-0.02	-0.05
3	6	0.14	-0.06	0.06	0.02	-0.18	-0.06	0.04	0.04	0.11
4	6	-0.04	0.07	0.06	-0.01	0.24	-0.11	0.01	0.01	0.06
5	6	0.05	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.13
6	6	-0.10	0.12	-0.05	-0.01	-0.13	0.13	0.11	0.04	0.00
7	6	0.07	0.03	0.00	-0.03	0.07	0.16	-0.12	-0.06	0.04
8	6	-0.02	0.06	-0.07	-0.13	0.21	0.09	-0.07	-0.02	-0.09
9	6	-0.03	-0.04	-0.07	-0.02	0.02	0.00	0.00	0.02	-0.07
10	6	-0.07	-0.13	-0.07	0.09	-0.15	0.09	0.09	0.04	-0.10
11	6	0.05	-0.19	0.00	0.01	0.00	0.00	-0.10	-0.02	-0.07
12	6	-0.03	0.05	0.02	0.01	-0.06	-0.07	0.09	-0.05	0.33

13	7	-0.03	0.03	0.00	0.02	0.03	0.00	-0.03	0.00	-0.05
14	8	0.00	-0.05	0.06	0.02	0.06	0.06	0.00	0.06	-0.01
15	8	0.04	0.05	0.00	-0.03	-0.08	0.04	-0.06	-0.03	-0.05
16	8	0.01	-0.04	-0.05	-0.03	-0.01	-0.06	0.01	0.00	-0.01
17	1	-0.21	-0.14	-0.13	-0.15	0.01	0.01	0.03	0.00	-0.08
18	1	0.12	0.24	0.11	0.10	0.01	-0.16	-0.03	-0.10	-0.10
19	1	0.27	-0.17	0.11	-0.12	-0.19	-0.02	-0.03	-0.06	0.19
20	1	-0.02	0.16	0.11	0.18	0.26	-0.08	0.18	0.13	0.13
21	1	-0.21	0.14	-0.10	-0.10	-0.05	0.15	0.22	0.13	0.16
22	1	0.22	0.00	0.14	0.13	0.10	-0.02	-0.14	-0.07	0.09
23	1	-0.09	0.13	-0.12	-0.27	0.11	0.08	-0.19	0.00	-0.13
24	1	-0.10	-0.29	-0.11	0.22	-0.10	0.04	0.20	-0.05	-0.19
25	1	0.06	-0.17	-0.01	0.09	-0.27	0.01	0.01	-0.11	-0.07
26	1	0.08	-0.31	-0.01	-0.04	0.17	0.00	-0.17	0.11	-0.14
27	1	-0.01	0.07	-0.01	0.00	-0.03	0.13	-0.15	-0.13	-0.44
28	1	0.03	-0.07	0.13	0.06	0.06	0.16	0.03	0.04	0.06
29	1	-0.06	0.08	-0.10	-0.06	0.11	-0.13	-0.08	0.08	-0.02

	19			20			21		
	?A			?A			?A		
Frequencies --	689.2612			708.1138			729.5863		
Red. masses --	5.5705			6.1244			7.2095		
Frc consts --	1.5592			1.8093			2.2610		
IR Inten --	29.2088			151.7544			90.9090		
Raman Activ --	8.9693			8.5327			4.8057		
Depolar --	0.2712			0.1973			0.1079		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.17	0.01	0.09	-0.07	0.07	-0.05	-0.03	0.03	-0.02
2 6	-0.15	0.01	0.10	-0.15	-0.05	-0.02	-0.08	-0.06	-0.03
3 6	-0.14	-0.08	-0.06	-0.14	-0.02	-0.05	-0.09	0.04	0.02
4 6	0.08	0.02	-0.05	0.00	0.07	0.00	0.01	0.05	0.03
5 6	0.00	-0.01	-0.05	-0.10	-0.01	0.03	0.11	-0.10	0.01

```
   6   6    -0.14  -0.07   0.10     0.07   0.00   0.06     0.08  -0.01
0.04
   7   6     0.07   0.01   0.13     0.03   0.11   0.11     0.04   0.06
0.00
   8   6     0.03  -0.01  -0.13     0.02   0.02   0.00    -0.07   0.08  -
0.05
   9   6    -0.05   0.03  -0.14     0.15  -0.08  -0.06    -0.10  -0.03  -
0.03
  10   6    -0.18  -0.04  -0.18     0.05   0.02  -0.12     0.03   0.11
0.08
  11   6     0.23   0.05   0.15     0.03   0.07   0.04     0.01   0.01
0.00
  12   6     0.09  -0.10   0.12    -0.05   0.37   0.09    -0.03  -0.24  -
0.05
  13   7     0.02   0.01  -0.03     0.03  -0.12  -0.03    -0.11   0.04
0.07
  14   8     0.00   0.10   0.01     0.00  -0.27   0.03     0.07  -0.10
0.00
  15   8    -0.05   0.00  -0.04     0.11   0.01  -0.04    -0.02   0.39  -
0.06
  16   8     0.00   0.03   0.00    -0.01  -0.07   0.01     0.15  -0.28  -
0.01
  17   1     0.16  -0.02   0.03    -0.09   0.06  -0.04    -0.05   0.02
0.01
  18   1    -0.20   0.17  -0.04    -0.18  -0.08  -0.04    -0.14  -0.15  -
0.05
  19   1     0.01  -0.21  -0.01    -0.20  -0.07   0.00    -0.22   0.14  -
0.01
  20   1    -0.06   0.09  -0.03     0.09   0.12   0.02     0.07   0.15
0.08
  21   1    -0.02  -0.19   0.07     0.22  -0.07   0.08     0.13  -0.07
0.01
  22   1     0.04   0.02   0.12     0.01   0.12   0.09     0.11   0.07  -
0.05
  23   1    -0.17  -0.12  -0.16    -0.19   0.01  -0.07    -0.13   0.09  -
0.07
  24   1    -0.06   0.00  -0.24     0.09   0.17  -0.08     0.12   0.15
0.04
  25   1     0.24   0.02   0.16     0.07  -0.08   0.04     0.03  -0.06
0.01
  26   1     0.21   0.12   0.15     0.02   0.09   0.04     0.02  -0.01
0.01
  27   1    -0.04  -0.13  -0.21     0.03   0.29  -0.06    -0.01  -0.19  -
0.22
  28   1     0.03   0.07   0.09    -0.04  -0.39  -0.02     0.11   0.02
0.00
  29   1     0.02  -0.05   0.05     0.10  -0.01  -0.11    -0.06  -0.37
0.19
                      22                    23                    24
                      ?A                    ?A                    ?A
 Frequencies --    806.3788              814.3334              829.5854
 Red. masses --      4.9336                3.9488                5.0563
 Frc consts  --      1.8901                1.5428                2.0502
 IR Inten    --     86.6399               52.6583                1.6788
```

Raman Activ --		3.8733			7.0941			15.4281		
Depolar --		0.3229			0.0615			0.0198		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.07	0.07	-0.08	-0.06	0.00	-0.07	0.05	-0.13	-0.07
2	6	-0.02	0.03	0.04	-0.09	0.04	0.05	-0.08	0.01	0.26
3	6	-0.02	-0.10	0.20	0.05	-0.13	-0.14	0.03	0.03	0.09
4	6	-0.09	-0.10	-0.16	0.07	-0.11	0.17	0.15	0.00	-0.16
5	6	-0.18	-0.04	-0.01	-0.05	0.00	0.01	-0.01	0.00	-0.02
6	6	0.05	0.10	-0.04	0.00	-0.02	0.01	-0.06	-0.05	0.24
7	6	0.06	0.10	0.06	0.00	0.08	0.01	-0.04	0.13	-0.07
8	6	0.06	-0.11	-0.06	0.09	0.07	0.22	0.10	0.08	-0.16
9	6	0.08	0.05	-0.02	0.07	0.01	0.01	-0.02	-0.01	-0.01
10	6	0.10	-0.16	0.10	0.06	0.01	-0.20	0.02	0.01	0.09
11	6	0.02	0.07	0.02	-0.08	0.00	-0.06	-0.20	-0.07	-0.15
12	6	0.06	-0.02	-0.05	0.00	-0.05	-0.03	-0.01	0.01	-0.01
13	7	0.07	-0.12	0.00	-0.02	-0.04	0.02	-0.01	0.01	0.00
14	8	-0.03	0.05	0.00	-0.03	0.08	-0.01	0.01	-0.03	0.01
15	8	-0.13	0.14	0.03	-0.09	0.06	0.01	0.02	-0.02	-0.02
16	8	0.05	0.08	-0.03	0.03	-0.01	-0.01	-0.01	0.03	0.00
17	1	-0.02	0.08	-0.16	0.10	0.08	-0.21	0.17	-0.03	-0.03
18	1	-0.09	-0.14	0.03	0.03	0.18	0.13	-0.10	0.28	0.11
19	1	-0.01	-0.05	0.17	0.28	-0.34	-0.05	0.24	0.08	0.01
20	1	-0.07	-0.10	-0.16	0.20	-0.31	0.10	0.14	0.18	-0.09
21	1	-0.09	0.09	-0.14	0.20	-0.13	0.03	0.10	-0.31	0.11
22	1	-0.09	0.08	0.22	0.08	0.08	-0.01	0.14	0.12	-0.05
23	1	0.08	-0.30	0.01	0.09	0.17	0.19	0.17	-0.07	-0.09
24	1	0.09	-0.46	0.00	0.06	0.16	-0.15	0.19	0.09	0.03
25	1	0.09	0.00	0.01	-0.20	-0.09	-0.04	-0.26	-0.10	-0.14

26	1	0.02	-0.02	-0.03	-0.01	-0.02	0.08	-0.16	-0.05	-0.06
27	1	0.05	-0.16	-0.06	-0.01	-0.11	-0.01	0.01	0.04	0.07
28	1	-0.04	-0.13	0.07	-0.04	-0.05	0.05	0.02	0.01	-0.01
29	1	0.03	-0.16	0.18	0.03	-0.08	0.05	0.02	0.01	0.00

	25	26	27
	?A	?A	?A
Frequencies --	881.5565	885.3654	903.3331
Red. masses --	3.3982	3.1640	2.7354
Frc consts --	1.5560	1.4613	1.3151
IR Inten --	0.2616	1.1757	2.6370
Raman Activ --	0.5148	13.3344	0.3580
Depolar --	0.6613	0.0449	0.6278

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.16	-0.12	0.06	-0.07	0.10	-0.11	0.12	-0.01	-0.06
2	6	0.13	0.06	-0.08	-0.05	0.18	0.06	0.00	-0.05	0.09
3	6	-0.04	0.00	-0.03	0.05	-0.01	0.03	0.10	0.11	0.08
4	6	-0.07	0.00	0.07	-0.08	0.06	-0.01	0.00	0.05	-0.04
5	6	-0.13	-0.01	0.02	-0.03	-0.01	0.03	-0.09	-0.01	-0.06
6	6	-0.13	0.02	0.08	0.02	-0.18	0.07	0.03	-0.02	-0.10
7	6	-0.03	-0.10	-0.06	-0.02	-0.18	-0.11	-0.06	-0.04	0.03
8	6	0.03	0.11	-0.02	-0.02	-0.07	-0.01	-0.09	0.09	0.08
9	6	0.06	0.02	-0.05	0.00	0.01	0.03	0.02	0.02	0.04
10	6	0.05	0.00	0.02	0.03	0.05	0.03	-0.12	0.02	-0.06
11	6	-0.02	0.01	-0.02	0.12	0.04	0.03	0.03	-0.04	-0.01
12	6	0.04	0.07	-0.02	0.01	0.01	0.00	0.03	0.03	-0.04
13	7	0.07	-0.10	-0.01	0.02	-0.02	0.00	0.06	-0.04	0.00
14	8	0.01	-0.05	0.01	0.00	-0.02	-0.01	0.01	-0.04	0.00
15	8	-0.12	0.07	0.03	-0.01	0.02	0.01	-0.06	0.02	0.03
16	8	0.03	-0.04	-0.01	0.01	-0.01	-0.01	0.01	-0.03	0.00
17	1	0.19	-0.09	0.13	-0.24	-0.08	-0.35	0.09	-0.03	-0.03
18	1	0.12	0.33	-0.23	0.03	0.38	0.07	-0.19	-0.25	-0.04

```
  19   1    -0.18   0.03  -0.02     0.20  -0.03   0.02     0.52   0.18  -
0.06
  20   1    -0.21   0.08   0.10     0.05   0.08   0.01     0.04   0.02  -
0.06
  21   1    -0.32   0.23   0.17     0.17  -0.24   0.13     0.24  -0.06
0.00
  22   1     0.07  -0.10  -0.09    -0.24  -0.14  -0.37     0.05  -0.03  -
0.02
  23   1     0.05   0.29  -0.09     0.11   0.03  -0.01    -0.15   0.09
0.06
  24   1     0.17   0.10  -0.01     0.12   0.17   0.03    -0.45  -0.16
0.04
  25   1    -0.11   0.20  -0.02    -0.01   0.02   0.04     0.02  -0.17
0.00
  26   1    -0.05   0.15   0.01     0.14   0.08   0.11    -0.02   0.17
0.03
  27   1     0.00  -0.05  -0.05     0.00  -0.01  -0.03     0.01  -0.03  -
0.01
  28   1     0.00  -0.15   0.04     0.00   0.01  -0.03     0.02  -0.02
0.00
  29   1     0.03  -0.14   0.07    -0.03   0.02  -0.01     0.06  -0.16
0.08
                     28                    29                    30
                     ?A                    ?A                    ?A
 Frequencies --   923.5507              955.7948              986.1846
 Red. masses --     2.6946                2.3121                2.0725
 Frc consts  --     1.3541                1.2445                1.1876
 IR Inten    --    16.9168                3.8992                4.5665
 Raman Activ --     0.8600                3.1660                4.9268
 Depolar     --     0.6801                0.7475                0.4441
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.05  -0.01   0.04    -0.05   0.06   0.01     0.03  -0.03
0.02
   2   6     0.04  -0.02   0.00     0.15  -0.01   0.08     0.06   0.14  -
0.04
   3   6     0.00  -0.07  -0.04    -0.05   0.05  -0.04    -0.07  -0.04
0.00
   4   6     0.05   0.17  -0.08     0.12   0.01  -0.01     0.00  -0.08  -
0.02
   5   6     0.00   0.01   0.08    -0.05  -0.01   0.04     0.00   0.00
0.03
   6   6     0.01   0.05  -0.02    -0.09  -0.07  -0.07     0.14  -0.08  -
0.04
   7   6    -0.08  -0.08   0.06    -0.01   0.07  -0.02     0.00   0.05
0.03
   8   6     0.17  -0.06  -0.04    -0.07  -0.06   0.02    -0.04   0.06  -
0.03
   9   6     0.06   0.02   0.10     0.01   0.00  -0.02    -0.01   0.01
0.04
  10   6    -0.06   0.04  -0.07     0.00   0.06   0.01    -0.08  -0.02
0.00
  11   6    -0.06  -0.01   0.03     0.02  -0.07   0.01    -0.07  -0.02
0.06
```

12	6	-0.01	-0.02	-0.05	0.04	0.03	0.02	0.01	0.00	-0.01
13	7	-0.01	-0.02	0.01	0.04	-0.04	-0.01	0.01	0.00	-0.01
14	8	-0.01	0.01	-0.02	0.00	0.00	-0.01	0.01	-0.02	0.00
15	8	-0.05	0.03	-0.01	-0.07	0.02	0.00	-0.01	0.01	-0.01
16	8	0.02	-0.05	-0.01	0.01	0.00	0.00	0.00	0.02	0.00
17	1	-0.20	-0.07	0.19	-0.08	0.06	0.09	0.13	0.01	-0.06
18	1	0.09	-0.04	0.07	0.36	0.02	0.30	0.15	0.41	-0.07
19	1	0.03	-0.21	0.04	-0.20	0.11	-0.05	-0.27	-0.10	0.08
20	1	0.15	0.39	0.02	0.43	0.04	0.03	-0.04	-0.07	-0.02
21	1	0.12	0.14	0.14	-0.25	-0.14	-0.24	0.38	-0.26	-0.06
22	1	-0.22	-0.11	0.20	-0.01	0.08	-0.07	0.10	0.06	-0.04
23	1	0.41	-0.15	0.07	-0.25	-0.19	0.01	-0.05	0.02	-0.01
24	1	-0.26	0.11	0.05	0.05	0.21	0.04	-0.28	-0.08	0.07
25	1	0.11	0.05	0.01	0.05	-0.12	0.01	0.32	0.09	0.01
26	1	-0.15	0.02	-0.14	0.07	-0.25	0.00	-0.22	-0.07	-0.30
27	1	0.03	-0.02	0.14	-0.01	-0.03	-0.05	0.04	0.02	0.13
28	1	-0.02	-0.02	-0.03	-0.01	-0.02	-0.01	0.02	0.04	-0.01
29	1	-0.06	0.09	-0.08	0.01	-0.04	0.03	-0.01	0.03	0.00

	31			32			33		
	?A			?A			?A		
Frequencies --	1000.4081			1008.0899			1027.4133		
Red. masses --	2.8659			2.3414			2.4215		
Frc consts --	1.6899			1.4019			1.5060		
IR Inten --	24.2001			2.8412			44.0547		
Raman Activ --	8.6418			5.5193			0.5314		
Depolar --	0.0883			0.1917			0.7335		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.05	0.15	0.04	0.08	0.17	0.04	-0.08	0.03	-0.07
2 6	-0.03	0.06	0.02	-0.02	0.02	0.00	0.08	-0.07	-0.04
3 6	-0.08	0.13	0.00	0.01	-0.09	0.01	0.08	0.07	-0.03
4 6	0.11	0.02	0.01	-0.06	0.02	-0.02	-0.05	-0.06	0.05

```
    5   6     0.04   0.00  -0.09     0.02  -0.01   0.01    -0.05   0.01
0.04
    6   6     0.00  -0.05   0.00    -0.01  -0.02  -0.02     0.00  -0.04
0.11
    7   6     0.01  -0.18   0.04     0.14  -0.09   0.04     0.11   0.00
0.04
    8   6     0.08   0.07   0.02    -0.05  -0.06  -0.02     0.05  -0.02  -
0.05
    9   6     0.07   0.00  -0.09     0.01   0.02   0.02    -0.04   0.00  -
0.03
   10   6     0.02  -0.14   0.01    -0.02   0.08   0.01    -0.14  -0.01  -
0.01
   11   6    -0.08  -0.04   0.01    -0.10  -0.05  -0.10    -0.02   0.08  -
0.03
   12   6    -0.02   0.00   0.00     0.00   0.01  -0.01     0.03  -0.02
0.06
   13   7    -0.04   0.00   0.01     0.01  -0.01   0.01     0.00  -0.01  -
0.07
   14   8     0.00   0.03   0.01     0.00  -0.02  -0.01     0.00   0.00
0.00
   15   8    -0.01  -0.01   0.00    -0.01   0.00   0.01    -0.02   0.03  -
0.03
   16   8    -0.01  -0.01   0.01     0.00   0.02  -0.01     0.01  -0.01
0.00
   17   1     0.04   0.21   0.00     0.33   0.40   0.21    -0.03   0.09
0.02
   18   1    -0.01  -0.08   0.13    -0.03   0.04  -0.02     0.15  -0.10
0.05
   19   1    -0.18   0.40  -0.15     0.11  -0.21   0.06     0.09   0.09  -
0.04
   20   1     0.22  -0.08  -0.03    -0.16   0.05  -0.01     0.07  -0.06
0.06
   21   1    -0.02   0.09   0.13    -0.02  -0.06  -0.06    -0.03   0.02
0.15
   22   1     0.15  -0.18   0.01     0.45  -0.13   0.24     0.15   0.00
0.02
   23   1     0.10   0.24  -0.04    -0.11  -0.13  -0.02    -0.01   0.02  -
0.09
   24   1     0.05  -0.43  -0.11    -0.01   0.24   0.07    -0.13   0.00  -
0.01
   25   1     0.09   0.02  -0.01    -0.21  -0.09  -0.09    -0.11   0.02  -
0.02
   26   1    -0.18  -0.04  -0.18    -0.05  -0.03   0.01     0.02   0.08
0.05
   27   1    -0.03  -0.01  -0.01    -0.05  -0.02  -0.15     0.23   0.10
0.80
   28   1    -0.03  -0.21   0.08     0.00   0.01  -0.03     0.01   0.05  -
0.01
   29   1     0.06  -0.13   0.07    -0.02   0.06  -0.03     0.00  -0.01
0.01
                     34                    35                    36
                     ?A                    ?A                    ?A
 Frequencies --  1028.4398             1034.8848             1037.7684
 Red. masses --     2.2343                1.9385                2.0680
```

Frc consts	--	1.3923			1.2232			1.3122		
IR Inten	--	39.5446			23.1125			2.8826		
Raman Activ	--	1.0004			2.5193			7.9362		
Depolar	--	0.7088			0.7238			0.5201		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	-0.02	-0.06	-0.06	-0.03	0.02	-0.05	-0.01	0.01
2	6	0.00	-0.03	-0.02	0.05	0.00	-0.07	-0.05	-0.01	-0.10
3	6	0.05	0.03	-0.10	0.02	0.08	0.07	0.12	0.01	0.05
4	6	-0.01	0.00	0.15	-0.01	0.02	-0.06	0.03	-0.06	-0.03
5	6	0.03	-0.02	0.01	0.01	0.01	0.03	0.00	-0.01	0.02
6	6	0.04	-0.03	0.02	0.00	-0.04	0.09	-0.09	-0.10	-0.04
7	6	0.01	0.04	0.06	0.08	0.04	-0.02	0.02	0.00	0.05
8	6	0.04	-0.04	-0.13	0.02	-0.05	0.09	0.04	0.06	-0.03
9	6	0.03	-0.03	-0.01	0.01	0.00	-0.04	0.03	0.01	-0.02
10	6	-0.07	-0.04	0.09	-0.08	-0.01	-0.08	0.02	0.08	0.01
11	6	-0.01	0.03	-0.01	-0.02	0.05	-0.04	-0.06	0.02	0.13
12	6	-0.02	0.04	-0.08	-0.01	0.00	-0.05	-0.01	0.00	0.00
13	7	0.03	-0.02	0.05	0.02	0.00	0.04	-0.01	0.00	0.01
14	8	-0.01	0.04	-0.01	0.00	0.01	0.00	0.01	-0.02	0.00
15	8	-0.03	-0.01	0.04	0.00	-0.01	0.03	-0.01	0.00	0.01
16	8	-0.01	0.03	0.00	0.00	-0.02	0.01	0.00	0.02	0.00
17	1	0.05	0.01	-0.14	-0.18	-0.05	0.25	-0.03	0.00	-0.02
18	1	0.11	0.00	0.10	-0.01	0.14	-0.22	-0.22	-0.13	-0.23
19	1	0.06	0.17	-0.19	-0.06	0.03	0.12	0.39	-0.06	0.04
20	1	-0.07	0.17	0.23	0.11	-0.05	-0.09	0.11	-0.05	-0.02
21	1	0.01	-0.15	-0.11	0.13	-0.01	0.21	-0.33	-0.07	-0.17
22	1	-0.13	0.02	0.16	0.16	0.06	-0.16	0.07	0.03	-0.08
23	1	-0.01	0.08	-0.20	-0.07	-0.23	0.13	0.00	0.02	-0.03
24	1	-0.20	0.02	0.18	-0.08	-0.16	-0.14	0.18	0.27	0.00

```
  25   1     0.03  -0.17   0.00    -0.17   0.22  -0.03     0.39   0.17
0.08
  26   1    -0.05   0.17   0.01     0.08  -0.14   0.06    -0.23  -0.08  -
0.31
  27   1    -0.19  -0.08  -0.61    -0.16  -0.10  -0.57    -0.03  -0.02  -
0.08
  28   1    -0.03  -0.10   0.03    -0.01  -0.04   0.00     0.00  -0.05
0.00
  29   1    -0.01   0.03   0.00    -0.04   0.05  -0.03     0.00   0.02
0.00
                     37                      38                      39
                     ?A                      ?A                      ?A
 Frequencies --  1045.7962               1056.4156               1068.9220
 Red. masses --     2.4999                  2.4051                  1.6867
 Frc consts  --     1.6109                  1.5815                  1.1355
 IR Inten    --    12.1933                 52.8085                  2.4176
 Raman Activ --     3.1023                  1.4784                  5.4923
 Depolar     --     0.7472                  0.6623                  0.7495
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.05  -0.05  -0.02    -0.01   0.05  -0.10    -0.02  -0.11  -
0.04
   2   6     0.01   0.04   0.02     0.13  -0.04   0.07     0.00   0.02
0.07
   3   6     0.00   0.10   0.04    -0.05   0.00   0.08    -0.03  -0.02  -
0.01
   4   6    -0.12   0.06  -0.01    -0.09  -0.08  -0.03     0.04   0.01  -
0.03
   5   6     0.07   0.05   0.00    -0.02   0.01   0.00     0.00   0.00
0.01
   6   6    -0.08  -0.12  -0.08    -0.06  -0.02  -0.01    -0.01   0.03  -
0.06
   7   6    -0.02   0.07   0.09    -0.02  -0.02   0.06     0.08  -0.09
0.03
   8   6     0.06  -0.06   0.04     0.11   0.09   0.00    -0.05   0.01
0.02
   9   6     0.13   0.01  -0.03    -0.07   0.04  -0.01     0.01   0.00  -
0.01
  10   6     0.05  -0.01  -0.03    -0.03   0.06  -0.08     0.01   0.01
0.02
  11   6    -0.02   0.00  -0.04     0.01   0.01   0.01    -0.03   0.11
0.00
  12   6    -0.02  -0.04   0.03    -0.02  -0.02  -0.04    -0.01  -0.01
0.01
  13   7    -0.08   0.01   0.00    -0.01   0.03   0.03    -0.01   0.01
0.01
  14   8     0.00   0.04  -0.01     0.01  -0.07   0.01     0.00   0.00
0.00
  15   8     0.01   0.00  -0.01     0.08  -0.02   0.01     0.02   0.00
0.00
  16   8     0.01  -0.07   0.02     0.00  -0.01   0.00     0.00   0.00
0.00
  17   1     0.04  -0.05   0.00     0.09   0.10  -0.19    -0.26  -0.33  -
0.25
```

18	1	0.01	0.23	-0.08	0.28	-0.13	0.30	0.11	-0.01	0.22
19	1	-0.11	0.16	0.03	-0.23	-0.10	0.18	-0.05	-0.02	-0.01
20	1	-0.40	0.07	-0.02	-0.18	-0.18	-0.08	0.15	0.01	-0.02
21	1	-0.07	-0.37	-0.32	-0.12	0.05	0.02	-0.06	-0.03	-0.16
22	1	-0.09	0.05	0.17	-0.07	-0.02	0.07	0.40	-0.12	0.23
23	1	-0.03	-0.19	0.06	0.32	0.21	0.03	-0.15	-0.03	0.00
24	1	0.05	-0.06	-0.04	0.08	0.05	-0.15	-0.01	0.03	0.04
25	1	-0.08	-0.17	-0.03	0.10	-0.22	0.02	-0.12	0.38	-0.01
26	1	0.00	0.15	0.08	-0.05	0.16	-0.02	-0.11	0.39	-0.01
27	1	0.06	0.02	0.28	-0.08	-0.03	-0.36	-0.01	0.00	-0.06
28	1	-0.05	-0.28	0.07	0.05	0.18	-0.07	0.00	-0.02	0.00
29	1	-0.07	0.12	-0.09	0.00	-0.01	0.00	-0.01	0.03	-0.01

	40			41			42		
	?A			?A			?A		
Frequencies --	1102.1963			1142.6531			1157.1578		
Red. masses --	2.1746			2.4478			2.6142		
Frc consts --	1.5565			1.8830			2.0624		
IR Inten --	67.3199			147.3902			16.1070		
Raman Activ --	7.5136			3.3792			1.4129		
Depolar --	0.7380			0.7271			0.6869		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.02	0.01	-0.02	0.00	0.00	-0.01	-0.07	-0.01	0.07
2 6	0.03	-0.03	0.02	-0.05	-0.02	0.03	-0.01	0.01	-0.06
3 6	0.00	-0.06	0.04	0.01	0.02	-0.06	0.05	-0.07	0.07
4 6	0.00	-0.08	-0.05	-0.01	-0.04	-0.05	0.06	-0.02	0.02
5 6	0.08	-0.02	0.00	0.19	0.06	0.06	0.12	-0.07	-0.08
6 6	-0.02	0.03	0.04	0.00	0.02	0.01	-0.01	-0.03	-0.05
7 6	-0.03	-0.02	-0.03	0.00	0.00	-0.02	-0.05	-0.02	0.08
8 6	-0.05	0.07	-0.04	-0.02	0.02	0.01	0.03	0.05	-0.01
9 6	0.21	-0.02	-0.02	-0.04	0.09	0.00	-0.03	0.14	-0.06
10 6	-0.06	0.07	0.03	0.00	-0.03	0.00	-0.02	0.09	0.05

11	6	0.04	0.00	0.00	0.00	0.01	0.02	0.06	0.02	-0.09
12	6	-0.03	-0.02	0.00	0.03	0.07	0.00	0.01	0.03	0.01
13	7	-0.08	0.00	0.02	0.05	-0.05	-0.01	0.00	-0.02	-0.01
14	8	0.01	0.05	-0.02	0.01	-0.06	0.01	0.02	-0.09	0.01
15	8	0.00	0.00	-0.01	-0.16	0.01	0.01	-0.08	-0.01	0.01
16	8	0.00	0.02	0.00	0.03	-0.05	0.05	-0.03	0.06	-0.02
17	1	-0.01	0.01	-0.05	0.09	0.01	-0.22	-0.29	-0.10	0.29
18	1	0.08	-0.11	0.12	0.01	-0.20	0.19	0.03	0.23	-0.10
19	1	-0.08	-0.14	0.11	-0.01	0.04	-0.07	-0.11	0.02	0.04
20	1	-0.03	-0.16	-0.09	-0.24	-0.18	-0.14	0.14	-0.15	-0.03
21	1	0.02	0.22	0.26	-0.03	0.08	0.05	0.19	-0.21	-0.10
22	1	-0.07	0.01	-0.23	0.05	0.01	-0.11	-0.21	-0.05	0.33
23	1	-0.27	0.10	-0.13	0.05	-0.13	0.09	0.07	0.17	-0.05
24	1	-0.35	0.15	0.21	0.08	-0.11	-0.07	0.00	-0.17	-0.06
25	1	-0.04	-0.01	0.00	0.04	0.02	0.01	-0.28	-0.09	-0.05
26	1	0.09	-0.06	0.06	-0.01	-0.02	-0.03	0.18	0.09	0.23
27	1	-0.02	0.00	0.03	-0.06	-0.02	0.01	-0.01	0.01	0.10
28	1	-0.08	-0.53	0.12	0.03	0.07	-0.02	0.04	0.03	-0.03
29	1	-0.03	0.08	-0.03	-0.28	0.61	-0.31	0.09	-0.16	0.11

	43			44			45		
	?A			?A			?A		
Frequencies --	1195.4407			1209.0325			1229.1241		
Red. masses --	1.5157			4.7425			2.3707		
Frc consts --	1.2762			4.0845			2.1102		
IR Inten --	50.3202			8.5974			15.3776		
Raman Activ --	2.2520			3.7793			8.5187		
Depolar --	0.6991			0.5804			0.7443		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.01	0.02	0.01	-0.06	0.02	0.02	0.03	-0.02	-0.03
2 6	-0.01	-0.02	0.01	-0.03	-0.04	-0.01	-0.03	-0.05	0.02
3 6	0.01	0.01	-0.03	0.01	0.13	-0.06	0.03	-0.06	-0.07

4	6	-0.01	-0.04	-0.06	0.01	-0.17	-0.05	-0.06	0.00	-0.03
5	6	-0.07	0.08	0.06	-0.02	-0.07	0.12	-0.08	-0.11	0.11
6	6	0.02	0.03	0.00	-0.12	-0.02	-0.01	-0.03	0.05	-0.02
7	6	-0.01	-0.04	0.00	-0.01	-0.04	0.05	0.01	-0.02	-0.03
8	6	-0.01	0.03	0.00	-0.11	0.11	-0.17	0.00	-0.01	0.07
9	6	-0.02	-0.07	-0.04	0.09	0.06	0.31	0.00	0.16	-0.11
10	6	0.00	-0.02	0.04	0.16	-0.09	-0.16	-0.01	0.03	0.04
11	6	0.03	0.01	-0.01	0.09	0.03	-0.03	-0.01	0.01	0.04
12	6	0.00	-0.01	0.01	-0.02	-0.04	-0.06	0.00	-0.06	0.02
13	7	0.01	0.01	0.00	-0.03	0.01	0.02	-0.05	0.02	0.01
14	8	0.00	0.03	0.00	-0.02	-0.03	0.00	0.03	-0.05	0.00
15	8	0.02	0.00	0.00	0.03	0.01	-0.01	0.07	0.00	-0.02
16	8	0.03	-0.06	0.03	0.00	0.04	0.00	0.01	0.05	0.00
17	1	-0.07	0.06	0.31	0.02	0.13	0.23	0.24	0.15	0.05
18	1	-0.06	0.19	-0.15	0.02	0.26	-0.09	0.08	0.21	0.02
19	1	0.06	-0.02	-0.01	-0.03	0.15	-0.06	0.03	0.42	-0.39
20	1	0.22	-0.36	-0.19	0.18	0.25	0.16	0.19	0.20	0.09
21	1	0.05	-0.21	-0.21	0.15	-0.06	0.15	0.16	-0.04	0.02
22	1	-0.17	-0.09	0.31	0.15	-0.04	0.12	-0.09	-0.01	-0.06
23	1	0.10	0.38	-0.10	-0.08	-0.12	-0.08	0.13	-0.10	0.15
24	1	-0.04	0.12	0.12	-0.06	-0.21	-0.08	-0.09	-0.25	-0.02
25	1	-0.04	-0.02	0.00	-0.13	-0.01	-0.01	0.10	0.09	0.03
26	1	0.06	-0.02	0.04	0.19	0.01	0.18	0.01	-0.19	-0.05
27	1	-0.01	-0.03	-0.09	0.01	0.00	-0.02	0.01	-0.01	-0.04
28	1	-0.01	-0.04	0.03	0.03	0.32	-0.08	0.00	-0.23	0.03
29	1	-0.15	0.30	-0.17	-0.03	0.08	0.00	-0.12	0.24	-0.07
			46			47			48	
			?A			?A			?A	

Frequencies --	1234.0097			1252.7627			1261.5962		
Red. masses --	2.5669			2.3050			2.6474		
Frc consts --	2.3030			2.1314			2.4826		
IR Inten --	61.9281			72.9492			14.9649		
Raman Activ --	1.6491			5.6671			4.1890		
Depolar --	0.6112			0.7327			0.7044		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	0.04	-0.10	-0.01	0.01	0.00	0.01	0.00	-0.04
2 6	0.02	-0.12	0.06	-0.07	-0.07	-0.03	0.05	0.00	0.02
3 6	0.00	0.01	0.03	0.14	-0.05	0.01	-0.05	0.04	-0.03
4 6	-0.08	0.04	0.04	0.06	0.03	0.03	0.01	0.02	0.06
5 6	0.14	-0.07	-0.06	-0.09	0.18	-0.07	-0.02	0.13	-0.06
6 6	-0.08	0.10	0.06	-0.08	0.02	-0.01	0.04	0.01	0.06
7 6	0.05	0.01	-0.10	0.01	-0.01	0.00	0.02	0.01	-0.03
8 6	-0.05	-0.07	0.01	0.01	-0.03	-0.04	-0.08	-0.05	-0.04
9 6	0.02	-0.04	0.05	0.01	0.02	0.01	0.05	0.25	0.05
10 6	0.02	0.02	-0.06	0.05	0.08	0.03	-0.05	-0.09	-0.01
11 6	-0.03	-0.01	0.10	-0.01	0.00	0.04	-0.01	0.00	0.01
12 6	0.01	0.04	0.00	0.00	-0.01	0.00	0.00	-0.04	-0.02
13 7	0.02	-0.02	-0.01	0.00	0.01	0.00	-0.04	0.01	0.01
14 8	0.00	0.02	-0.01	-0.01	-0.01	0.00	0.03	-0.06	-0.01
15 8	-0.05	0.01	0.01	0.00	-0.02	0.01	0.02	-0.04	0.00
16 8	-0.02	0.03	-0.01	0.01	-0.08	0.00	0.00	-0.05	0.00
17 1	-0.15	-0.03	0.14	0.15	0.07	-0.21	0.05	0.00	-0.11
18 1	-0.06	0.29	-0.23	0.16	0.19	0.12	-0.11	-0.10	-0.12
19 1	-0.20	0.01	0.07	-0.46	0.04	0.09	0.21	-0.36	0.18
20 1	0.26	-0.12	0.00	-0.15	-0.08	-0.04	0.16	-0.04	0.04
21 1	0.18	-0.29	-0.15	0.25	-0.08	0.12	-0.16	-0.06	-0.14
22 1	0.15	-0.02	0.12	0.05	0.00	-0.06	-0.23	-0.04	0.27
23 1	0.22	0.28	-0.04	-0.23	-0.06	-0.10	0.09	0.08	-0.03

24	1	-0.02	-0.11	-0.09	-0.23	-0.43	0.00	0.15	0.10	-0.04
25	1	0.30	0.03	0.07	0.05	0.12	0.03	-0.05	0.27	-0.01
26	1	-0.20	0.09	-0.20	-0.01	-0.14	-0.04	0.06	-0.32	-0.03
27	1	-0.01	0.04	0.08	0.00	-0.06	-0.02	0.00	-0.06	-0.02
28	1	-0.02	-0.07	0.01	0.02	0.17	-0.05	0.00	-0.33	0.05
29	1	0.06	-0.12	0.07	0.03	-0.09	-0.01	0.09	-0.19	0.05

	49			50			51		
	?A			?A			?A		
Frequencies --	1269.9901			1292.9725			1309.9729		
Red. masses --	1.1851			1.6111			1.6969		
Frc consts --	1.1261			1.5870			1.7157		
IR Inten --	9.3286			40.1166			9.5260		
Raman Activ --	13.2662			1.9703			1.0665		
Depolar --	0.7484			0.7239			0.7282		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	0.01	-0.01	-0.01	0.03	0.05	0.05	0.11	0.05
2	6	0.02	-0.01	-0.02	-0.07	-0.03	-0.05	0.04	0.01	-0.03
3	6	0.01	0.00	0.02	0.10	0.06	-0.02	-0.01	-0.04	0.00
4	6	-0.01	0.01	-0.02	0.02	-0.04	-0.05	-0.01	-0.03	0.04
5	6	0.03	-0.05	0.01	-0.01	0.00	0.06	-0.06	0.01	0.00
6	6	-0.02	-0.02	0.01	0.02	0.03	0.03	-0.02	-0.04	0.02
7	6	-0.02	0.00	0.02	-0.05	-0.01	-0.04	-0.09	0.08	-0.04
8	6	0.01	0.03	0.02	-0.04	0.04	0.03	0.03	-0.03	-0.04
9	6	-0.01	-0.07	0.00	-0.03	0.00	-0.03	0.01	0.04	0.01
10	6	0.00	0.01	-0.01	-0.04	-0.04	0.00	0.00	0.01	0.00
11	6	0.01	-0.01	0.00	0.04	-0.02	0.00	0.02	-0.09	0.00
12	6	0.00	0.02	0.00	0.00	0.00	0.01	0.00	-0.02	0.00
13	7	0.01	-0.01	0.00	0.01	0.00	0.00	-0.01	0.01	0.00
14	8	-0.01	0.02	0.00	0.03	0.02	-0.01	0.01	0.00	-0.01
15	8	-0.01	0.01	0.00	-0.01	-0.01	0.00	0.02	0.00	0.00
16	8	-0.01	0.02	0.00	-0.01	0.01	-0.02	0.02	0.00	0.01

17	1	0.17	0.03	-0.38	0.04	0.03	-0.10	-0.42	-0.27	-0.19
18	1	-0.01	-0.15	0.01	0.17	0.03	0.20	-0.11	-0.19	-0.12
19	1	-0.05	0.08	-0.02	-0.30	-0.13	0.20	0.06	0.21	-0.18
20	1	-0.07	0.12	0.02	-0.15	0.16	0.02	0.00	-0.18	-0.02
21	1	0.12	-0.13	0.00	0.04	-0.18	-0.16	0.16	-0.02	0.17
22	1	-0.14	-0.06	0.38	0.19	-0.04	0.12	0.46	0.05	0.19
23	1	0.00	0.12	-0.01	0.33	-0.20	0.24	0.09	-0.04	-0.02
24	1	-0.01	0.07	0.02	0.11	0.22	0.01	0.02	-0.02	-0.02
25	1	-0.17	0.53	-0.02	0.01	-0.04	0.01	-0.07	0.19	-0.01
26	1	0.15	-0.46	0.02	-0.01	0.21	0.04	-0.08	0.25	-0.01
27	1	0.00	0.03	0.02	-0.01	-0.01	-0.01	0.01	-0.02	-0.01
28	1	0.00	0.07	0.00	-0.04	-0.39	0.08	-0.01	-0.10	0.01
29	1	0.00	0.00	0.01	0.11	-0.24	0.11	-0.08	0.17	-0.08

		52			53			54		
		?A			?A			?A		
Frequencies --		1336.5973			1352.3431			1359.9461		
Red. masses --		1.7507			1.4723			1.4366		
Frc consts --		1.8427			1.5865			1.5654		
IR Inten --		1.3712			3.6533			0.5583		
Raman Activ --		1.1942			0.6750			3.3430		
Depolar --		0.7495			0.7208			0.7136		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.05	-0.02	0.05	-0.03	0.00	0.01	0.02	-0.02	0.02
2	6	-0.06	0.04	-0.03	-0.01	-0.06	-0.05	0.00	0.06	0.04
3	6	0.08	-0.04	0.02	-0.08	0.00	0.04	0.04	-0.01	-0.04
4	6	-0.01	0.04	-0.03	0.08	0.01	0.00	-0.05	-0.01	-0.01
5	6	-0.03	-0.04	0.01	-0.02	-0.01	-0.01	0.01	0.02	0.00
6	6	0.06	-0.03	0.05	0.04	-0.04	0.03	0.00	-0.07	0.01
7	6	0.05	0.03	-0.01	0.01	0.02	-0.01	0.02	0.03	0.05
8	6	-0.04	-0.04	0.00	-0.07	-0.02	0.00	-0.06	-0.02	-0.02
9	6	0.06	0.00	0.10	-0.02	-0.03	0.02	-0.04	-0.01	-0.04

```
  10   6    -0.09   0.03  -0.06     0.03   0.08  -0.02     0.08   0.04  -
0.03
  11   6    -0.02  -0.01  -0.02     0.00   0.01   0.00    -0.01   0.01  -
0.03
  12   6     0.00  -0.01  -0.02     0.00   0.00   0.01     0.00   0.01
0.01
  13   7    -0.01   0.00   0.00     0.01   0.00   0.00     0.01   0.00
0.00
  14   8     0.00   0.00  -0.01     0.01   0.02  -0.01     0.01   0.00
0.00
  15   8     0.01   0.01   0.00     0.00   0.00  -0.01     0.00   0.00
0.00
  16   8     0.01   0.01   0.00     0.01   0.00   0.01     0.00   0.00
0.00
  17   1     0.01  -0.08  -0.05     0.02   0.00  -0.12     0.01  -0.04  -
0.03
  18   1     0.07  -0.17   0.23     0.28   0.32   0.09    -0.26  -0.27  -
0.09
  19   1    -0.34   0.28  -0.09     0.44  -0.02  -0.06    -0.29  -0.05
0.06
  20   1     0.15  -0.14  -0.10    -0.30   0.02  -0.03     0.29   0.05
0.05
  21   1    -0.33   0.05  -0.14    -0.30   0.11  -0.05    -0.23   0.11
0.04
  22   1    -0.25   0.02   0.05     0.05   0.00   0.14     0.02   0.05  -
0.08
  23   1    -0.06   0.34  -0.14     0.29   0.14   0.06     0.47   0.09
0.11
  24   1     0.31  -0.10  -0.33    -0.18  -0.38  -0.08    -0.48  -0.16
0.19
  25   1     0.00  -0.07  -0.02     0.01  -0.02   0.00    -0.03  -0.03  -
0.02
  26   1    -0.05   0.09  -0.01     0.02  -0.01   0.01     0.04  -0.06
0.04
  27   1     0.01  -0.01   0.02     0.00   0.01   0.00    -0.01   0.01  -
0.01
  28   1     0.00  -0.01  -0.01    -0.02  -0.20   0.04    -0.01  -0.09
0.02
  29   1    -0.05   0.10  -0.03    -0.04   0.08  -0.04     0.02  -0.04
0.02
                     55                    56                    57
                     ?A                    ?A                    ?A
 Frequencies --  1365.1350             1384.6495             1390.0537
 Red. masses --     1.6255                1.5387                1.6037
 Frc consts  --     1.7848                1.7381                1.8258
 IR Inten    --     8.6307                4.5429               17.7147
 Raman Activ --     2.4219                1.9256                1.2448
 Depolar     --     0.7357                0.6514                0.6943
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.05  -0.06  -0.02    -0.04   0.01  -0.02    -0.07   0.01  -
0.01
   2   6     0.06   0.07  -0.01     0.01  -0.05   0.09     0.07   0.03
0.01
```

3	6	-0.01	-0.05	0.03	0.04	-0.04	0.02	0.00	-0.05	0.01
4	6	0.05	0.00	0.02	-0.01	-0.02	0.03	0.06	-0.04	0.01
5	6	-0.03	0.02	-0.05	0.00	0.02	-0.07	-0.03	0.00	-0.04
6	6	-0.09	0.02	-0.03	0.08	-0.03	-0.06	0.03	0.06	0.11
7	6	0.04	-0.01	0.03	-0.04	-0.01	0.00	-0.03	-0.05	-0.04
8	6	-0.05	-0.01	-0.02	0.01	0.04	-0.01	-0.01	0.02	0.03
9	6	-0.06	-0.03	0.06	-0.03	-0.03	0.03	0.06	0.00	-0.03
10	6	-0.02	0.02	0.01	-0.06	0.01	-0.01	-0.01	0.03	-0.03
11	6	0.00	0.06	0.00	0.02	0.03	0.00	0.03	-0.01	0.00
12	6	0.00	0.01	0.00	0.00	0.01	-0.01	0.00	-0.01	0.00
13	7	0.03	0.00	-0.01	0.01	0.00	0.00	-0.02	0.00	0.00
14	8	0.03	0.03	-0.02	0.01	0.01	-0.01	-0.02	-0.01	0.01
15	8	0.00	0.00	0.00	-0.01	0.00	0.01	0.00	0.00	0.00
16	8	0.01	-0.01	0.01	0.01	-0.01	0.02	0.01	0.00	0.02
17	1	0.12	0.10	0.12	0.05	0.06	-0.09	0.04	0.10	0.01
18	1	-0.11	-0.33	-0.02	-0.20	0.41	-0.36	-0.24	-0.23	-0.23
19	1	0.00	0.12	-0.09	-0.25	0.17	-0.05	-0.09	0.06	-0.05
20	1	-0.12	0.13	0.06	0.10	0.12	0.10	-0.23	0.31	0.14
21	1	0.44	-0.17	0.13	-0.28	0.35	0.06	-0.21	-0.37	-0.46
22	1	0.03	0.00	-0.05	0.15	-0.04	0.14	0.02	-0.06	-0.03
23	1	0.18	0.10	0.02	-0.02	-0.24	0.08	-0.05	-0.11	0.07
24	1	0.30	-0.02	-0.17	0.19	0.12	-0.11	-0.15	-0.13	-0.02
25	1	0.06	-0.18	0.01	-0.01	-0.01	0.01	-0.02	-0.04	0.01
26	1	0.06	-0.08	0.03	0.08	-0.14	0.02	-0.03	0.14	-0.02
27	1	0.00	0.02	0.01	0.00	0.00	0.02	0.01	-0.02	0.00
28	1	-0.05	-0.49	0.10	-0.02	-0.19	0.03	0.02	0.25	-0.05
29	1	-0.07	0.14	-0.07	-0.07	0.14	-0.06	-0.08	0.16	-0.07

		58			59			60		
		?A			?A			?A		
Frequencies --		1393.8129			1416.9034			1426.7345		
Red. masses --		1.4611			1.6156			1.4484		
Frc consts --		1.6724			1.9110			1.7372		
IR Inten --		0.5721			20.7599			6.5326		
Raman Activ --		1.9429			13.4812			0.9729		
Depolar --		0.6848			0.6644			0.7470		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	-0.01	-0.01	-0.07	-0.09	-0.01	0.00	-0.03	-0.11
2	6	-0.02	0.02	-0.02	-0.02	0.04	-0.04	-0.02	0.04	0.00
3	6	-0.03	0.02	-0.04	0.00	0.01	0.05	0.00	-0.05	0.02
4	6	-0.09	-0.02	0.00	-0.02	0.04	-0.01	0.01	0.05	0.05
5	6	0.01	0.02	-0.04	0.00	-0.01	-0.06	0.02	0.03	0.06
6	6	0.02	0.00	0.01	0.00	-0.05	0.00	0.03	-0.01	0.02
7	6	-0.05	0.00	0.01	-0.08	0.04	-0.06	-0.03	-0.01	0.01
8	6	0.06	0.04	-0.01	-0.01	-0.07	0.02	-0.01	0.04	-0.05
9	6	-0.03	-0.04	0.03	0.05	0.03	-0.03	-0.01	-0.01	0.02
10	6	-0.01	0.07	0.04	0.00	-0.03	0.00	0.01	0.00	-0.04
11	6	0.04	-0.06	0.00	0.05	0.02	0.03	0.03	-0.02	0.02
12	6	-0.01	0.01	0.00	0.00	-0.01	0.00	0.00	0.01	0.00
13	7	0.01	0.00	0.00	-0.02	0.00	0.00	0.00	0.00	0.00
14	8	0.01	0.02	-0.01	-0.02	-0.01	0.01	0.00	0.00	0.00
15	8	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	-0.01	0.01	0.01	0.00	0.01	-0.01	0.00	-0.02
17	1	0.16	0.13	0.15	0.42	0.29	0.15	0.03	0.15	0.47
18	1	0.08	-0.10	0.16	0.11	-0.07	0.17	0.02	-0.11	0.13
19	1	0.13	-0.29	0.12	0.00	0.01	0.05	-0.02	0.29	-0.20
20	1	0.44	0.10	0.11	0.18	0.06	0.02	-0.18	-0.43	-0.17
21	1	-0.05	-0.09	-0.12	0.00	0.11	0.16	-0.15	-0.01	-0.10
22	1	0.05	0.01	-0.07	0.47	-0.01	0.30	0.07	-0.01	0.00

```
  23   1    -0.18  -0.18  -0.01     0.08   0.24  -0.07     0.08  -0.31
0.10
  24   1     0.13  -0.45  -0.21    -0.06   0.19   0.11    -0.07   0.05
0.02
  25   1    -0.08   0.28   0.00     0.11  -0.05   0.04    -0.05   0.29
0.01
  26   1    -0.01   0.16   0.03     0.05   0.10   0.06     0.03  -0.08  -
0.01
  27   1     0.00   0.02   0.01     0.00  -0.02   0.01     0.00   0.01
0.00
  28   1    -0.02  -0.20   0.04     0.02   0.23  -0.05    -0.01  -0.06
0.01
  29   1    -0.03   0.07  -0.03    -0.06   0.12  -0.06     0.10  -0.22
0.10
                      61                     62                     63
                      ?A                     ?A                     ?A
 Frequencies --  1429.7381              1436.1231              1448.2018
 Red. masses --     1.5490                 1.4631                 1.5673
 Frc consts  --     1.8655                 1.7778                 1.9367
 IR Inten    --    11.0690                13.3089                19.9587
 Raman Activ --     1.0538                 0.1675                 1.0828
 Depolar     --     0.7361                 0.6348                 0.7173
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.04   0.01  -0.06    -0.05  -0.02   0.05     0.06   0.02  -
0.06
   2   6    -0.01   0.03   0.04     0.04   0.02   0.01    -0.04   0.02  -
0.02
   3   6     0.02   0.02  -0.09    -0.01   0.00  -0.04     0.00  -0.02
0.03
   4   6     0.02  -0.05  -0.04    -0.01   0.03  -0.01     0.00  -0.09
0.02
   5   6     0.01   0.01   0.08     0.01   0.01   0.07     0.00   0.05  -
0.07
   6   6     0.02  -0.03  -0.01    -0.03  -0.05   0.01    -0.01  -0.04  -
0.01
   7   6    -0.06   0.00  -0.03     0.05   0.01  -0.12     0.08   0.03  -
0.06
   8   6     0.03  -0.03   0.04     0.00   0.05   0.00    -0.05   0.05
0.02
   9   6     0.01   0.00   0.00     0.00  -0.01   0.00     0.03  -0.03  -
0.04
  10   6    -0.03   0.04   0.05     0.01   0.04   0.02    -0.01   0.00
0.01
  11   6    -0.01   0.07   0.02     0.00   0.01   0.01    -0.02  -0.03
0.02
  12   6     0.00   0.00   0.00     0.00   0.01   0.00     0.00   0.00
0.00
  13   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   8     0.00   0.00   0.00     0.00   0.00   0.00    -0.01   0.00
0.01
  15   8     0.00   0.00   0.00     0.00   0.00  -0.01     0.00   0.00
0.01
```

16	8	-0.01	0.01	-0.02	-0.01	0.00	-0.02	0.01	-0.01	0.02
17	1	-0.25	-0.10	0.28	0.19	0.08	-0.20	-0.27	-0.09	0.39
18	1	-0.12	-0.11	-0.01	-0.16	-0.12	-0.16	0.13	-0.04	0.22
19	1	-0.06	-0.18	0.06	0.05	-0.03	-0.04	0.00	0.06	-0.01
20	1	-0.31	0.18	0.03	0.05	-0.22	-0.12	-0.01	0.37	0.22
21	1	-0.07	0.08	0.04	0.04	0.07	0.18	0.05	0.15	0.22
22	1	0.32	-0.04	0.19	-0.23	-0.10	0.53	-0.36	-0.04	0.35
23	1	-0.15	0.28	-0.14	-0.16	-0.28	0.07	0.12	-0.17	0.16
24	1	0.12	-0.31	-0.15	-0.02	-0.21	-0.06	0.02	0.06	0.02
25	1	0.08	-0.14	0.02	0.11	-0.28	0.02	0.06	0.10	0.00
26	1	0.10	-0.35	-0.01	-0.08	0.23	-0.03	-0.07	0.07	-0.04
27	1	0.00	0.00	-0.02	0.00	0.02	-0.01	0.00	-0.02	0.00
28	1	0.00	0.02	0.00	0.00	-0.01	0.00	0.01	0.14	-0.02
29	1	0.08	-0.17	0.08	0.08	-0.17	0.07	-0.04	0.10	-0.05

	64			65			66		
	?A			?A			?A		
Frequencies --	1458.3679			1476.9914			1508.6585		
Red. masses --	1.5209			1.8426			1.9792		
Frc consts --	1.9058			2.3683			2.6542		
IR Inten --	4.3628			21.9485			20.7578		
Raman Activ --	1.9036			4.6024			4.7689		
Depolar --	0.7250			0.7193			0.5320		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.07	-0.01	0.04	-0.03	-0.01	0.01	-0.01	0.00	0.04
2 6	-0.01	0.00	-0.05	0.03	-0.02	0.03	0.00	-0.01	-0.02
3 6	-0.03	-0.02	0.03	-0.01	-0.02	-0.04	-0.05	-0.09	0.05
4 6	-0.06	0.01	0.03	-0.01	-0.01	-0.01	-0.06	-0.08	-0.08
5 6	0.00	0.02	-0.03	0.03	0.07	0.05	0.09	0.18	0.06
6 6	0.00	0.03	0.04	-0.01	0.01	-0.05	0.01	0.02	0.02
7 6	-0.05	-0.04	-0.01	0.00	0.02	0.06	-0.01	0.00	-0.01
8 6	-0.01	0.05	-0.04	-0.10	-0.01	-0.02	0.04	-0.02	0.04

```
    9   6     0.05  -0.03  -0.01     0.14  -0.06  -0.05    -0.04   0.00
0.02
   10   6    -0.02   0.01   0.00    -0.09   0.03   0.07     0.02  -0.01  -
0.04
   11   6    -0.04   0.11  -0.01     0.02  -0.04  -0.02     0.01   0.00  -
0.01
   12   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.01
0.00
   13   7    -0.01   0.00   0.00    -0.02   0.00   0.00     0.01   0.00
0.00
   14   8    -0.01   0.00   0.01    -0.03   0.00   0.01     0.01   0.00  -
0.01
   15   8     0.00   0.00   0.00     0.00   0.00   0.00    -0.02  -0.02
0.00
   16   8     0.00  -0.01   0.00    -0.01  -0.01  -0.02    -0.02  -0.03  -
0.03
   17   1    -0.12  -0.19  -0.14     0.12   0.07  -0.10     0.05   0.01  -
0.10
   18   1     0.15  -0.07   0.17    -0.07   0.08  -0.14     0.06   0.03
0.02
   19   1     0.13   0.06  -0.05     0.11   0.00  -0.08     0.21   0.45  -
0.35
   20   1     0.31  -0.13   0.01     0.04  -0.01  -0.02     0.20   0.36
0.13
   21   1     0.02  -0.16  -0.13     0.13   0.05   0.08    -0.04  -0.04  -
0.07
   22   1     0.20  -0.06   0.05     0.03   0.07  -0.20     0.04   0.01  -
0.03
   23   1     0.14  -0.33   0.15     0.51   0.05   0.15    -0.18   0.23  -
0.13
   24   1     0.05  -0.02  -0.04     0.39  -0.14  -0.23    -0.09   0.12
0.05
   25   1     0.13  -0.41   0.01    -0.07   0.17  -0.02     0.01  -0.07
0.00
   26   1     0.16  -0.46   0.03     0.00   0.13   0.05     0.00   0.08
0.03
   27   1     0.00   0.01   0.01    -0.01  -0.01  -0.02    -0.02  -0.02  -
0.02
   28   1     0.01   0.15  -0.03     0.03   0.39  -0.08    -0.01  -0.10
0.02
   29   1    -0.01   0.02  -0.01     0.09  -0.19   0.08     0.16  -0.36
0.14
                     67                    68                    69
                     ?A                    ?A                    ?A
 Frequencies --  1639.5799             2029.5970             2101.2216
 Red. masses --     1.1004                3.7727                1.3024
 Frc consts  --     1.7429                9.1563                3.3880
 IR Inten    --     5.7422              295.9273               90.1973
 Raman Activ --    10.0110               31.1232              122.0639
 Depolar     --     0.6442                0.3524                0.1173
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.01   0.01   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

2	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	-0.01	0.01	0.00	0.00	0.01	0.00
6	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	6	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	-0.06	-0.04	0.01	0.02	0.02	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	-0.07	-0.02	-0.04	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.36	0.07	-0.09	-0.11	-0.08	0.03
13	7	0.00	0.00	0.00	-0.27	-0.05	0.07	0.07	-0.01	-0.02
14	8	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	-0.02	-0.03	0.01	-0.03	0.00	0.01
16	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	1	-0.02	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
18	1	-0.02	0.00	-0.02	0.00	0.01	0.00	0.00	0.00	0.00
19	1	-0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
20	1	-0.03	-0.01	-0.01	0.00	0.01	0.00	0.00	0.00	0.00
21	1	-0.01	-0.01	-0.02	0.00	0.00	0.00	0.00	0.00	0.00
22	1	-0.01	-0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
23	1	-0.03	-0.01	-0.01	0.01	0.00	0.00	0.00	0.00	0.00
24	1	-0.01	0.00	0.00	0.01	0.00	-0.01	0.00	0.00	0.00
25	1	0.67	0.21	-0.10	0.00	0.00	0.00	0.00	0.00	0.00
26	1	0.24	0.10	0.65	0.00	0.00	0.00	0.00	0.00	0.00
27	1	0.00	0.00	0.00	0.59	0.58	-0.27	0.50	0.81	-0.26
28	1	0.00	0.00	0.00	0.00	-0.01	0.01	0.00	0.01	0.00

```
  29   1     0.00   0.00   0.00    -0.01   0.01  -0.01     0.00   0.00
0.00
                     70                    71                    72
                     ?A                    ?A                    ?A
 Frequencies --  3210.7190             3254.2217             3272.6439
 Red. masses --     1.0582                1.1066                1.0878
 Frc consts  --     6.4272                6.9048                6.8645
 IR Inten    --    43.0742               24.3105                8.9700
 Raman Activ --   138.6104               93.5104               46.3986
 Depolar     --     0.1755                0.7444                0.5332
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.01
0.00
   2   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   3   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.01
0.03
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   7   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.01
0.00
   8   6     0.00   0.00   0.00     0.00   0.00   0.00     0.02  -0.03  -
0.07
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  11   6    -0.06  -0.02  -0.03    -0.05  -0.01   0.08     0.00   0.00
0.00
  12   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  17   1    -0.05   0.06  -0.02     0.00   0.00   0.00     0.04  -0.06
0.01
  18   1    -0.01   0.00   0.01    -0.01   0.00   0.00    -0.03   0.01
0.03
  19   1     0.00   0.00   0.00     0.00   0.00   0.00    -0.01  -0.02  -
0.04
  20   1     0.00   0.00  -0.01     0.00   0.00   0.01     0.03   0.14  -
0.33
  21   1    -0.01  -0.01   0.01     0.00  -0.01   0.00     0.01   0.01  -
0.01
```

```
  22   1     0.00  -0.06  -0.01     0.00   0.00   0.00     0.00  -0.14  -
0.02
  23   1     0.00  -0.01  -0.02    -0.01   0.01   0.03    -0.27   0.30
0.82
  24   1     0.00   0.00   0.00     0.00   0.00   0.00     0.01  -0.01
0.03
  25   1     0.04   0.03   0.70    -0.07  -0.04  -0.70     0.00   0.00
0.03
  26   1     0.60   0.18  -0.31     0.62   0.18  -0.29    -0.01   0.00
0.01
  27   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  29   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     73                    74                    75
                     ?A                    ?A                    ?A
 Frequencies --  3276.9444             3290.3046             3293.2804
 Red. masses --     1.0881                1.0889                1.0874
 Frc consts  --     6.8845                6.9453                6.9487
 IR Inten    --    13.6471                6.8142                8.5783
 Raman Activ --    53.5009               94.9700               96.4568
 Depolar     --     0.5600                0.6106                0.6705
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00  -0.01   0.00     0.02  -0.03   0.01     0.02  -0.02
0.01
   2   6    -0.03   0.01   0.02    -0.04   0.01   0.03     0.01   0.00  -
0.01
   3   6    -0.01  -0.04  -0.06     0.01   0.02   0.03     0.00   0.00  -
0.01
   4   6     0.00   0.00   0.00     0.00   0.01  -0.02     0.00   0.02  -
0.05
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.01   0.01  -0.01     0.02   0.02  -0.03    -0.02  -0.02
0.03
   7   6     0.00   0.00   0.00     0.00  -0.01   0.00     0.00   0.02
0.00
   8   6     0.00   0.00  -0.01     0.00   0.00  -0.01     0.01  -0.01  -
0.02
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.01   0.00   0.01     0.00   0.00   0.00     0.00   0.00  -
0.01
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	1	-0.06	0.08	-0.02	-0.27	0.39	-0.10	-0.19	0.28	-0.07
18	1	0.30	-0.12	-0.26	0.40	-0.16	-0.34	-0.14	0.06	0.13
19	1	0.16	0.46	0.71	-0.08	-0.22	-0.34	0.02	0.05	0.08
20	1	0.00	-0.02	0.04	-0.02	-0.09	0.21	-0.05	-0.28	0.64
21	1	-0.06	-0.09	0.09	-0.19	-0.27	0.29	0.20	0.29	-0.30
22	1	0.00	0.01	0.00	0.00	0.10	0.01	0.00	-0.20	-0.03
23	1	-0.03	0.03	0.09	-0.05	0.05	0.14	-0.07	0.09	0.23
24	1	-0.08	0.05	-0.15	0.02	-0.01	0.03	0.06	-0.05	0.12
25	1	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00
26	1	0.00	0.00	0.00	-0.02	-0.01	0.01	-0.02	-0.01	0.01
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	76			77			78		
	?A			?A			?A		
Frequencies --	3299.8784			3308.2431			3314.8992		
Red. masses --	1.0882			1.0887			1.0894		
Frc consts --	6.9819			7.0201			7.0528		
IR Inten --	39.8876			48.3628			28.1840		
Raman Activ --	71.2122			117.6051			66.7972		
Depolar --	0.7309			0.2275			0.7491		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.01	-0.02	0.00	0.03	-0.05	0.01	-0.01	0.01	0.00
2 6	-0.03	0.01	0.02	0.03	-0.01	-0.02	0.00	0.00	0.00
3 6	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	-0.01	-0.01
4 6	0.00	-0.02	0.03	0.00	-0.01	0.03	0.00	0.00	0.00
5 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6 6	-0.02	-0.03	0.03	0.00	0.00	0.00	0.00	0.00	0.00
7 6	0.00	0.01	0.00	0.00	-0.03	-0.01	0.00	-0.06	-0.01

8	6	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	-0.01
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	-0.01	0.01	-0.02	0.01	-0.01	0.02	-0.03	0.02	-0.05
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	1	-0.16	0.22	-0.06	-0.39	0.56	-0.15	0.06	-0.09	0.02
18	1	0.33	-0.14	-0.28	-0.33	0.13	0.28	-0.02	0.01	0.02
19	1	-0.01	-0.02	-0.04	0.02	0.05	0.08	0.03	0.08	0.12
20	1	0.04	0.18	-0.40	0.03	0.13	-0.29	-0.01	-0.02	0.05
21	1	0.26	0.38	-0.39	0.00	0.00	0.00	-0.02	-0.03	0.02
22	1	0.00	-0.15	-0.02	0.00	0.37	0.06	0.00	0.64	0.10
23	1	0.05	-0.06	-0.16	0.01	-0.01	-0.02	-0.03	0.03	0.08
24	1	0.13	-0.10	0.26	-0.10	0.07	-0.20	0.32	-0.22	0.61
25	1	0.00	0.00	-0.03	0.00	0.00	-0.03	0.00	0.00	0.04
26	1	0.00	0.00	0.00	-0.02	-0.01	0.01	0.03	0.01	-0.01
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	79	80	81
	?A	?A	?A
Frequencies --	3323.6940	3855.0528	3862.2875
Red. masses --	1.0925	1.0677	1.0669
Frc consts --	7.1106	9.3489	9.3771
IR Inten --	19.5865	99.7930	80.3423
Raman Activ --	381.8786	90.8211	127.9654
Depolar --	0.0226	0.2449	0.2546

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z

1	6	-0.01	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6	-0.02	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.00	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	-0.02	-0.02	0.03	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	-0.05	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
8	6	0.00	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.02	-0.01	0.04	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	8	0.00	0.00	0.00	-0.06	0.02	0.02	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	8	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.04	0.04
17	1	0.12	-0.18	0.05	0.00	0.00	0.00	0.00	0.00	0.00
18	1	0.19	-0.08	-0.16	0.00	0.00	0.00	0.00	0.00	0.00
19	1	-0.03	-0.09	-0.13	0.00	0.00	0.00	0.00	0.00	0.00
20	1	-0.01	-0.05	0.12	0.00	0.00	0.00	0.00	0.00	0.00
21	1	0.19	0.28	-0.29	0.00	0.00	0.00	0.00	0.00	0.00
22	1	0.00	0.57	0.09	0.00	0.00	0.00	0.00	0.00	0.00
23	1	-0.04	0.04	0.12	0.00	0.00	0.00	0.00	0.00	0.00
24	1	-0.23	0.16	-0.44	0.00	0.00	0.00	0.00	0.00	0.00
25	1	0.01	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00
26	1	0.04	0.01	-0.02	0.00	0.00	0.00	0.00	0.00	0.00
27	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  28   1     0.00   0.00   0.00     0.89  -0.23  -0.39    -0.02   0.01
0.01
  29   1     0.00   0.00   0.00    -0.01  -0.01  -0.02    -0.42  -0.59  -
0.69

 -------------------
 - Thermochemistry -
 -------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Atom  1 has atomic number  6 and mass  12.00000
 Atom  2 has atomic number  6 and mass  12.00000
 Atom  3 has atomic number  6 and mass  12.00000
 Atom  4 has atomic number  6 and mass  12.00000
 Atom  5 has atomic number  6 and mass  12.00000
 Atom  6 has atomic number  6 and mass  12.00000
 Atom  7 has atomic number  6 and mass  12.00000
 Atom  8 has atomic number  6 and mass  12.00000
 Atom  9 has atomic number  6 and mass  12.00000
 Atom 10 has atomic number  6 and mass  12.00000
 Atom 11 has atomic number  6 and mass  12.00000
 Atom 12 has atomic number  6 and mass  12.00000
 Atom 13 has atomic number  7 and mass  14.00307
 Atom 14 has atomic number  8 and mass  15.99491
 Atom 15 has atomic number  8 and mass  15.99491
 Atom 16 has atomic number  8 and mass  15.99491
 Atom 17 has atomic number  1 and mass   1.00783
 Atom 18 has atomic number  1 and mass   1.00783
 Atom 19 has atomic number  1 and mass   1.00783
 Atom 20 has atomic number  1 and mass   1.00783
 Atom 21 has atomic number  1 and mass   1.00783
 Atom 22 has atomic number  1 and mass   1.00783
 Atom 23 has atomic number  1 and mass   1.00783
 Atom 24 has atomic number  1 and mass   1.00783
 Atom 25 has atomic number  1 and mass   1.00783
 Atom 26 has atomic number  1 and mass   1.00783
 Atom 27 has atomic number  1 and mass   1.00783
 Atom 28 has atomic number  1 and mass   1.00783
 Atom 29 has atomic number  1 and mass   1.00783
 Molecular mass:   219.08954 amu.
 Principal axes and moments of inertia in atomic units:
                           1         2         3
     EIGENVALUES --  2011.79323 2488.08445 3465.68699
           X            0.99955   0.02924   0.00719
           Y           -0.02933   0.99949   0.01263
           Z           -0.00681  -0.01284   0.99989
 THIS MOLECULE IS AN ASYMMETRIC TOP.
 ROTATIONAL SYMMETRY NUMBER  1.
 WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
           MAY CAUSE SIGNIFICANT ERROR
 ROTATIONAL TEMPERATURES (KELVIN)      0.04305     0.03481     0.02499
 ROTATIONAL CONSTANTS (GHZ)            0.89708     0.72535     0.52075
    1 IMAGINARY FREQUENCIES IGNORED.
 Zero-point vibrational energy     647641.7 (Joules/Mol)
                                  154.79007 (Kcal/Mol)
```

WARNING-- EXPLICIT CONSIDERATION OF 15 DEGREES OF FREEDOM AS VIBRATIONS MAY CAUSE SIGNIFICANT ERROR

VIBRATIONAL TEMPERATURES:	109.57	208.61	350.69	368.63	376.00
(KELVIN)	463.67	498.10	506.32	550.84	622.36
	643.21	684.51	727.34	770.45	842.54
	907.42	984.02	991.69	1018.81	1049.71
	1160.19	1171.64	1193.58	1268.36	1273.84
	1299.69	1328.78	1375.17	1418.89	1439.36
	1450.41	1478.21	1479.69	1488.96	1493.11
	1504.66	1519.94	1537.93	1585.81	1644.01
	1664.88	1719.96	1739.52	1768.43	1775.45
	1802.44	1815.15	1827.22	1860.29	1884.75
	1923.05	1945.71	1956.65	1964.11	1992.19
	1999.97	2005.37	2038.60	2052.74	2057.06
	2066.25	2083.63	2098.25	2125.05	2170.61
	2358.98	2920.12	3023.17	4619.48	4682.07
	4708.58	4714.76	4733.99	4738.27	4747.76
	4759.80	4769.37	4782.03	5546.53	5556.94

Zero-point correction=	0.246674
(Hartree/Particle)	
Thermal correction to Energy=	0.256908
Thermal correction to Enthalpy=	0.257852
Thermal correction to Gibbs Free Energy=	0.211143
Sum of electronic and zero-point Energies=	-736.627383
Sum of electronic and thermal Energies=	-736.617149
Sum of electronic and thermal Enthalpies=	-736.616204
Sum of electronic and thermal Free Energies=	-736.662914

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	161.212	44.920	98.308
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	42.056
ROTATIONAL	0.889	2.981	31.229
VIBRATIONAL	159.435	38.959	25.023
VIBRATION 1	0.599	1.965	3.988
VIBRATION 2	0.616	1.908	2.737
VIBRATION 3	0.659	1.773	1.775
VIBRATION 4	0.666	1.752	1.687
VIBRATION 5	0.669	1.744	1.653
VIBRATION 6	0.707	1.631	1.299
VIBRATION 7	0.724	1.583	1.183
VIBRATION 8	0.728	1.571	1.158
VIBRATION 9	0.752	1.507	1.028
VIBRATION 10	0.793	1.399	0.850
VIBRATION 11	0.806	1.367	0.805
VIBRATION 12	0.832	1.304	0.722
VIBRATION 13	0.861	1.238	0.644
VIBRATION 14	0.890	1.172	0.575
VIBRATION 15	0.943	1.063	0.475

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.761579D-97	-97.118285	-223.623115
TOTAL V=0	0.220273D+17	16.342962	37.631060

VIB (BOT)		0.400732-111	-111.397146	-256.501408
VIB (BOT)	1	0.270593D+01	0.432316	0.995444
VIB (BOT)	2	0.140048D+01	0.146278	0.336818
VIB (BOT)	3	0.803072D+00	-0.095245	-0.219311
VIB (BOT)	4	0.759501D+00	-0.119472	-0.275094
VIB (BOT)	5	0.742749D+00	-0.129158	-0.297396
VIB (BOT)	6	0.582513D+00	-0.234695	-0.540404
VIB (BOT)	7	0.534242D+00	-0.272262	-0.626907
VIB (BOT)	8	0.523623D+00	-0.280982	-0.646984
VIB (BOT)	9	0.471311D+00	-0.326693	-0.752238
VIB (BOT)	10	0.401999D+00	-0.395775	-0.911305
VIB (BOT)	11	0.384511D+00	-0.415091	-0.955782
VIB (BOT)	12	0.352809D+00	-0.452460	-1.041828
VIB (BOT)	13	0.323512D+00	-0.490110	-1.128519
VIB (BOT)	14	0.297128D+00	-0.527056	-1.213591
VIB (BOT)	15	0.258759D+00	-0.587105	-1.351858
VIB (V=0)		0.115905D+03	2.064100	4.752767
VIB (V=0)	1	0.325173D+01	0.512115	1.179188
VIB (V=0)	2	0.198706D+01	0.298212	0.686657
VIB (V=0)	3	0.144600D+01	0.160170	0.368804
VIB (V=0)	4	0.140931D+01	0.149006	0.343099
VIB (V=0)	5	0.139536D+01	0.144688	0.333155
VIB (V=0)	6	0.126767D+01	0.103007	0.237183
VIB (V=0)	7	0.123172D+01	0.090512	0.208411
VIB (V=0)	8	0.122400D+01	0.087783	0.202127
VIB (V=0)	9	0.118712D+01	0.074495	0.171530
VIB (V=0)	10	0.114156D+01	0.057500	0.132399
VIB (V=0)	11	0.113075D+01	0.053368	0.122883
VIB (V=0)	12	0.111194D+01	0.046083	0.106109
VIB (V=0)	13	0.109553D+01	0.039626	0.091241
VIB (V=0)	14	0.108162D+01	0.034076	0.078463
VIB (V=0)	15	0.106299D+01	0.026529	0.061084
ELECTRONIC		0.100000D+01	0.000000	0.000000
TRANSLATIONAL		0.127466D+09	8.105393	18.663357
ROTATIONAL		0.149097D+07	6.173468	14.214936

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000000366	0.000000152	0.000000149
2	6	-0.000000258	0.000000289	0.000000067
3	6	-0.000000260	-0.000000381	0.000000700
4	6	-0.000000129	0.000000370	0.000000150
5	6	0.000002054	0.000000843	0.000001446
6	6	0.000000592	-0.000000697	-0.000000042
7	6	-0.000000567	0.000000571	-0.000000012
8	6	0.000000254	-0.000001867	0.000001432
9	6	0.000000902	-0.000000369	0.000001568
10	6	-0.000000049	0.000001208	-0.000001214
11	6	-0.000000383	-0.000000276	0.000000267
12	6	0.000008108	-0.000012750	-0.000005104
13	7	-0.000002946	0.000006319	0.000003073
14	8	-0.000003708	0.000002426	-0.000002173

15	8	-0.000001856	0.000011490	-0.000002125
16	8	-0.000000388	-0.000000436	-0.000000769
17	1	0.000000142	-0.000000318	-0.000000019
18	1	0.000000186	-0.000000161	-0.000000134
19	1	-0.000000096	0.000000245	-0.000000139
20	1	0.000000107	-0.000000197	-0.000000130
21	1	-0.000000149	0.000000110	-0.000000039
22	1	-0.000000332	-0.000000544	0.000000009
23	1	0.000000024	0.000000033	-0.000000405
24	1	0.000000039	0.000000067	0.000000877
25	1	-0.000000017	-0.000000054	-0.000000101
26	1	0.000000246	0.000000005	-0.000000164
27	1	-0.000003345	-0.000006988	0.000001724
28	1	0.000001430	0.000000642	0.000000360
29	1	0.000000033	0.000000268	0.000000749

Cartesian Forces: Max 0.000012750 RMS 0.000002554

Internal Coordinate Forces (Hartree/Bohr or radian)

Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	C		0.000000(1)		0.000000(30)		0.000000(59)	
2	C		0.000000(2)		0.000000(31)		0.000000(60)	
3	C		0.000000(3)		0.000000(32)		0.000001(61)	
4	C		0.000000(4)		0.000000(33)		0.000000(62)	
5	C		0.000002(5)		0.000001(34)		0.000001(63)	
6	C		0.000001(6)		-0.000001(35)		0.000000(64)	
7	C		-0.000001(7)		0.000001(36)		0.000000(65)	
8	C		0.000000(8)		-0.000002(37)		0.000001(66)	
9	C		0.000001(9)		0.000000(38)		0.000002(67)	
10	C		0.000000(10)		0.000001(39)		-0.000001(68)	
11	C		0.000000(11)		0.000000(40)		0.000000(69)	
12	C		0.000008(12)		-0.000013(41)		-0.000005(70)	
13	N		-0.000003(13)		0.000006(42)		0.000003(71)	
14	O		-0.000004(14)		0.000002(43)		-0.000002(72)	
15	O		-0.000002(15)		0.000011(44)		-0.000002(73)	
16	O		0.000000(16)		0.000000(45)		-0.000001(74)	
17	H		0.000000(17)		0.000000(46)		0.000000(75)	
18	H		0.000000(18)		0.000000(47)		0.000000(76)	
19	H		0.000000(19)		0.000000(48)		0.000000(77)	
20	H		0.000000(20)		0.000000(49)		0.000000(78)	
21	H		0.000000(21)		0.000000(50)		0.000000(79)	
22	H		0.000000(22)		-0.000001(51)		0.000000(80)	
23	H		0.000000(23)		0.000000(52)		0.000000(81)	
24	H		0.000000(24)		0.000000(53)		0.000001(82)	
25	H		0.000000(25)		0.000000(54)		0.000000(83)	
26	H		0.000000(26)		0.000000(55)		0.000000(84)	
27	H		-0.000003(27)		-0.000007(56)		0.000002(85)	
28	H		0.000001(28)		0.000001(57)		0.000000(86)	
29	H		0.000000(29)		0.000000(58)		0.000001(87)	

Internal Forces: Max 0.000012750 RMS 0.000002554

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

```
Berny optimization.
Search for a local minimum.
Step number   1 out of a maximum of  97
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
    Eigenvalues ---   -0.25972   0.00072   0.00317   0.00457   0.01086
    Eigenvalues ---    0.01221   0.01409   0.02075   0.02333   0.02673
    Eigenvalues ---    0.03632   0.03849   0.04303   0.04459   0.04576
    Eigenvalues ---    0.04766   0.04845   0.04977   0.05068   0.05100
    Eigenvalues ---    0.05135   0.05220   0.05379   0.05399   0.05501
    Eigenvalues ---    0.05779   0.05952   0.06905   0.07693   0.08274
    Eigenvalues ---    0.09974   0.10405   0.10663   0.11575   0.12620
    Eigenvalues ---    0.15066   0.16191   0.16999   0.18795   0.19059
    Eigenvalues ---    0.19602   0.20763   0.23387   0.25680   0.26701
    Eigenvalues ---    0.29976   0.31570   0.33249   0.36973   0.37596
    Eigenvalues ---    0.39144   0.40576   0.43036   0.49242   0.49889
    Eigenvalues ---    0.50369   0.51928   0.54840   0.57936   0.58697
    Eigenvalues ---    0.62227   0.63650   0.68004   0.69609   0.71928
    Eigenvalues ---    0.72973   0.77165   0.81438   0.87943   0.94121
    Eigenvalues ---    0.96069   0.96508   0.97785   0.99938   1.01716
    Eigenvalues ---    1.06416   1.06683   1.09734   1.14417   1.15135
    Eigenvalues ---    1.98825
Eigenvalue   1 out of range, new value =    0.259724 Eigenvector:
                          1
          X1           0.01784
          Y1           0.00467
          Z1          -0.00409
          X2           0.00927
          Y2           0.00490
          Z2           0.00263
          X3          -0.01162
          Y3          -0.01125
          Z3           0.00505
          X4           0.00370
          Y4          -0.01375
          Z4           0.00424
          X5           0.00822
          Y5          -0.07991
          Z5           0.02273
          X6          -0.00326
          Y6           0.00252
          Z6           0.00064
          X7          -0.00478
          Y7          -0.00003
          Z7           0.00233
          X8          -0.00307
          Y8          -0.01705
          Z8          -0.00118
          X9          -0.00246
          Y9          -0.04161
          Z9           0.00507
          X10         -0.00388
          Y10         -0.01501
          Z10          0.00467
```

X11	0.00484
Y11	0.01368
Z11	-0.00021
X12	-0.18650
Y12	0.26411
Z12	0.02615
X13	-0.06937
Y13	0.31892
Z13	-0.00952
X14	0.00273
Y14	-0.02575
Z14	0.00602
X15	-0.14720
Y15	-0.13403
Z15	0.00661
X16	0.08680
Y16	-0.04202
Z16	-0.01812
X17	0.02122
Y17	0.00790
Z17	-0.00451
X18	0.00829
Y18	0.00908
Z18	-0.00293
X19	0.01482
Y19	-0.00613
Z19	-0.00339
X20	0.01988
Y20	-0.00794
Z20	0.00441
X21	-0.00422
Y21	0.00603
Z21	0.00158
X22	-0.01066
Y22	0.00048
Z22	0.00292
X23	-0.00010
Y23	-0.01436
Z23	-0.00089
X24	-0.00001
Y24	-0.01139
Z24	0.00322
X25	0.00513
Y25	0.00824
Z25	-0.00044
X26	0.00365
Y26	0.01515
Z26	-0.00099
X27	0.67418
Y27	-0.50396
Z27	-0.11747
X28	-0.00621
Y28	-0.02949
Z28	-0.00124

```
          X29          0.04130
          Y29         -0.01919
          Z29         -0.00621
 Angle between quadratic step and forces=  77.75 degrees.
 Linear search not attempted -- first point.
 TrRot= -0.000008 -0.000003 -0.000026 -0.000001  0.000002 -0.000001
```

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
X1	-3.71576	0.00000	0.00000	-0.00004	-0.00004	-3.71580
Y1	1.43071	0.00000	0.00000	0.00001	0.00002	1.43073
Z1	-0.90674	0.00000	0.00000	0.00005	0.00003	-0.90672
X2	-3.21201	0.00000	0.00000	0.00004	0.00003	-3.21198
Y2	0.93372	0.00000	0.00000	0.00000	0.00000	0.93372
Z2	1.95051	0.00000	0.00000	0.00003	0.00001	1.95052
X3	-0.38553	0.00000	0.00000	0.00005	0.00005	-0.38548
Y3	1.63267	0.00000	0.00000	0.00000	0.00000	1.63267
Z3	2.47091	0.00000	0.00000	-0.00004	-0.00006	2.47085
X4	-0.98673	0.00000	0.00000	-0.00007	-0.00007	-0.98680
Y4	1.38795	0.00000	0.00000	0.00003	0.00003	1.38798
Z4	-1.98210	0.00000	0.00000	-0.00002	-0.00004	-1.98214
X5	0.53242	0.00000	0.00000	-0.00001	-0.00001	0.53240
Y5	2.81574	0.00000	0.00000	0.00003	0.00002	2.81576
Z5	0.00594	0.00000	0.00000	-0.00006	-0.00008	0.00585
X6	-2.50367	0.00000	0.00000	0.00005	0.00004	-2.50363
Y6	-1.95262	0.00000	0.00000	0.00000	0.00000	-1.95262
Z6	2.01810	0.00000	0.00000	-0.00001	-0.00003	2.01807
X7	-2.70166	0.00000	0.00000	-0.00002	-0.00004	-2.70169
Y7	-2.75135	0.00000	0.00000	0.00001	0.00002	-2.75134
Z7	-0.79658	0.00000	0.00000	-0.00001	-0.00003	-0.79661
X8	-0.28444	0.00000	0.00000	-0.00004	-0.00006	-0.28450
Y8	-1.51607	0.00000	0.00000	0.00003	0.00003	-1.51604
Z8	-1.90540	0.00000	0.00000	-0.00006	-0.00009	-1.90549
X9	1.73176	0.00000	0.00000	-0.00002	-0.00003	1.73173
Y9	-2.07042	0.00000	0.00000	-0.00002	-0.00003	-2.07045
Z9	0.13735	0.00000	0.00000	-0.00012	-0.00015	0.13720
X10	0.32902	0.00000	0.00000	0.00005	0.00005	0.32907
Y10	-1.25031	0.00000	0.00000	0.00000	0.00000	-1.25031
Z10	2.53725	0.00000	0.00000	-0.00007	-0.00010	2.53715
X11	-4.85180	0.00000	0.00000	-0.00005	-0.00006	-4.85187
Y11	-1.08352	0.00000	0.00000	0.00001	0.00002	-1.08350
Z11	-1.81809	0.00000	0.00000	0.00006	0.00004	-1.81805
X12	4.08446	0.00001	0.00000	0.00006	0.00004	4.08451
Y12	-0.63140	-0.00001	0.00000	-0.00013	-0.00014	-0.63154
Z12	-0.34883	-0.00001	0.00000	-0.00004	-0.00007	-0.34890
X13	6.28170	0.00000	0.00000	0.00014	0.00013	6.28183
Y13	-0.48884	0.00001	0.00000	0.00002	0.00000	-0.48884
Z13	-0.96225	0.00000	0.00000	0.00039	0.00035	-0.96189
X14	2.21789	0.00000	0.00000	-0.00015	-0.00017	2.21773
Y14	-4.74299	0.00000	0.00000	-0.00006	-0.00007	-4.74306
Z14	0.28705	0.00000	0.00000	-0.00030	-0.00033	0.28672
X15	3.20406	0.00000	0.00000	-0.00005	-0.00006	3.20400
Y15	2.23264	0.00001	0.00000	0.00001	-0.00001	2.23264
Z15	-0.20617	0.00000	0.00000	-0.00021	-0.00024	-0.20641
X16	0.10643	0.00000	0.00000	-0.00006	-0.00006	0.10637

```
  Y16        5.43573   0.00000   0.00000   0.00003   0.00002   5.43576
  Z16       -0.23557   0.00000   0.00000  -0.00002  -0.00004  -0.23561
  X17       -4.74692   0.00000   0.00000  -0.00005  -0.00006  -4.74698
  Y17        3.13912   0.00000   0.00000   0.00001   0.00002   3.13914
  Z17       -1.32263   0.00000   0.00000   0.00008   0.00006  -1.32256
  X18       -4.63817   0.00000   0.00000   0.00007   0.00007  -4.63811
  Y18        1.62781   0.00000   0.00000  -0.00002  -0.00001   1.62780
  Z18        3.22979   0.00000   0.00000   0.00007   0.00005   3.22985
  X19        0.08357   0.00000   0.00000   0.00008   0.00009   0.08366
  Y19        2.70757   0.00000   0.00000  -0.00001  -0.00001   2.70756
  Z19        4.14067   0.00000   0.00000  -0.00004  -0.00006   4.14061
  X20       -0.78331   0.00000   0.00000  -0.00011  -0.00012  -0.78343
  Y20        2.21267   0.00000   0.00000   0.00004   0.00003   2.21271
  Z20       -3.83702   0.00000   0.00000  -0.00002  -0.00004  -3.83707
  X21       -3.45101   0.00000   0.00000   0.00008   0.00007  -3.45094
  Y21       -3.16722   0.00000   0.00000  -0.00002  -0.00001  -3.16723
  Z21        3.35126   0.00000   0.00000   0.00001  -0.00001   3.35125
  X22       -2.82882   0.00000   0.00000  -0.00002  -0.00004  -2.82886
  Y22       -4.75845   0.00000   0.00000   0.00001   0.00002  -4.75843
  Z22       -1.11718   0.00000   0.00000  -0.00002  -0.00004  -1.11722
  X23        0.26327   0.00000   0.00000  -0.00008  -0.00011   0.26316
  Y23       -2.23828   0.00000   0.00000   0.00004   0.00004  -2.23824
  Z23       -3.73574   0.00000   0.00000  -0.00007  -0.00010  -3.73584
  X24        1.20654   0.00000   0.00000   0.00009   0.00008   1.20662
  Y24       -1.93493   0.00000   0.00000   0.00000  -0.00001  -1.93494
  Z24        4.24248   0.00000   0.00000  -0.00009  -0.00011   4.24237
  X25       -5.04722   0.00000   0.00000  -0.00010  -0.00012  -5.04734
  Y25       -1.18348   0.00000   0.00000   0.00003   0.00003  -1.18344
  Z25       -3.85578   0.00000   0.00000   0.00006   0.00004  -3.85574
  X26       -6.65911   0.00000   0.00000  -0.00003  -0.00004  -6.65915
  Y26       -1.49700   0.00000   0.00000   0.00000   0.00001  -1.49699
  Z26       -0.94492   0.00000   0.00000   0.00010   0.00008  -0.94484
  X27        5.39349   0.00000   0.00000   0.00007   0.00007   5.39356
  Y27        2.24521  -0.00001   0.00000  -0.00008  -0.00010   2.24511
  Z27       -0.92868   0.00000   0.00000   0.00028   0.00024  -0.92844
  X28        3.81749   0.00000   0.00000   0.00041   0.00039   3.81788
  Y28       -5.23331   0.00000   0.00000   0.00006   0.00005  -5.23326
  Z28       -0.45393   0.00000   0.00000   0.00083   0.00080  -0.45314
  X29        0.97482   0.00000   0.00000  -0.00004  -0.00003   0.97479
  Y29        6.42854   0.00000   0.00000   0.00003   0.00002   6.42856
  Z29        1.03098   0.00000   0.00000  -0.00003  -0.00006   1.03092
        Item               Value     Threshold  Converged?
Maximum Force            0.000013     0.000450     YES
RMS     Force            0.000003     0.000300     YES
Maximum Displacement     0.000796     0.001800     YES
RMS     Displacement     0.000129     0.001200     YES
Predicted change in Energy=-3.027748D-09
Optimization completed.
   -- Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1|1|UNPC-UNK|Freq|RHF|3-21+G*|C12H13N1O3|PCUSER|12-Mar-2002|0||#N RHF/
3-21+G* FREQ||Freq calc of output str of mech1s10ts3||0,1|C,-1.9662930
69,0.7571009397,-0.4798278707|C,-1.699725069,0.4941049397,1.0321651293
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,-0.150520069,-0.8022710603,-1.0082938707|C,0.916406931,-1.0956210603,
0.0726831293|C,0.174111931,-0.6616330603,1.3426531293|C,-2.567463069,-
0.5733760603,-0.9620928707|C,2.161404931,-0.3341200603,-0.1845918707|N
,3.324132931,-0.2586820603,-0.5091988707|O,1.173657931,-2.5098830603,0
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.454416069,0.8613989397,1.7091321293|H,0.044223931,1.4327859397,2.1911
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14,0.00000032,0.00000002,-0.00000019,0.00000016,0.00000013,0.00000010,
-0.00000024,0.00000014,-0.00000011,0.00000020,0.00000013,0.00000015,-0
.00000011,0.00000004,0.00000033,0.00000054,0.,-0.00000002,-0.00000003,
0.00000040,-0.00000004,-0.00000007,-0.00000088,0.00000002,0.00000005,0
.00000010,-0.00000025,0.,0.00000016,0.00000335,0.00000699,-0.00000172,
-0.00000143,-0.00000064,-0.00000036,-0.00000003,-0.00000027,-0.0000007
5|||@

A MAN IS EXACTLY AS GREAT AS THE TIDE SURGING
BENEATH HIM.   - BISMARCK
Job cpu time: 0 days 18 hours 16 minutes 1.0 seconds.
File lengths (MBytes): RWF= 319 Int=   0 D2E=   0 Chk=   6 Scr=
1
Normal termination of Gaussian 98.

```
%nproc=2
%chk=mech1s8ts2
%nosave

#N RHF/3-21+G* OPT=(CALCFC,TS,NOEIGENTEST,GDIIS) OPTCYC=200

TS search for mech1s8 using input@1.73A from mech1st8.out
optcyc=200&calcfc

-1   1
C,-2.052388,-0.489945,-0.445780
C,-1.635613,-0.508442,1.050601
C,-0.689336,0.709575,1.282410
C,-0.931900,0.387942,-1.056190
C,-0.684120,1.515481,-0.030195
C,-0.398943,-1.483215,1.055784
C,-0.273544,-1.892238,-0.451415
C,0.321268,-0.591056,-1.069143
C,1.322022,-0.161034,0.005110
C,0.559808,-0.254839,1.310990
C,-1.734308,-1.914114,-0.914688
O,-1.940830,2.350664,-0.018334
C,2.524103,0.573434,-0.212785
N,3.525770,1.098487,-0.410228
O,0.385875,2.321510,-0.256121
H,-3.044527,-0.111137,-0.626997
H,-2.443327,-0.689433,1.744693
H,-0.846255,1.336780,2.143684
H,-1.166664,0.798733,-2.026552
H,-0.377759,-2.296140,1.768169
H,0.305134,-2.776467,-0.661770
H,0.763852,-0.695692,-2.047304
H,1.192948,-0.233917,2.181334
H,-1.826605,-2.037829,-1.989679
H,-2.320951,-2.680855,-0.413296
H,-1.625520,3.255768,-0.154034
O,2.406024,-1.495217,0.199536
H,1.938438,-2.324176,0.404511
```

```
%chk=mech1s10ts3
# opt=(calcfc,gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity
optcyc=200

TS search for mech1str10 using input@1.2964A from m1s10S2
optcyc=200&calcfc

0  1
 C
 C                  1             B1
 C                  2             B2    1             A1
 C                  1             B3    2             A2    3
D1
 C                  4             B4    1             A3    2
D2
 C                  2             B5    1             A4    4
D3
 C                  6             B6    2             A5    1
D4
 C                  7             B7    6             A6    2
D5
 C                  8             B8    7             A7    6
D6
 C                  9             B9    8             A8    7
D7
 C                  1            B10    2             A9    3
D8
 C                  9            B11    8            A10    7
D9
 N                 12            B12    9            A11    8
D10
 O                  9            B13    8            A12    7
D11
 O                 12            B14    9            A13    8
D12
 O                  5            B15    4            A14    1
D13
 H                  1            B16    2            A15    3
D14
 H                  2            B17    1            A16   11
D15
 H                  3            B18    2            A17    1
D16
 H                  4            B19    1            A18    2
D17
 H                  6            B20    2            A19    1
D18
 H                  7            B21    6            A20    2
D19
 H                  8            B22    7            A21    6
D20
 H                 10            B23    9            A22    8
D21
```

```
 H                 11             B24    1             A23    2
D22
 H                 11             B25    1             A24    2
D23
 H                 13             B26   12             A25    9
D24
 H                 14             B27    9             A26    8
D25
 H                 16             B28    5             A27    4
D26
```

B1	1.556590
B2	1.565617
B3	1.550033
B4	1.524962
B5	1.573864
B6	1.550674
B7	1.551278
B8	1.543286
B9	1.537236
B10	1.538516
B11	1.475498
B12	1.241411
B13	1.434889
B14	1.448832
B15	1.411047
B16	1.078607
B17	1.078252
B18	1.079639
B19	1.079392
B20	1.078174
B21	1.078253
B22	1.080214
B23	1.077915
B24	1.084453
B25	1.084403
B26	1.181212
B27	0.968568
B28	0.967640
A1	107.282842
A2	101.190747
A3	103.764595
A4	103.061763
A5	103.187108
A6	101.229330
A7	103.616208
A8	101.152971
A9	103.055461
A10	110.582882
A11	147.517976
A12	110.458738
A13	111.639962
A14	109.760535
A15	115.233619

```
  A16          115.635738
  A17          119.077435
  A18          114.964920
  A19          118.815843
  A20          115.164790
  A21          114.383836
  A22          113.077456
  A23          113.015016
  A24          112.716206
  A25           78.008567
  A26          113.631146
  A27          113.133573
  D1            20.422540
  D2           -40.577318
  D3           -73.635629
  D4            -0.031840
  D5            73.588327
  D6            41.561814
  D7           -46.723415
  D8           127.418596
  D9          -163.695538
  D10         -123.281567
  D11           70.796390
  D12           56.029111
  D13          -76.895501
  D14         -103.213604
  D15          -97.947119
  D16          135.817365
  D17         -162.983459
  D18         -129.694996
  D19         -162.898293
  D20          163.540383
  D21          163.664157
  D22         -170.762307
  D23           64.743891
  D24          179.022603
  D25          124.335322
  D26         -175.307547

1  2 1.0  4 1.0  11 1.0  17 1.0
2  3 1.0  6 1.0  18 1.0
3  5 1.0  10 1.0  19 1.0
4  5 1.0  8 1.0  20 1.0
5  15 1.0  16 1.0
6  7 1.0  10 1.0  21 1.0
7  8 1.0  11 1.0  22 1.0
8  9 1.0  23 1.0
9  10 1.0  12 1.0  14 1.0
10  24 1.0
11  25 1.0  26 1.0
12  13 2.0  15 1.0
13
14  28 1.0
15
```

16 29 1.0
17
18
19
20
21
22
23
24
25
26
27
28
29

```
%nproc=2
# opt=(gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity optcyc=100

TS search for mech1str5 using input@1.65A from mech1str8S2

-1  1
 C                 -0.384972   -0.457912   -2.206216
 C                 -0.340283    1.042067   -1.809950
 C                  0.886244    1.255289   -0.864965
 C                  0.443991   -1.107184   -1.073894
 C                  1.549392   -0.119096   -0.652103
 C                 -1.301500    1.110144   -0.559316
 C                 -1.777969   -0.352824   -0.396529
 C                 -0.517124   -1.034070    0.170459
 C                  0.216923   -0.019004    1.084904
 C                 -0.071666    1.325402    0.370338
 C                 -1.834259   -0.859830   -1.854865
 O                  2.840640   -0.314264   -1.227268
 C                 -0.076279   -0.087411    2.553956
 N                  0.502447   -0.335314    3.583153
 O                  1.634382   -0.258939    0.769047
 H                 -0.051660   -0.682356   -3.213579
 H                 -0.501147    1.741658   -2.619065
 H                  1.577792    2.064343   -1.043082
 H                  0.823961   -2.098175   -1.280748
 H                 -2.083688    1.854443   -0.554876
 H                 -2.656772   -0.475145    0.212642
 H                 -0.685106   -1.985602    0.651143
 H                 -0.036681    2.187632    1.012765
 H                 -2.004436   -1.930221   -1.926078
 H                 -2.572581   -0.336729   -2.457384
 H                  2.811933   -0.258637   -2.190988
 O                 -1.600311    0.297659    2.500111
 H                 -1.891420    0.296913    3.421134

 1  2 1.0  4 1.0  11 1.0  16 1.0
 2  3 1.0  6 1.0  17 1.0
 3  5 1.0  10 1.0  18 1.0
 4  5 1.0  8 1.0  19 1.0
 5  12 1.0  15 1.0
 6  7 1.0  10 1.0  20 1.0
 7  8 1.0  11 1.0  21 1.0
 8  9 1.0  22 1.0
 9  10 1.0  13 1.0  15 1.0
 10  23 1.0
 11  24 1.0  25 1.0
 12  26 1.0
 13  14 2.0
 14
 15
 16
 17
 18
 19
```

```
20
21
22
23
24
25
26
27  28 1.0
28
```

Entering Link 1 = C:\G98W\l1.exe PID=   121.

Gaussian, Inc. access to this program. By using this program,
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Cite this work as:
Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

****
Gaussian 98: x86-Win32-G98RevA.7 11-Apr-1999
23-Apr-2002
****
%chk=mech1st8tsF
Default route: MaxDisk=2000MB

#N RHF/3-21+G* FREQ

1/10=4,30=1,38=1/1,3;
2/17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11,27=262144000/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Freq calc of output str of mech1st8ts

Symbolic Z-matrix:
Charge = -1 Multiplicity = 1
C -0.38497 -0.45791 -2.20622

C	-0.34028	1.04207	-1.80995
C	0.88624	1.25529	-0.86497
C	0.44399	-1.10718	-1.07389
C	1.54939	-0.1191	-0.6521
C	-1.3015	1.11014	-0.55932
C	-1.77797	-0.35282	-0.39653
C	-0.51712	-1.03407	0.17046
C	0.21692	-0.019	1.0849
C	-0.07167	1.3254	0.37034
C	-1.83426	-0.85983	-1.85487
O	2.84064	-0.31426	-1.22727
C	-0.07628	-0.08741	2.55396
N	0.50245	-0.33531	3.58315
O	1.63438	-0.25894	0.76905
H	-0.05166	-0.68236	-3.21358
H	-0.50115	1.74166	-2.61907
H	1.57779	2.06434	-1.04308
H	0.82396	-2.09817	-1.28075
H	-2.08369	1.85444	-0.55488
H	-2.65677	-0.47514	0.21264
H	-0.68511	-1.9856	0.65114
H	-0.03668	2.18763	1.01276
H	-2.00444	-1.93022	-1.92608
H	-2.57258	-0.33673	-2.45738
H	2.81193	-0.25864	-2.19099
O	-1.60031	0.29766	2.50011
H	-1.89142	0.29691	3.42113

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 94 maximum allowed number of steps= 168.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

---

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C	0	-0.384972		-0.457912		-2.206216	
2	2	C	0	-0.340283		1.042067		-1.809950	
3	3	C	0	0.886244		1.255289		-0.864965	
4	4	C	0	0.443991		-1.107184		-1.073894	
5	5	C	0	1.549392		-0.119096		-0.652103	
6	6	C	0	-1.301500		1.110144		-0.559316	
7	7	C	0	-1.777969		-0.352824		-0.396529	
8	8	C	0	-0.517124		-1.034070		0.170459	
9	9	C	0	0.216923		-0.019004		1.084904	
10	10	C	0	-0.071666		1.325402		0.370338	
11	11	C	0	-1.834259		-0.859830		-1.854865	
12	12	O	0	2.840640		-0.314264		-1.227268	
13	13	C	0	-0.076279		-0.087411		2.553956	
14	14	N	0	0.502447		-0.335314		3.583153	
15	15	O	0	1.634382		-0.258939		0.769047	

16	16	H	0	-0.051660	-0.682356	-3.213579
17	17	H	0	-0.501147	1.741658	-2.619065
18	18	H	0	1.577792	2.064343	-1.043082
19	19	H	0	0.823961	-2.098175	-1.280748
20	20	H	0	-2.083688	1.854443	-0.554876
21	21	H	0	-2.656772	-0.475145	0.212642
22	22	H	0	-0.685106	-1.985602	0.651143
23	23	H	0	-0.036681	2.187632	1.012765
24	24	H	0	-2.004436	-1.930221	-1.926078
25	25	H	0	-2.572581	-0.336729	-2.457384
26	26	H	0	2.811933	-0.258637	-2.190988
27	27	O	0	-1.600311	0.297659	2.500111
28	28	H	0	-1.891420	0.296913	3.421134

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.384972	-0.457912	-2.206216
2	6	0	-0.340283	1.042067	-1.809950
3	6	0	0.886244	1.255289	-0.864965
4	6	0	0.443991	-1.107184	-1.073894
5	6	0	1.549392	-0.119096	-0.652103
6	6	0	-1.301500	1.110144	-0.559316
7	6	0	-1.777969	-0.352824	-0.396529
8	6	0	-0.517124	-1.034070	0.170459
9	6	0	0.216923	-0.019004	1.084904
10	6	0	-0.071666	1.325402	0.370338
11	6	0	-1.834259	-0.859830	-1.854865
12	8	0	2.840640	-0.314264	-1.227268
13	6	0	-0.076279	-0.087411	2.553956
14	7	0	0.502447	-0.335314	3.583153
15	8	0	1.634382	-0.258939	0.769047
16	1	0	-0.051660	-0.682356	-3.213579
17	1	0	-0.501147	1.741658	-2.619065
18	1	0	1.577792	2.064343	-1.043082
19	1	0	0.823961	-2.098175	-1.280748
20	1	0	-2.083688	1.854443	-0.554876
21	1	0	-2.656772	-0.475145	0.212642
22	1	0	-0.685106	-1.985602	0.651143
23	1	0	-0.036681	2.187632	1.012765
24	1	0	-2.004436	-1.930221	-1.926078
25	1	0	-2.572581	-0.336729	-2.457384
26	1	0	2.811933	-0.258637	-2.190988
27	8	0	-1.600311	0.297659	2.500111
28	1	0	-1.891420	0.296913	3.421134

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.552083	0.000000			
3	C	2.519921	1.562955	0.000000		
4	C	1.546249	2.403361	2.412575	0.000000	

5	C	2.504362	2.501955	1.540782	1.541472	0.000000
6	C	2.451755	1.578815	2.213755	2.868462	3.105998
7	C	2.286143	2.451616	3.146981	2.442333	3.345337
8	C	2.449083	2.874654	2.877970	1.574008	2.405052
9	C	3.374372	3.133134	2.423593	2.428190	2.191503
10	C	3.149127	2.214969	1.564762	2.875619	2.399956
11	C	1.544480	2.418924	3.585355	2.421058	3.666663
12	O	3.373951	3.506768	2.532671	2.529065	1.426964
13	C	4.784538	4.515428	3.797146	3.804197	3.594805
14	N	5.858271	5.629648	4.739522	4.720941	4.368093
15	O	3.601329	3.499020	2.350020	2.352229	1.430541
16	H	1.084552	2.242122	3.185925	2.237052	3.072749
17	H	2.240993	1.081652	2.288728	3.375906	3.396477
18	H	3.401043	2.304809	1.079135	3.368240	2.218350
19	H	2.237962	3.390669	3.379715	1.081309	2.199590
20	H	3.310520	2.296656	3.045593	3.928075	4.135647
21	H	3.318470	3.429130	4.087616	3.416047	4.308871
22	H	3.253985	3.916971	3.907825	2.241033	3.189871
23	H	4.181154	3.061407	2.290617	3.929504	3.257055
24	H	2.206544	3.408429	4.430515	2.720000	4.187228
25	H	2.205313	2.702481	4.127201	3.406956	4.505226
26	H	3.203146	3.431251	2.785424	2.752286	1.995407
27	O	4.919090	4.551751	4.292289	4.350433	4.475574
28	H	5.874199	5.506861	5.196590	5.256511	5.348225

		6	7	8	9	10
6	C	0.000000				
7	C	1.547190	0.000000			
8	C	2.396971	1.541201	0.000000		
9	C	2.506799	2.507125	1.550933	0.000000	
10	C	1.556626	2.513165	2.409459	1.549618	0.000000
11	C	2.417246	1.544981	2.422218	3.681926	3.582388
12	O	4.430849	4.692884	3.707606	3.509588	3.704373
13	C	3.553557	3.416366	2.602223	1.499587	2.600817
14	N	4.743798	4.586771	3.629637	2.534329	3.661934
15	O	3.501191	3.607149	2.363919	1.471912	2.362140
16	H	3.438062	3.320317	3.433959	4.357652	4.108035
17	H	2.298247	3.310105	3.935272	4.163525	3.048648
18	H	3.071620	4.185912	3.932114	3.274236	2.294450
19	H	3.915528	3.255477	2.244288	3.207453	3.905011
20	H	1.079731	2.233957	3.365077	3.389910	2.276870
21	H	2.223921	1.076265	2.211848	3.037602	3.154300
22	H	3.380650	2.226641	1.079207	2.206652	3.379039
23	H	2.287397	3.387050	3.364472	2.222332	1.075815
24	H	3.406755	2.208843	2.722251	4.201571	4.428116
25	H	2.704025	2.208798	3.408335	4.519965	4.124714
26	H	4.632089	4.929113	4.154558	4.186045	4.169498
27	O	3.179546	2.974090	2.893799	2.324957	2.815838
28	H	4.105281	3.874220	3.771882	3.162734	3.698196

		11	12	13	14	15
11	C	0.000000				
12	O	4.748284	0.000000			
13	C	4.808828	4.780955	0.000000		
14	N	5.941999	5.348620	1.206493	0.000000	
15	O	4.390610	2.333108	2.478242	3.034189	0.000000

16	H	2.248391	3.527935	5.798192	6.828107	4.345495
17	H	3.021412	4.163106	5.503286	6.617290	4.476849
18	H	4.566385	2.699348	4.506071	5.321350	2.946974
19	H	2.988184	2.692990	4.422506	5.183491	2.870754
20	H	3.019845	5.422583	4.179154	5.348496	4.476963
21	H	2.258118	5.685135	3.505857	4.621749	4.332474
22	H	2.977917	4.330437	2.755811	3.567971	2.894010
23	H	4.554296	4.422240	2.748210	3.641814	2.972803
24	H	1.086171	5.155038	5.213870	6.259378	4.826788
25	H	1.087099	5.551275	5.604214	6.778192	5.302306
26	H	4.696968	0.965751	5.557480	6.219350	3.185661
27	O	4.512242	5.830081	1.572848	2.448515	3.710744
28	H	5.401619	6.661349	2.048033	2.481242	4.446776

		16	17	18	19	20
16	H	0.000000				
17	H	2.536007	0.000000			
18	H	3.861415	2.628657	0.000000		
19	H	2.550900	4.276835	4.236898	0.000000	
20	H	4.199189	2.603466	3.699843	4.960293	0.000000
21	H	4.309122	4.192791	5.094838	4.120673	2.518827
22	H	4.127442	4.961912	4.938943	2.454009	4.261040
23	H	5.108722	3.688470	2.616912	4.936502	2.599760
24	H	2.651068	4.027754	5.437700	2.905940	4.026184
25	H	2.654493	2.938822	4.999099	4.002957	2.942752
26	H	3.070081	3.893704	2.870022	2.857354	5.577551
27	O	6.000417	5.431322	5.076980	5.090384	3.462683
28	H	6.954358	6.364287	5.923552	5.934428	4.274520

		21	22	23	24	25
21	H	0.000000				
22	H	2.522148	0.000000			
23	H	3.820400	4.238762	0.000000		
24	H	2.667754	2.895819	5.428220	0.000000	
25	H	2.674937	3.993029	4.984488	1.773215	0.000000
26	H	5.977545	4.825909	4.935876	5.105074	5.391665
27	O	2.635498	3.077266	2.868647	4.971712	5.091612
28	H	3.387663	3.786544	3.579821	5.793580	5.951677

		26	27	28
26	H	0.000000		
27	O	6.464037	0.000000	
28	H	7.343438	0.965934	0.000000

Interatomic angles:

C1-C2-C3=107.9871	C2-C1-C4=101.736	C1-C4-C3= 75.5528
C3-C2-C4= 71.3822	C1-C2-C5= 72.0237	C1-C5-C3= 72.6931
C2-C3-C5=107.4331	C1-C4-C5=108.4013	C2-C4-C5= 75.2017
C3-C5-C4=103.0225	C1-C2-C6=103.0842	C1-C6-C3= 65.1501
C3-C2-C6= 89.5963	C4-C1-C6= 88.6856	C4-C2-C6= 89.6925
C4-C3-C6= 76.5024	C5-C1-C6= 77.6061	C5-C2-C6= 96.5033
C5-C3-C6=110.3517	C5-C4-C6= 83.7875	C2-C1-C7= 76.7628
C3-C1-C7= 81.6512	C3-C2-C7=100.9084	C4-C1-C7= 76.484
C2-C4-C7= 60.7808	C3-C4-C7= 80.8105	C5-C1-C7= 88.4637
C5-C2-C7= 84.9544	C5-C4-C7=112.2425	C1-C7-C6= 76.852
C2-C6-C7=103.3008	C3-C6-C7=112.3871	C4-C7-C6= 89.009
C2-C1-C8= 88.9197	C3-C1-C8= 70.77	C3-C2-C8= 74.3519
C1-C4-C8=103.4188	C2-C4-C8= 90.0757	C3-C4-C8= 89.8845

C1-C8-C5= 62.1106 C2-C5-C8= 71.6919 C3-C5-C8= 90.962
C5-C4-C8=101.0568 C1-C8-C6= 60.7747 C2-C6-C8= 90.1931
C3-C6-C8= 77.1321 C4-C8-C6= 90.0387 C5-C8-C6= 80.6029
C1-C7-C8= 76.8451 C2-C7-C8= 89.0743 C3-C8-C7= 85.1209
C4-C8-C7=103.252 C5-C8-C7=114.139 C6-C7-C8=101.8137
C1-C3-C9= 86.0688 C2-C3-C9=101.419 C1-C4-C9=114.3776
C2-C4-C9= 80.8515 C4-C3-C9= 60.2762 C1-C5-C9= 91.6281
C2-C5-C9= 83.4761 C3-C5-C9= 78.8763 C4-C5-C9= 79.0556
C1-C6-C9= 85.7603 C2-C6-C9= 97.5485 C6-C3-C9= 65.2615
C4-C9-C6= 71.0566 C5-C9-C6= 82.4718 C1-C7-C9= 89.3715
C2-C7-C9= 78.3633 C3-C9-C7= 79.3016 C7-C4-C9= 61.9613
C5-C9-C7= 90.5366 C7-C6-C9= 72.0379 C1-C8-C9=113.1206
C2-C8-C9= 84.5138 C3-C9-C8= 90.0268 C4-C8-C9=101.9773
C5-C9-C8= 77.9097 C6-C8-C9= 75.4584 C7-C8-C9=108.3493
C1-C2-C10=112.2365 C1-C3-C10= 98.1539 C2-C3-C10= 90.1731
C1-C4-C10= 85.2069 C4-C2-C10= 76.9003 C4-C3-C10= 90.0014
C1-C5-C10= 79.8681 C2-C10-C5= 65.5165 C5-C3-C10=101.2087
C4-C5-C10= 91.032 C1-C6-C10=101.2018 C2-C6-C10= 89.8875
C3-C10-C6= 90.3428 C4-C6-C10= 74.5302 C5-C10-C6=101.3024
C1-C7-C10= 81.8679 C7-C2-C10= 64.9379 C3-C10-C7= 98.3269
C4-C7-C10= 70.9253 C5-C10-C7= 85.7951 C7-C6-C10=108.1332
C1-C8-C10= 80.802 C2-C10-C8= 76.7416 C3-C10-C8= 90.2183
C4-C8-C10= 89.8957 C8-C5-C10= 60.1915 C8-C6-C10= 71.5387
C7-C8-C10= 75.4582 C2-C10-C9=111.439 C3-C10-C9=102.19
C4-C9-C10= 89.785 C5-C9-C10= 77.7232 C6-C10-C9=107.6113
C7-C9-C10= 72.2334 C8-C9-C10=101.9928 C2-C1-C11=102.7343
C3-C1-C11=121.9522 C3-C2-C11=127.097 C4-C1-C11=103.1328
C4-C2-C11= 60.2712 C3-C4-C11= 95.7615 C5-C1-C11=128.2306
C5-C2-C11= 96.3248 C5-C4-C11=134.2335 C1-C11-C6= 72.7244
C2-C6-C11= 71.0035 C3-C6-C11=101.3758 C4-C11-C6= 72.7211
C1-C11-C7= 95.4596 C2-C11-C7= 72.6595 C4-C11-C7= 72.2273
C6-C7-C11=102.8386 C1-C11-C8= 72.4628 C2-C11-C8= 72.8538
C3-C8-C11= 84.6701 C8-C4-C11= 71.0751 C5-C8-C11= 98.8525
C8-C6-C11= 60.414 C8-C7-C11=103.4152 C9-C4-C11= 98.801
C9-C6-C11= 96.7739 C9-C7-C11=129.0823 C9-C8-C11=134.691
C10-C2-C11=101.172 C10-C4-C11= 84.6544 C10-C6-C11=127.3668
C10-C7-C11=122.1341 C10-C8-C11= 95.7077 C1-C3-O12= 83.7894
C2-C3-O12=115.7557 C1-C4-O12=109.3892 C2-C4-O12= 90.5897
C3-C4-O12= 61.6098 C1-C5-O12=115.4868 C2-C5-O12=124.0828
C3-C5-O12=117.115 C4-C5-O12=116.8042 C6-C3-O12=137.8786
C6-C4-O12=110.1925 C7-C4-O12=141.4549 C8-C3-O12= 86.2604
C8-C4-O12=127.7361 C8-C5-O12=149.6938 C9-C3-O12= 90.1353
C9-C4-O12= 90.1163 C9-C5-O12=151.1531 C10-C3-O12=127.814
C10-C4-O12= 86.2829 C10-C5-O12=149.9113 C11-C4-O12=147.156
C1-C8-C13=142.5743 C2-C8-C13=110.9686 C3-C8-C13= 87.5666
C4-C8-C13=129.6106 C5-C8-C13= 91.6792 C6-C8-C13= 90.5086
C7-C8-C13=108.3461 C3-C9-C13=150.0127 C4-C9-C13=150.3188
C5-C9-C13=153.2868 C6-C9-C13=123.0017 C7-C9-C13=114.6585
C8-C9-C13=117.0784 C2-C10-C13=139.1777 C3-C10-C13=129.759
C4-C10-C13= 87.8486 C5-C10-C13= 91.8297 C6-C10-C13=115.1445
C7-C10-C13= 83.8138 C8-C10-C13= 62.4432 C10-C9-C13=117.0584
C11-C8-C13=146.2857 C3-C9-N14=145.8522 C4-C9-N14=144.0892
C5-C9-N14=135.0015 C6-C9-N14=140.4462 C7-C9-N14=130.9578
C8-C9-N14=123.5629 C10-C9-N14=125.7198 C8-C13-N14=141.9859

C9-C13-N14=138.7 C10-C13-N14=145.7894 C1-C3-O15= 95.3144
C2-C3-O15=125.6142 C1-C4-O15=133.9187 C2-C4-O15= 94.7385
C3-O15-C4= 61.7368 C1-C5-O15=130.4777 C2-C5-O15=123.3656
C3-C5-O15=104.4783 C4-C5-O15=104.5826 C6-C3-O15=100.1581
C6-C4-O15= 83.6064 C7-C4-O15= 97.5695 C1-C8-O15= 96.8621
C2-C8-O15= 83.2026 C3-O15-C8= 75.2541 C8-C4-O15= 70.9052
C5-O15-C8= 74.1229 C6-C8-O15= 94.6807 C7-C8-O15=133.852
C3-O15-C9= 74.7873 C4-O15-C9= 74.9041 C5-O15-C9= 98.0497
C6-C9-O15=121.0635 C7-C9-O15=128.152 C8-C9-O15=102.8602
C2-C10-O15= 99.6681 C10-C3-O15= 71.0248 C4-O15-C10= 75.1742
C5-O15-C10= 73.9689 C6-C10-O15=125.3575 C7-C10-O15= 95.3926
C8-O15-C10= 61.3042 C10-C9-O15=102.8155 C11-C4-O15=133.7972
C11-C8-O15=133.0825 C3-O15-O12= 65.4761 C4-O15-O12= 65.3363
O12-C5-O15=109.4687 C8-O15-O12=104.248 C9-O15-O12=133.2646
C10-O15-O12=104.1755 C3-O15-C13=103.6767 C4-O15-C13=103.8822
C5-O15-C13=131.892 C8-O15-C13= 64.9648 C13-C9-O15=113.0213
C10-O15-C13= 64.9505 O12-O15-C13=167.1068 N14-C9-O15= 94.7435
N14-C13-O15=105.6086 C2-C1-H16=115.3592 C3-C1-H16=118.6878
C3-C2-H16=112.483 C4-C1-H16=115.374 C2-H16-C4= 64.8999
C3-C4-H16= 86.4158 C5-C1-H16=111.5317 C5-C2-H16= 80.5343
C5-C4-H16=107.39 C6-C1-H16=150.5935 C6-C2-H16=127.4041
C6-C4-H16= 83.6825 C7-C1-H16=158.7527 C7-C2-H16= 89.9321
C7-C4-H16= 90.289 C8-C1-H16=150.3735 C8-C2-H16= 83.3237
C8-C4-H16=127.7373 C9-C4-H16=138.1193 C10-C2-H16=134.3465
C10-C4-H16=106.2599 C11-C1-H16=116.4764 C2-H16-C11= 65.1867
C4-H16-C11= 65.3339 C6-C11-H16= 94.8654 C7-C11-H16=121.0393
C8-C11-H16= 94.5796 O12-C4-H16= 95.3028 O15-C4-H16=142.4696
C1-C2-H17=115.455 C1-H17-C3= 67.5922 C3-C2-H17=118.7342
C4-C1-H17=125.0885 C4-C2-H17=148.8727 C4-C3-H17= 91.7536
C5-C1-H17= 91.2363 C5-C2-H17=139.3472 C5-C3-H17=123.8029
C1-H17-C6= 65.37 C6-C2-H17=118.3016 C6-C3-H17= 61.3595
C4-C6-H17= 80.7768 C7-C1-H17= 93.9638 C7-C2-H17=135.4016
C7-C6-H17=117.4751 C8-C1-H17=114.0095 C8-C2-H17=166.7319
C8-C3-H17= 98.5799 C8-C6-H17=113.8729 C9-C3-H17=124.1199
C9-C6-H17=120.0443 C10-C2-H17=132.1926 C10-C3-H17=102.9693
C10-C6-H17=102.8332 C11-C1-H17=104.3995 C11-C2-H17=113.7529
C11-C6-H17= 79.6505 O12-C3-H17=119.3298 O15-C3-H17=149.6332
H16-C1-H17= 92.7477 H16-C2-H17= 92.7681 C3-H17-H16= 82.4787
C4-H16-H17= 89.8031 C6-H17-H16= 90.5259 C11-H16-H17= 78.0685
C1-C2-H18=122.5178 C1-C3-H18=138.1709 C2-C3-H18=120.3565
C4-C2-H18= 91.328 C4-C3-H18=146.8596 C1-C5-H18= 91.9299
C2-H18-C5= 67.1343 C5-C3-H18=114.5664 C4-C5-H18=126.2898
C6-C2-H18=102.9427 C6-C3-H18=134.8498 C7-C2-H18=123.2683
C8-C2-H18= 98.1814 C8-C3-H18=165.5254 C8-C5-H18=116.4701
C9-C3-H18=134.7462 C9-C5-H18= 95.8846 C2-C10-H18= 61.4456
C10-C3-H18=119.2758 C4-C10-H18= 80.4529 C5-H18-C10= 64.2298
C6-C10-H18=104.1585 C7-C10-H18=121.0093 C8-C10-H18=113.402
C9-C10-H18=115.4413 C11-C2-H18=150.3313 C2-H18-O12= 88.6129
O12-C3-H18= 86.9328 C4-O12-H18= 80.1419 O12-C5-H18= 92.9804
C10-H18-O12= 95.4263 C13-C10-H18=133.9017 C2-H18-O15= 82.5828
O15-C3-H18=113.1934 C4-O15-H18= 78.0417 O15-C5-H18=105.6968
C8-O15-H18= 94.8944 C9-O15-H18= 89.1377 O15-C10-H18= 78.5082
O15-O12-H18= 71.267 C13-O15-H18=112.0279 H16-C2-H18=116.2504
C1-H17-H18= 88.2257 H17-C2-H18= 94.9211 H17-C3-H18= 95.8914

C5-H18-H17= 88.5513 C6-H17-H18= 76.8104 C10-H18-H17= 76.1866
O12-H18-H17=102.763 O15-H18-H17=106.6829 H16-H17-H18= 96.7599
C2-C1-H19=125.9578 C3-C1-H19= 90.3251 C1-C4-H19=115.6662
C2-C4-H19=151.1227 C3-C4-H19=148.1674 C1-H19-C5= 68.709
C2-C5-H19= 92.0757 C3-C5-H19=128.4002 C5-C4-H19=112.8187
C6-C1-H19=113.1359 C6-C4-H19=163.0547 C7-C1-H19= 92.0342
C7-C4-H19=130.9816 C1-H19-C8= 66.24 C2-C8-H19= 81.9638
C3-C8-H19= 81.5553 C8-C4-H19=114.1028 C5-H19-C8= 65.5225
C6-C8-H19=115.0124 C7-C8-H19=117.4227 C9-C4-H19=127.8538
C9-C5-H19= 93.8473 C9-C8-H19=114.1266 C10-C4-H19=159.1261
C10-C5-H19=116.1382 C10-C8-H19=114.0459 C11-C1-H19=102.8322
C2-C11-H19= 76.8705 C11-C4-H19=111.2597 C5-H19-C11= 88.5919
C6-C11-H19= 92.2178 C7-C11-H19= 85.5396 C11-C8-H19= 79.5353
C1-H19-O12= 85.827 C3-O12-H19= 80.5309 O12-C4-H19= 86.7171
O12-C5-H19= 93.45 C8-H19-O12= 96.9245 C11-H19-O12=113.2951
C13-C8-H19=131.5693 C1-H19-O15= 88.7508 C3-O15-H19= 80.007
O15-C4-H19=107.6103 O15-C5-H19=102.4486 O15-C8-H19= 77.0175
C9-O15-H19= 89.1864 C10-O15-H19= 96.0448 C11-H19-O15= 97.0542
O15-O12-H19= 69.2387 C13-O15-H19=111.3302 H16-C1-H19= 93.8077
C2-H16-H19= 89.8118 H16-C4-H19= 93.9524 C5-H19-H16= 80.234
C8-H19-H16= 91.2419 C11-H16-H19= 76.7295 O12-H19-H16= 84.5162
O15-H19-H16=106.3993 H17-C1-H19=145.4435 H17-H16-H19=114.4393
H18-C5-H19=147.081 H18-O12-H19=103.5756 H18-O15-H19= 93.4745
C1-C2-H20=117.3557 C3-C2-H20=102.5354 C4-C2-H20=113.3702
C5-C2-H20=118.9864 C1-C6-H20=135.598 C2-C6-H20=118.2961
C3-C6-H20=132.1666 C4-C6-H20=167.0128 C1-C7-H20= 94.1688
C2-H20-C7= 65.5031 C4-C7-H20=114.2063 C7-C6-H20=115.3589
C8-C2-H20= 80.3451 C8-C6-H20=148.4797 C8-C7-H20=125.0839
C9-C6-H20=138.2972 C9-C7-H20= 91.1011 C2-C10-H20= 61.482
C3-C10-H20=103.3313 C4-C10-H20= 98.6811 C5-C10-H20=124.3064
C10-C6-H20=118.331 C7-H20-C10= 67.7088 C8-C10-H20= 91.745
C9-C10-H20=123.6098 C11-C2-H20= 79.5967 C11-C6-H20=113.849
C11-C7-H20=104.6166 C13-C10-H20=117.7634 O15-C10-H20=149.6176
H16-C2-H20=135.3878 C1-H17-H20= 85.8692 H17-C2-H20= 93.8481
C3-H17-H20= 76.7044 H17-C6-H20= 93.8157 C7-H20-H17= 85.9981
C10-H20-H17= 76.995 H16-H17-H20=109.5735 H18-C2-H20=107.0386
H18-C10-H20=108.0663 H18-H17-H20= 90.0041 C1-C6-H21= 90.2907
C2-C6-H21=127.9698 C3-C6-H21=134.1795 C4-C6-H21= 83.2278
C1-C7-H21=160.1102 C2-C7-H21=150.4371 C4-C7-H21=149.8517
C6-C7-H21=114.7384 C1-C8-H21= 90.6451 C2-C8-H21= 83.6931
C3-C8-H21=106.1143 C4-C8-H21=128.1338 C5-C8-H21=137.8662
C6-H21-C8= 65.4175 C8-C7-H21=114.1756 C9-C6-H21= 79.6518
C9-C7-H21=109.2925 C9-C8-H21=106.3326 C10-C6-H21=111.8846
C10-C7-H21=117.23 C10-C8-H21= 85.975 C1-C11-H21=120.3812
C2-C11-H21= 94.245 C4-C11-H21= 93.7166 C6-H21-C11= 65.2693
C11-C7-H21=117.8537 C8-H21-C11= 65.6149 C13-C8-H21= 93.1233
O15-C8-H21=142.4429 H16-C11-H21=145.9588 H17-C6-H21=135.9877
H19-C8-H21=135.2507 H19-C11-H21=102.6334 C2-H20-H21= 90.6924
H20-C6-H21= 92.7791 H20-C7-H21= 92.331 C8-H21-H20= 90.4473
C10-H20-H21= 82.0873 C11-H21-H20= 78.2111 H17-H20-H21=109.8664
C1-C4-H22=117.2691 C2-C4-H22=114.9521 C3-C4-H22=114.1751
C5-C4-H22=113.6987 C6-C4-H22= 81.855 C1-C7-H22= 92.2744
C2-C7-H22=113.6195 C4-H22-C7= 66.2765 C6-C7-H22=126.2799
C1-C8-H22=130.3954 C2-C8-H22=162.4024 C3-C8-H22=159.6383

C4-C8-H22=113.9669 C5-C8-H22=128.4264 C6-C8-H22=150.8554
C7-C8-H22=115.2298 C3-C9-H22=115.0451 C4-H22-C9= 66.1732
C5-C9-H22= 92.9828 C6-C9-H22= 91.4266 C7-H22-C9= 68.8754
C9-C8-H22=112.8371 C10-C4-H22= 81.6419 C10-C7-H22= 90.7371
C10-C8-H22=148.7853 C10-C9-H22=127.3312 C1-C11-H22= 85.8543
C2-C11-H22= 92.4804 C11-C4-H22= 79.2945 C6-C11-H22= 76.8214
C11-C7-H22=102.7896 C11-C8-H22=110.5611 C9-H22-C11= 89.2121
O12-C4-H22=130.3175 C4-H22-C13= 98.6383 C7-H22-C13= 85.884
C13-C8-H22= 86.5116 C13-C9-H22= 94.1282 C10-C13-H22= 78.1614
C11-H22-C13=113.9485 N14-C9-H22= 97.3883 N14-C13-H22=123.604
C3-O15-H22= 95.7943 O15-C4-H22= 78.067 C5-O15-H22= 88.2943
C7-H22-O15= 88.5697 O15-C8-H22=108.5415 O15-C9-H22=101.8996
C10-O15-H22= 79.3058 C11-H22-O15= 96.7777 O12-O15-H22=111.4304
O15-C13-H22= 66.8913 H16-C4-H22=134.3512 H16-C11-H22=103.4404
H18-O15-H22=115.4625 C1-H19-H22= 87.6926 H19-C4-H22= 87.9981
C5-H19-H22= 86.3616 C7-H22-H19= 87.9971 H19-C8-H22= 87.8781
C9-H22-H19= 86.8045 C11-H22-H19= 65.9306 O12-H19-H22=114.4868
C13-H22-H19=116.0598 O15-H19-H22= 65.2979 H16-H19-H22=111.0972
H20-C7-H22=145.5936 C4-H22-H21= 91.4493 C6-H21-H22= 90.6218
H21-C7-H22= 92.9295 H21-C8-H22= 93.6542 C9-H22-H21= 79.6306
C11-H21-H22= 76.8451 C13-H22-H21= 83.1222 O15-H22-H21=106.0408
H19-H22-H21=111.7974 H20-H21-H22=115.4041 C1-C3-H23=120.6494
C2-C3-H23=103.59 C4-C3-H23=113.31 C5-C3-H23=115.0389
C1-C6-H23=123.795 C2-C6-H23=103.1841 C3-C6-H23= 61.1546
C4-C6-H23= 98.6815 C7-C6-H23=122.9144 C8-C3-H23= 80.3507
C8-C6-H23= 91.7873 C3-H23-C9= 64.9429 C4-C9-H23=115.2641
C5-C9-H23= 95.1064 C6-H23-C9= 67.5227 C7-C9-H23= 91.2736
C8-C9-H23=125.2198 C2-C10-H23=133.9691 C3-C10-H23=119.1717
C4-C10-H23=166.4262 C5-C10-H23=135.6291 C6-C10-H23=119.5484
C7-C10-H23=137.6883 C8-C10-H23=147.1813 C9-C10-H23=114.4509
C11-C6-H23=150.9408 O12-C3-H23=132.8772 C3-H23-C13= 97.387
C6-H23-C13= 89.2841 C8-C13-H23= 77.8738 C13-C9-H23= 93.1404
C13-C10-H23= 86.2195 N14-C9-H23= 99.7171 N14-C13-H23=129.9092
O15-C3-H23= 79.6623 C4-O15-H23= 94.3898 C5-O15-H23= 88.1431
C6-H23-O15= 82.3459 C8-O15-H23= 77.2328 O15-C9-H23=105.3543
O15-C10-H23=114.4111 O12-O15-H23=112.3515 O15-C13-H23= 69.1113
H17-C3-H23=107.309 H17-C6-H23=107.0951 C2-H18-H23= 76.6362
H18-C3-H23= 95.0686 C5-H18-H23= 84.2616 C6-H23-H18= 77.2332
C9-H23-H18= 84.7397 H18-C10-H23= 94.9543 O12-H18-H23=112.5658
C13-H23-H18=114.2332 O15-H18-H23= 64.2728 H17-H18-H23= 89.3617
H19-O15-H23=115.285 C2-H20-H23= 77.1235 C3-H23-H20= 76.7488
H20-C6-H23= 94.1882 C7-H20-H23= 88.6325 C9-H23-H20= 88.9784
H20-C10-H23= 94.8857 C13-H23-H20=102.7512 O15-H23-H20=106.7198
H17-H20-H23= 90.2879 H18-H23-H20= 90.3447 H21-C6-H23=115.7338
H21-H20-H23= 96.5424 H22-C9-H23=146.2934 H22-C13-H23=100.7294
H22-O15-H23= 92.5124 C2-C1-H24=129.3137 C3-C1-H24=139.1398
C4-C1-H24= 91.1645 C2-C4-H24= 83.1598 C3-C4-H24=119.2384
C5-C1-H24=125.3366 C5-C4-H24=157.6981 C6-C1-H24= 93.8476
C6-C4-H24= 75.0693 C1-H24-C7= 62.3652 C2-C7-H24= 93.8541
C4-C7-H24= 71.3766 C6-C7-H24=129.3437 C8-C1-H24= 71.3504
C2-C8-H24= 74.9768 C3-C8-H24=104.5486 C8-C4-H24= 73.2672
C5-C8-H24=109.3468 C6-C8-H24= 83.1782 C8-C7-H24= 91.3159
C9-C4-H24=109.267 C9-C7-H24=125.8621 C9-C8-H24=158.1446
C10-C4-H24=104.5902 C10-C7-H24=139.2694 C10-C8-H24=119.1608

C1-C11-H24=112.8645 C2-C11-H24=150.7878 C4-C11-H24= 93.8934
C6-C11-H24=150.7853 C7-C11-H24=113.0161 C8-C11-H24= 93.9639
O12-C4-H24=158.2631 C13-C8-H24=156.5965 O15-C4-H24=144.1084
O15-C8-H24=143.1511 H16-C1-H24=101.8527 C2-H16-H24= 87.8891
C4-H16-H24= 67.0019 C7-H24-H16= 85.6778 C8-H24-H16= 79.4338
H16-C11-H24= 99.3453 H17-C1-H24=129.8108 H17-H16-H24=101.8593
H19-C1-H24= 81.6583 H19-C4-H24= 88.8005 C5-H19-H24=109.4187
C7-H24-H19= 77.7431 H19-C8-H24= 70.8766 C11-H24-H19= 83.679
O12-H19-H24=134.0275 O15-H19-H24=113.3474 H19-H16-H24= 67.8897
H20-C7-H24=129.9771 C1-H24-H21= 85.2569 C4-H24-H21= 78.6909
C6-H21-H24= 87.7939 H21-C7-H24=103.124 C8-H21-H24= 67.0665
H21-C11-H24= 99.8368 H16-H24-H21=108.2237 H19-H24-H21= 95.2494
H20-H21-H24=101.8021 C1-H24-H22= 77.9579 H22-C4-H24= 70.6727
H22-C7-H24= 81.5164 H22-C8-H24= 88.1511 C9-H22-H24=110.1291
C11-H24-H22= 83.6337 C13-H22-H24=134.5867 O15-H22-H24=112.9545
H16-H24-H22= 96.0635 H19-H22-H24= 65.1917 H22-H21-H24= 67.7642
C2-C1-H25= 90.2598 C3-C1-H25=121.5793 C3-C2-H25=149.6173
C4-C1-H25=129.6641 C4-C2-H25= 83.4926 C5-C1-H25=146.0413
C5-C2-H25=119.865 C6-C1-H25= 70.7637 C6-C2-H25= 73.0746
C3-C6-H25=113.7479 C4-C6-H25= 75.3154 C1-H25-C7= 62.3852
C2-C7-H25= 70.6649 C4-C7-H25= 94.0583 C6-C7-H25= 90.3283
C8-C1-H25= 94.0097 C8-C2-H25= 75.2712 C8-C6-H25= 83.62
C8-C7-H25=129.8496 C9-C6-H25=120.2729 C9-C7-H25=146.7817
C10-C2-H25=113.6568 C10-C6-H25=149.8365 C10-C7-H25=121.6067
C1-C11-H25=112.7061 C2-C11-H25= 92.9474 C4-C11-H25=150.118
C6-C11-H25= 93.1292 C7-C11-H25=112.9544 C8-C11-H25=150.1527
H16-C1-H25=102.1484 C2-H16-H25= 66.3762 C4-H16-H25= 87.8605
C6-H25-H16= 79.8176 C7-H25-H16= 85.5952 H16-C11-H25= 99.5293
H17-C1-H25= 82.7418 H17-C2-H25= 91.6006 C3-H17-H25=103.5809
H17-C6-H25= 71.4357 C7-H25-H17= 78.6334 C11-H25-H17= 83.8049
H17-H16-H25= 68.9268 H18-C2-H25=173.4238 H18-H17-H25=127.6822
H19-C1-H25=128.5524 H19-C11-H25=155.5151 H19-H16-H25=100.5098
C1-H25-H20= 78.6082 H20-C2-H25= 71.6001 H20-C6-H25= 91.7883
H20-C7-H25= 82.9598 C10-H20-H25=103.6806 C11-H25-H20= 83.5197
H16-H25-H20= 97.0854 H20-H17-H25= 63.8046 C1-H25-H21= 85.1064
C2-H25-H21= 79.2379 C6-H21-H25= 66.2626 H21-C7-H25=103.602
C8-H21-H25= 87.9136 H21-C11-H25=100.2592 H16-H25-H21=107.9088
H17-H25-H21= 96.5283 H20-H21-H25= 68.9506 H22-C7-H25=128.3829
H22-C11-H25=155.5618 H22-H21-H25=100.3654 H23-C6-H25=173.938
H23-H20-H25=128.0305 C1-H25-H24= 66.3381 C2-H25-H24= 97.0101
C4-H24-H25= 96.3366 C6-H25-H24= 96.8872 C7-H25-H24= 66.336
C8-H24-H25= 96.3143 H24-C11-H25=109.3569 H16-H24-H25= 70.5793
H17-H25-H24=115.2257 H19-H24-H25=115.4886 H20-H25-H24=114.9729
H21-H24-H25= 70.8352 H22-H24-H25=115.4565 C1-C3-H26= 74.0891
C2-C3-H26=100.402 C1-C4-H26= 91.9807 C2-C4-H26= 83.1506
C3-C4-H26= 64.883 C1-C5-H26= 90.0382 C2-C5-H26= 98.8262
C3-C5-H26=103.1886 C4-C5-H26=101.4129 C6-C3-H26=135.5052
C6-C4-H26=110.979 C7-C4-H26=143.1364 C8-C3-H26= 94.3607
C8-C4-H26=146.2942 C8-C5-H26=141.336 C9-C3-H26=106.7478
C9-C4-H26=107.6462 C9-C5-H26=177.6677 C10-C3-H26=145.4269
C10-C4-H26= 95.5847 C10-C5-H26=142.9416 C11-C4-H26=130.3294
C3-O12-H26= 94.8253 C4-O12-H26= 92.8893 C5-O12-H26=111.5582
O15-C3-H26= 76.1551 O15-C4-H26= 76.7866 O15-C5-H26=136.197
O15-O12-H26=146.8365 H16-C4-H26= 75.159 H17-C3-H26= 99.772

```
    C2-H18-H26= 82.2865     H18-C3-H26= 83.4468     C4-H26-H18= 73.5752
    H18-C5-H26= 85.6876    C10-H18-H26=107.1483    H18-O12-H26= 90.1964
   O15-H18-H26= 66.3962    H17-H18-H26= 90.0534     C1-H19-H26= 76.8352
    C3-H26-H19= 73.5763     H19-C4-H26= 84.4096     H19-C5-H26= 85.7183
    C8-H19-H26=108.4504    C11-H19-H26=106.9126    H19-O12-H26= 89.7753
   O15-H19-H26= 67.5788    H16-H19-H26= 68.9073    H18-H26-H19= 95.4221
    H22-C4-H26=150.0824    H22-H19-H26=130.4729     H23-C3-H26=152.8767
   H23-H18-H26=128.1436     H24-C4-H26=137.7809    H24-H19-H26=124.6959
     C1-C7-O27=138.1274      C2-C7-O27=113.7057      C4-C7-O27=106.4591
     C6-C7-O27= 82.9502      C1-C8-O27=133.8825      C2-C8-O27=104.1981
     C3-C8-O27= 96.0895      C4-C8-O27=152.4219      C5-C8-O27=114.9537
     C6-C8-O27= 73.1984      C7-C8-O27= 77.6739      C3-C9-O27=129.3436
     C4-C9-O27=132.4775      C5-C9-O27=164.5626      C6-C9-O27= 82.2099
     C7-C9-O27= 75.8704      C8-C9-O27= 94.4795     C2-C10-O27=129.1969
    C3-C10-O27=155.9353     C4-C10-O27= 99.6983     C5-C10-O27=117.9845
    C6-C10-O27= 88.4148     C7-C10-O27= 67.5724     C8-C10-O27= 66.7318
    C10-C9-O27= 90.9718     C11-C7-O27=173.3579     C11-C8-O27=115.8803
    C7-O27-C13= 92.1592     C8-C13-O27= 83.8895     C9-C13-O27= 98.3227
   C10-C13-O27= 80.7921     C7-O27-N14=115.1865     C8-O27-N14= 85.1625
    C9-O27-N14= 64.0739    C10-O27-N14= 87.8621    N14-C13-O27=122.9766
    O15-C8-O27= 89.1935     O15-C9-O27=154.8945    O15-C10-O27= 91.1241
   O15-C13-O27=131.3866    H18-C10-O27=166.8405     H19-C8-O27=164.2457
    H20-C7-O27= 82.0162    H20-C10-O27= 84.976      C6-H21-O27= 81.2553
    C7-H21-O27= 97.5055     C8-H21-O27= 72.7151     C9-O27-H21= 75.23
   C10-O27-H21= 70.6198    C11-H21-O27=134.3166    C13-O27-H21=110.2637
   N14-O27-H21=130.7201    H20-H21-O27= 84.3801     H22-C7-O27= 70.9011
    H22-C8-O27= 89.3652     H22-C9-O27= 85.4993    H22-C13-O27= 86.0393
   H22-H21-O27= 73.2222     C3-H23-O27=112.1159     C6-H23-O27= 75.2024
    C7-O27-H23= 70.833      C8-O27-H23= 71.4437     H23-C9-O27= 78.1895
   H23-C10-O27= 81.8664    H23-C13-O27= 78.0002    N14-O27-H23= 86.0751
   O15-H23-O27= 78.854     H18-H23-O27=135.4435    H20-H23-O27= 78.4058
   H21-O27-H23= 87.8035     H24-C7-O27=146.7984     H24-C8-O27=124.541
   H24-H21-O27=139.2655     H25-C7-O27=158.2206    H25-H21-O27=146.9886
    C8-C13-H28=107.8154     C9-C13-H28=125.4172    C10-C13-H28=104.7815
    C9-N14-H28= 78.1784    N14-C13-H28= 95.8826    O15-C13-H28=158.3922
   H22-C13-H28=103.0507    H23-C13-H28= 95.4443     C7-O27-H28=155.5749
    C8-O27-H28=151.6511     C9-O27-H28=144.6722    C10-O27-H28=152.2613
   C13-O27-H28=105.022     N14-O27-H28= 80.6107    H21-O27-H28=134.9553
   H23-O27-H28=131.2357
Stoichiometry    C12H12NO3(1-)
Framework group  C1[X(C12H12NO3)]
Deg. of freedom   78
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0       -2.142557   -0.677604   -0.419022
   2          6             0       -1.717950   -0.613258    1.072464
   3          6             0       -0.946977    0.727578    1.297386
   4          6             0       -1.153135    0.315901   -1.070850
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     5          6             0       -0.863451    1.445856   -0.063169
     6          6             0       -0.344800   -1.392298    1.087095
     7          6             0       -0.155128   -1.807122   -0.391331
     8          6             0        0.213912   -0.464031   -1.051043
     9          6             0        1.043505    0.366257   -0.037243
    10          6             0        0.410589   -0.050371    1.314479
    11          6             0       -1.604103   -2.054053   -0.867212
    12          8             0       -1.616895    2.648646   -0.210967
    13          6             0        2.536775    0.282143   -0.146005
    14          7             0        3.469095    1.004174   -0.401106
    15          8             0        0.528131    1.731147   -0.232157
    16          1             0       -3.191826   -0.482649   -0.612096
    17          1             0       -2.478726   -0.901529    1.785268
    18          1             0       -1.198426    1.368480    2.128379
    19          1             0       -1.436033    0.686432   -2.046505
    20          1             0       -0.212862   -2.183435    1.809946
    21          1             0        0.566655   -2.589440   -0.550563
    22          1             0        0.688663   -0.541152   -2.017144
    23          1             0        1.063876    0.053555    2.162885
    24          1             0       -1.678482   -2.207414   -1.939926
    25          1             0       -2.084819   -2.881105   -0.350800
    26          1             0       -2.565581    2.484737   -0.134780
    27          8             0        2.704640   -1.243122    0.199303
    28          1             0        3.656802   -1.403054    0.170364
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9380707      0.6522842      0.4912465
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,O-16,C-
12,N-14,
 O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,O-16,H-1
 Standard basis: 3-21+G* (6D, 7F)
 There are   232 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    262144 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
   232 basis functions      340 primitive gaussians
    58 alpha electrons       58 beta electrons
       nuclear repulsion energy      1209.0193959051 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   232 RedAO= T  NBF=   232
 NBsUse=   232 1.00D-04 NBFU=   232
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -736.377852591     A.U. after   18 cycles
             Convg  =    0.8126D-08             -V/T =  2.0022
             S**2   =   0.0000
 Range of M.O.s used for correlation:     1   232
 NBasis=   232 NAE=    58 NBE=    58 NFC=     0 NFV=     0
 NROrb=    232 NOA=    58 NOB=    58 NVA=   174 NVB=   174

 **** Warning!!: The largest alpha MO coefficient is  0.10693241D+03

          Differentiating once with respect to electric field.
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               with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   3 vectors were produced by pass 12.
   1 vectors were produced by pass 13.
 Inv2:  IOpt= 1 Iter= 1 AM= 7.15D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  40 with in-core refinement.
 G2DrvN: will do   28 atoms at a time, making    1 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  87 IRICut=      82 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
          There are  87 degrees of freedom in the 1st order CPHF.
  84 vectors were produced by pass  0.
 AX will form  84 AO Fock derivatives at one time.
  84 vectors were produced by pass  1.
  84 vectors were produced by pass  2.
  84 vectors were produced by pass  3.
  84 vectors were produced by pass  4.
  84 vectors were produced by pass  5.
  84 vectors were produced by pass  6.
  47 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   2 vectors were produced by pass  9.
 Inv2:  IOpt= 1 Iter= 1 AM= 4.48D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 640 with in-core refinement.

 ********************************************************************

            Population analysis using the SCF density.

 ********************************************************************
```

```
 Alpha  occ. eigenvalues --  -20.38413 -20.34406 -20.27521 -15.23829 -
11.17335
 Alpha  occ. eigenvalues --  -11.10153 -11.07842 -11.07340 -11.06768 -
11.06535
 Alpha  occ. eigenvalues --  -11.06316 -11.06128 -11.05724 -11.05576 -
11.05444
 Alpha  occ. eigenvalues --  -11.05368  -1.30379  -1.23888  -1.14322  -
1.10613
 Alpha  occ. eigenvalues --   -0.97663  -0.97284  -0.93471  -0.91143  -
0.82041
 Alpha  occ. eigenvalues --   -0.80300  -0.75384  -0.69139  -0.67311  -
0.64711
 Alpha  occ. eigenvalues --   -0.63651  -0.59730  -0.58596  -0.54138  -
0.52801
 Alpha  occ. eigenvalues --   -0.51246  -0.50833  -0.48885  -0.47544  -
0.45362
 Alpha  occ. eigenvalues --   -0.41537  -0.40586  -0.40202  -0.38775  -
0.38303
 Alpha  occ. eigenvalues --   -0.36086  -0.35828  -0.35573  -0.34041  -
0.33118
 Alpha  occ. eigenvalues --   -0.32650  -0.32286  -0.30619  -0.29843  -
0.28679
 Alpha  occ. eigenvalues --   -0.27305  -0.19283  -0.12550
 Alpha virt. eigenvalues --    0.14094   0.15435   0.16109   0.16844
0.18155
 Alpha virt. eigenvalues --    0.18410   0.19183   0.20074   0.20745
0.22227
 Alpha virt. eigenvalues --    0.22916   0.23660   0.24731   0.25298
0.25595
 Alpha virt. eigenvalues --    0.25766   0.27839   0.28186   0.28821
0.29316
 Alpha virt. eigenvalues --    0.29529   0.29661   0.30008   0.30543
0.31147
 Alpha virt. eigenvalues --    0.32595   0.33652   0.34233   0.34429
0.35149
 Alpha virt. eigenvalues --    0.35900   0.36381   0.36600   0.36784
0.37210
 Alpha virt. eigenvalues --    0.38152   0.38289   0.38467   0.39202
0.39970
 Alpha virt. eigenvalues --    0.40276   0.40729   0.40910   0.41891
0.42871
 Alpha virt. eigenvalues --    0.44168   0.45217   0.45809   0.46475
0.47255
 Alpha virt. eigenvalues --    0.47602   0.48588   0.48793   0.49377
0.50556
 Alpha virt. eigenvalues --    0.51304   0.52125   0.52697   0.53542
0.54550
 Alpha virt. eigenvalues --    0.55091   0.55577   0.56948   0.57598
0.57980
 Alpha virt. eigenvalues --    0.58477   0.59362   0.59919   0.60149
0.60533
 Alpha virt. eigenvalues --    0.61563   0.62043   0.63166   0.63808
0.65259
```

```
 Alpha virt. eigenvalues --    0.65455   0.65855   0.66889   0.68065
0.68779
 Alpha virt. eigenvalues --    0.69413   0.70627   0.71227   0.72116
0.72854
 Alpha virt. eigenvalues --    0.73346   0.74183   0.74606   0.74884
0.75768
 Alpha virt. eigenvalues --    0.77088   0.77817   0.79569   0.83333
0.83664
 Alpha virt. eigenvalues --    0.86632   0.91899   1.04900   1.22582
1.24366
 Alpha virt. eigenvalues --    1.25769   1.26643   1.26955   1.28110
1.28892
 Alpha virt. eigenvalues --    1.29990   1.30452   1.31069   1.32080
1.33530
 Alpha virt. eigenvalues --    1.33815   1.35128   1.36201   1.37144
1.37831
 Alpha virt. eigenvalues --    1.38210   1.40569   1.43097   1.44763
1.44807
 Alpha virt. eigenvalues --    1.45888   1.49046   1.50458   1.52419
1.54230
 Alpha virt. eigenvalues --    1.55313   1.57022   1.60027   1.61739
1.63366
 Alpha virt. eigenvalues --    1.64657   1.64968   1.67249   1.67541
1.70094
 Alpha virt. eigenvalues --    1.71717   1.73368   1.75430   1.75798
1.85255
 Alpha virt. eigenvalues --    1.87430   1.89254   1.92967   1.94817
1.97727
 Alpha virt. eigenvalues --    2.01998   2.04359   2.09947   2.11304
2.23882
 Alpha virt. eigenvalues --    2.27152   2.28048   2.31884   2.37178
2.39771
 Alpha virt. eigenvalues --    2.41571   2.43881   2.46860   2.50683
2.55001
 Alpha virt. eigenvalues --    2.60431   2.67565   2.68312   2.71343
3.00535
 Alpha virt. eigenvalues --    3.12648   3.30764   3.34587   3.40549
3.79444
 Alpha virt. eigenvalues --    3.80917   3.89220   4.07807   4.26034
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   13.814998  -5.756567   2.123760  -7.087087   1.311958   3.205198
  2  C   -5.756567  18.753374 -13.413833  -0.455095   7.828073  -9.534454
  3  C    2.123760 -13.413833  50.395832  24.146626 -56.350193   9.381166
  4  C   -7.087087  -0.455095  24.146626  46.272726 -53.251198  -0.492053
  5  C    1.311958   7.828073 -56.350193 -53.251198 114.051906  -3.522036
  6  C    3.205198  -9.534454   9.381166  -0.492053  -3.522036  19.142194
  7  C   -0.967974   2.424239   0.134047   3.805408  -2.839063  -5.236431
  8  C    4.080247  -0.214292 -19.239550 -31.155494  44.235313   1.972376
  9  C   -1.099599  -5.088682  40.136193  37.992063 -72.927003   4.599602
 10  C   -1.882427  10.542261 -34.857712 -18.241279  44.657778 -11.846505
 11  C   -3.314791   0.728243   0.397486   1.891189  -1.190764  -0.272933
 12  O    0.023609  -0.142719   1.452376   1.332903  -2.944120   0.044184
 13  C    0.977080   0.148301   0.562103  -0.077158 -10.214993  -1.293663
```

14	N	-0.029188	-0.001143	0.115291	0.157370	-0.040022	-0.010178
15	O	0.003662	-0.095180	0.084169	0.079360	-0.055113	0.023949
16	H	0.542067	-0.127725	0.052510	-0.132190	-0.027886	0.052747
17	H	-0.093160	0.601449	-0.169720	0.006863	0.027360	-0.170123
18	H	0.009457	-0.135743	0.723659	0.099985	-0.288773	0.084760
19	H	-0.080049	-0.009402	0.102597	0.714804	-0.288824	0.003768
20	H	0.001298	-0.125581	0.073860	0.007227	-0.005710	0.570102
21	H	-0.062561	0.054516	-0.021550	0.060415	0.036424	-0.079601
22	H	0.022240	0.007862	-0.052980	-0.241289	0.168477	0.003380
23	H	0.002736	0.040872	-0.176728	-0.040447	0.133990	-0.060482
24	H	-0.086772	0.027568	0.007565	0.036564	-0.024519	0.044790
25	H	-0.054381	-0.013535	0.001074	0.004115	0.003455	0.040011
26	H	0.005648	0.002423	-0.123384	-0.116596	0.310415	0.003732
27	O	-0.015812	-0.034722	0.056958	0.019419	-0.037903	0.157957
28	H	0.000111	0.000639	-0.002826	-0.002612	0.003586	-0.010512

		7	8	9	10	11	12
1	C	-0.967974	4.080247	-1.099599	-1.882427	-3.314791	0.023609
2	C	2.424239	-0.214292	-5.088682	10.542261	0.728243	-0.142719
3	C	0.134047	-19.239550	40.136193	-34.857712	0.397486	1.452376
4	C	3.805408	-31.155494	37.992063	-18.241279	1.891189	1.332903
5	C	-2.839063	44.235313	-72.927003	44.657778	-1.190764	-2.944120
6	C	-5.236431	1.972376	4.599602	-11.846505	-0.272933	0.044184
7	C	13.923165	-7.846811	3.606805	0.139789	-2.628708	0.066856
8	C	-7.846811	54.870631	-59.867132	29.581152	-1.777274	-0.887051
9	C	3.606805	-59.867132	134.836547	-61.088093	2.455568	1.519324
10	C	0.139789	29.581152	-61.088093	58.212518	-0.665180	-0.868350
11	C	-2.628708	-1.777274	2.455568	-0.665180	11.801647	0.011660
12	O	0.066856	-0.887051	1.519324	-0.868350	0.011660	8.617149
13	C	0.547004	-7.109072	-20.999877	-6.711264	-0.545232	0.174420
14	N	0.049173	-0.030550	0.770410	0.027899	0.017903	0.000997
15	O	-0.055528	1.419292	-2.640732	1.384095	-0.080628	-0.071105
16	H	-0.027471	0.027595	0.027150	-0.036812	-0.001181	0.002960
17	H	0.016277	0.017630	-0.033836	0.137852	0.020775	0.000595
18	H	-0.007709	-0.012574	0.050998	-0.170260	0.002271	-0.000061
19	H	0.032715	-0.207354	0.081144	-0.026651	0.016308	-0.000479
20	H	-0.097595	0.052007	-0.052387	-0.065517	0.009453	-0.000011
21	H	0.508673	-0.083954	-0.020609	0.061064	-0.008863	-0.000048
22	H	-0.092009	0.889978	-0.417389	0.165544	0.004061	-0.000863
23	H	-0.020876	0.163733	-0.350686	0.803111	-0.003988	-0.000648
24	H	-0.124579	0.032275	-0.012414	-0.002544	0.417628	0.000118
25	H	-0.117957	0.082952	-0.022739	-0.000285	0.389101	-0.000001
26	H	0.004239	0.020863	-0.058589	0.016843	-0.015547	0.145429
27	O	-0.105686	0.459725	-1.037082	0.217455	-0.049844	0.000888
28	H	0.033196	-0.053981	0.097623	-0.024713	0.003375	-0.000004

		13	14	15	16	17	18
1	C	0.977080	-0.029188	0.003662	0.542067	-0.093160	0.009457
2	C	0.148301	-0.001143	-0.095180	-0.127725	0.601449	-0.135743
3	C	0.562103	0.115291	0.084169	0.052510	-0.169720	0.723659
4	C	-0.077158	0.157370	0.079360	-0.132190	0.006863	0.099985
5	C	-10.214993	-0.040022	-0.055113	-0.027886	0.027360	-0.288773
6	C	-1.293663	-0.010178	0.023949	0.052747	-0.170123	0.084760
7	C	0.547004	0.049173	-0.055528	-0.027471	0.016277	-0.007709
8	C	-7.109072	-0.030550	1.419292	0.027595	0.017630	-0.012574
9	C	-20.999877	0.770410	-2.640732	0.027150	-0.033836	0.050998

10	C	-6.711264	0.027899	1.384095	-0.036812	0.137852	-0.170260
11	C	-0.545232	0.017903	-0.080628	-0.001181	0.020775	0.002271
12	O	0.174420	0.000997	-0.071105	0.002960	0.000595	-0.000061
13	C	50.999473	-1.112400	-0.787981	-0.001259	-0.000218	-0.007003
14	N	-1.112400	8.086480	0.021052	0.000004	0.000000	-0.000090
15	O	-0.787981	0.021052	8.890756	-0.001325	0.000190	0.008111
16	H	-0.001259	0.000004	-0.001325	0.425007	-0.000537	-0.000020
17	H	-0.000218	0.000000	0.000190	-0.000537	0.407317	-0.000256
18	H	-0.007003	-0.000090	0.008111	-0.000020	-0.000256	0.384202
19	H	0.002595	-0.000224	0.006783	-0.000477	-0.000020	-0.000024
20	H	-0.007980	-0.000158	0.000955	-0.000019	-0.000412	-0.000094
21	H	-0.084485	0.000223	0.000416	-0.000014	-0.000014	0.000000
22	H	-0.115529	0.000508	0.016644	-0.000026	0.000001	0.000001
23	H	-0.139994	-0.000931	0.017957	0.000000	-0.000079	-0.000767
24	H	-0.000033	0.000016	-0.000045	-0.000049	-0.000033	0.000000
25	H	0.001857	-0.000004	0.000205	-0.000257	0.000174	0.000000
26	H	-0.000246	-0.000043	0.008348	-0.000209	-0.000014	-0.000126
27	O	-0.373290	-0.144180	0.092671	-0.000005	0.000036	-0.000006
28	H	0.017417	-0.007340	-0.002266	0.000000	0.000000	0.000000

		19	20	21	22	23	24
1	C	-0.080049	0.001298	-0.062561	0.022240	0.002736	-0.086772
2	C	-0.009402	-0.125581	0.054516	0.007862	0.040872	0.027568
3	C	0.102597	0.073860	-0.021550	-0.052980	-0.176728	0.007565
4	C	0.714804	0.007227	0.060415	-0.241289	-0.040447	0.036564
5	C	-0.288824	-0.005710	0.036424	0.168477	0.133990	-0.024519
6	C	0.003768	0.570102	-0.079601	0.003380	-0.060482	0.044790
7	C	0.032715	-0.097595	0.508673	-0.092009	-0.020876	-0.124579
8	C	-0.207354	0.052007	-0.083954	0.889978	0.163733	0.032275
9	C	0.081144	-0.052387	-0.020609	-0.417389	-0.350686	-0.012414
10	C	-0.026651	-0.065517	0.061064	0.165544	0.803111	-0.002544
11	C	0.016308	0.009453	-0.008863	0.004061	-0.003988	0.417628
12	O	-0.000479	-0.000011	-0.000048	-0.000863	-0.000648	0.000118
13	C	0.002595	-0.007980	-0.084485	-0.115529	-0.139994	-0.000033
14	N	-0.000224	-0.000158	0.000223	0.000508	-0.000931	0.000016
15	O	0.006783	0.000955	0.000416	0.016644	0.017957	-0.000045
16	H	-0.000477	-0.000019	-0.000014	-0.000026	0.000000	-0.000049
17	H	-0.000020	-0.000412	-0.000014	0.000001	-0.000079	-0.000033
18	H	-0.000024	-0.000094	0.000000	0.000001	-0.000767	0.000000
19	H	0.383618	0.000001	-0.000020	-0.000663	0.000001	0.000121
20	H	0.000001	0.399722	-0.000318	-0.000010	-0.000182	-0.000041
21	H	-0.000020	-0.000318	0.356028	0.000031	0.000006	-0.000196
22	H	-0.000663	-0.000010	0.000031	0.373277	-0.000012	0.000015
23	H	0.000001	-0.000182	0.000006	-0.000012	0.368429	0.000000
24	H	0.000121	-0.000041	-0.000196	0.000015	0.000000	0.462337
25	H	-0.000036	0.000069	-0.000250	-0.000041	0.000001	-0.019763
26	H	-0.000087	0.000000	0.000000	0.000003	0.000003	0.000000
27	O	0.000082	0.003739	-0.004031	0.004740	0.002327	-0.000128
28	H	0.000000	-0.000004	-0.000011	0.000022	0.000059	0.000000

		25	26	27	28
1	C	-0.054381	0.005648	-0.015812	0.000111
2	C	-0.013535	0.002423	-0.034722	0.000639
3	C	0.001074	-0.123384	0.056958	-0.002826
4	C	0.004115	-0.116596	0.019419	-0.002612
5	C	0.003455	0.310415	-0.037903	0.003586

6	C	0.040011	0.003732	0.157957	-0.010512
7	C	-0.117957	0.004239	-0.105686	0.033196
8	C	0.082952	0.020863	0.459725	-0.053981
9	C	-0.022739	-0.058589	-1.037082	0.097623
10	C	-0.000285	0.016843	0.217455	-0.024713
11	C	0.389101	-0.015547	-0.049844	0.003375
12	O	-0.000001	0.145429	0.000888	-0.000004
13	C	0.001857	-0.000246	-0.373290	0.017417
14	N	-0.000004	-0.000043	-0.144180	-0.007340
15	O	0.000205	0.008348	0.092671	-0.002266
16	H	-0.000257	-0.000209	-0.000005	0.000000
17	H	0.000174	-0.000014	0.000036	0.000000
18	H	0.000000	-0.000126	-0.000006	0.000000
19	H	-0.000036	-0.000087	0.000082	0.000000
20	H	0.000069	0.000000	0.003739	-0.000004
21	H	-0.000250	0.000000	-0.004031	-0.000011
22	H	-0.000041	0.000003	0.004740	0.000022
23	H	0.000001	0.000003	0.002327	0.000059
24	H	-0.019763	0.000000	-0.000128	0.000000
25	H	0.470299	0.000000	-0.000074	0.000000
26	H	0.000000	0.389398	0.000004	0.000000
27	O	-0.000074	0.000004	9.452483	0.141419
28	H	0.000000	0.000000	0.141419	0.349527

Total atomic charges:

		1
1	C	0.406299
2	C	-0.011147
3	C	0.461206
4	C	0.665458
5	C	-2.760616
6	C	-0.800944
7	C	0.876810
8	C	-3.420678
9	C	5.543421
10	C	-3.459769
11	C	-1.611736
12	O	-0.478011
13	C	2.151426
14	N	-0.870874
15	O	-0.268712
16	H	0.227422
17	H	0.231904
18	H	0.260063
19	H	0.269771
20	H	0.237584
21	H	0.288730
22	H	0.264027
23	H	0.262597
24	H	0.242115
25	H	0.236010
26	H	0.407491
27	O	-0.807140
28	H	0.457292

Sum of Mulliken charges= -1.00000

```
 Atomic charges with hydrogens summed into heavy atoms:
                1
  1  C    0.633721
  2  C    0.220757
  3  C    0.721269
  4  C    0.935229
  5  C   -2.760616
  6  C   -0.563360
  7  C    1.165540
  8  C   -3.156651
  9  C    5.543421
 10  C   -3.197172
 11  C   -1.133611
 12  O   -0.070519
 13  C    2.151426
 14  N   -0.870874
 15  O   -0.268712
 16  H    0.000000
 17  H    0.000000
 18  H    0.000000
 19  H    0.000000
 20  H    0.000000
 21  H    0.000000
 22  H    0.000000
 23  H    0.000000
 24  H    0.000000
 25  H    0.000000
 26  H    0.000000
 27  O   -0.349848
 28  H    0.000000
 Sum of Mulliken charges=  -1.00000
 Electronic spatial extent (au):  <R**2>=  2561.8725
 Charge=    -1.0000 electrons
 Dipole moment (Debye):
    X=   -13.7042    Y=    -6.0026    Z=     1.6993  Tot=    15.0574
 Quadrupole moment (Debye-Ang):
   XX=  -138.5886   YY=  -123.4568   ZZ=   -97.8254
   XY=   -13.6384   XZ=     4.3322   YZ=     4.7844
 Octapole moment (Debye-Ang**2):
  XXX=  -175.1694  YYY=   -41.1513  ZZZ=     0.4051  XYY=   -25.0877
  XXY=   -32.7011  XXZ=    19.7182  XZZ=    -5.7924  YZZ=     2.2677
  YYZ=     9.6996  XYZ=     9.3006
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -2369.7758 YYYY= -1326.0285 ZZZZ=  -526.6891 XXXY=  -309.2131
 XXXZ=    83.6083 YYYX=   -48.8634 YYYZ=    13.8428 ZZZX=    11.2612
 ZZZY=     1.9110 XXYY=  -568.6534 XXZZ=  -423.5531 YYZZ=  -289.0886
 XXYZ=    24.4511 YYXZ=     1.6532 ZZXY=   -16.8035
 N-N= 1.209019395905D+03 E-N=-4.158917409376D+03  KE= 7.347708536906D+02
  Exact polarizability: 149.155   3.707 133.682  -1.490  -1.761 111.529
 Approx polarizability: 124.746   3.750 123.643  -2.073  -3.403 107.675
 Full mass-weighted force constant matrix:
 Low frequencies --- -134.0487   -1.0391   -0.7421    0.0007    0.0011
0.0014
 Low frequencies ---    0.4647   66.9455  154.8559
```

****** 1 imaginary frequencies (negative Signs) ******
Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
Raman scattering activities (A**4/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

		1			2			3		
		?A			?A			?A		
Frequencies --		-134.0487			66.9455			154.8559		
Red. masses --		1.0453			10.0782			6.5953		
Frc consts --		0.0111			0.0266			0.0932		
IR Inten --		147.5413			1.0057			5.2413		
Raman Activ --		2.4278			2.2142			0.2778		
Depolar --		0.7486			0.7497			0.1061		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.01	0.00	-0.01	0.04	0.06	-0.06	0.03
2	6	0.00	0.00	0.00	-0.01	0.05	0.04	0.10	-0.04	0.02
3	6	0.01	0.00	0.00	0.00	0.05	-0.02	0.02	0.02	0.00
4	6	-0.01	0.00	0.00	0.01	-0.05	0.00	-0.03	0.01	0.01
5	6	0.00	0.00	0.01	0.00	-0.01	-0.05	-0.06	0.03	0.00
6	6	0.00	0.00	0.00	-0.01	0.04	0.07	0.15	0.06	-0.03
7	6	0.00	0.00	0.00	-0.01	-0.02	0.09	0.13	0.08	-0.04
8	6	0.00	0.00	0.00	0.00	-0.05	0.03	0.02	0.10	-0.04
9	6	0.00	0.00	0.00	0.00	-0.01	0.00	-0.01	0.12	-0.05
10	6	0.00	0.00	0.00	0.00	0.04	0.02	0.05	0.11	-0.04
11	6	0.00	0.00	0.00	-0.01	-0.03	0.10	0.14	-0.02	0.01
12	8	0.00	0.01	0.05	0.01	-0.01	-0.11	-0.17	-0.03	0.03
13	6	0.00	0.00	0.00	0.01	0.02	0.06	-0.02	-0.03	0.00
14	7	0.00	0.00	0.00	0.04	0.14	0.51	0.16	-0.25	0.08
15	8	0.00	0.00	0.00	0.00	-0.01	-0.05	-0.06	0.11	-0.04
16	1	-0.01	-0.01	0.01	0.00	-0.01	0.03	0.04	-0.13	0.07
17	1	0.00	0.00	0.00	-0.01	0.08	0.05	0.14	-0.09	0.04
18	1	-0.01	0.01	-0.01	0.01	0.09	-0.04	-0.01	0.00	0.01
19	1	0.00	-0.01	-0.01	0.01	-0.08	-0.02	-0.09	0.00	0.02
20	1	0.00	0.00	0.00	-0.02	0.07	0.10	0.24	0.06	-0.04

21	1	0.00	0.00	-0.01	-0.01	-0.03	0.11	0.18	0.13	-0.06
22	1	-0.01	0.01	0.00	0.00	-0.10	0.04	0.00	0.15	-0.05
23	1	0.01	-0.01	0.00	0.00	0.08	0.01	0.08	0.15	-0.07
24	1	0.00	0.00	0.00	-0.01	-0.08	0.10	0.11	-0.02	0.01
25	1	0.00	0.00	0.00	-0.02	-0.01	0.13	0.21	-0.05	0.02
26	1	-0.05	-0.15	-0.99	0.01	0.00	-0.05	-0.15	-0.12	0.04
27	8	0.00	0.00	-0.01	-0.02	-0.11	-0.55	-0.34	-0.13	0.03
28	1	0.00	0.00	-0.01	-0.02	-0.09	-0.48	-0.37	-0.30	0.12

	4			5			6		
	?A			?A			?A		
Frequencies --	176.1361			266.6364			318.2864		
Red. masses --	5.3230			5.1377			6.5420		
Frc consts --	0.0973			0.2152			0.3905		
IR Inten --	5.9824			2.3075			2.3366		
Raman Activ --	1.9135			1.0930			0.3945		
Depolar --	0.7409			0.7009			0.6816		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.06	0.02	0.10	0.00	-0.14	0.02	0.01	-0.04	-0.15
2 6	0.08	0.00	0.05	0.02	-0.10	0.00	-0.07	0.09	-0.11
3 6	0.12	-0.01	-0.01	-0.07	-0.03	-0.01	-0.02	0.05	-0.12
4 6	-0.10	-0.01	0.00	-0.09	-0.03	0.01	0.00	-0.02	-0.12
5 6	0.01	-0.01	-0.02	-0.03	0.03	0.00	-0.01	0.01	-0.06
6 6	0.07	-0.02	-0.09	0.06	-0.02	0.00	-0.08	0.08	0.06
7 6	-0.08	-0.02	-0.11	0.08	-0.01	-0.01	0.02	-0.02	0.12
8 6	-0.09	-0.03	-0.13	-0.04	0.02	-0.01	0.01	-0.06	0.01
9 6	0.00	-0.04	-0.17	-0.06	0.01	-0.01	0.00	-0.01	-0.04
10 6	0.09	-0.04	-0.14	-0.03	0.02	0.00	-0.05	0.07	-0.01
11 6	-0.14	0.01	0.04	0.11	-0.11	0.02	0.08	-0.10	0.05
12 8	0.02	0.00	0.06	0.33	0.25	0.01	-0.03	0.06	0.46
13 6	0.02	0.02	0.02	-0.09	0.02	-0.01	0.02	-0.04	-0.01
14 7	0.03	0.09	0.27	-0.11	0.05	0.01	0.03	-0.03	0.01

15	8	0.00	-0.04	-0.17	-0.03	-0.04	-0.01	-0.01	-0.01	-0.18
16	1	-0.07	0.05	0.20	-0.02	-0.24	0.04	0.01	-0.12	-0.23
17	1	0.14	0.01	0.13	0.05	-0.13	0.01	-0.13	0.16	-0.15
18	1	0.21	-0.01	0.01	-0.11	-0.08	0.02	-0.07	0.10	-0.18
19	1	-0.19	-0.01	0.03	-0.13	-0.08	0.00	0.08	-0.04	-0.16
20	1	0.13	-0.03	-0.11	0.11	-0.02	-0.01	-0.15	0.13	0.13
21	1	-0.12	-0.06	-0.18	0.15	0.06	-0.02	0.07	0.01	0.22
22	1	-0.19	-0.02	-0.18	-0.05	0.06	-0.02	0.04	-0.16	0.02
23	1	0.17	-0.06	-0.20	-0.02	0.07	-0.02	-0.07	0.13	-0.01
24	1	-0.26	0.01	0.05	0.10	-0.14	0.02	0.15	-0.27	0.07
25	1	-0.10	0.02	0.09	0.17	-0.14	0.04	0.05	-0.03	0.15
26	1	0.01	0.00	0.01	0.27	0.59	-0.07	-0.03	-0.02	0.28
27	8	0.04	0.06	0.20	-0.11	0.01	0.00	0.08	-0.02	-0.01
28	1	0.05	0.11	0.40	-0.12	-0.01	0.04	0.09	0.05	0.04

	7			8			9		
	?A			?A			?A		
Frequencies --	348.7780			395.8886			415.0454		
Red. masses --	6.2217			7.8663			2.2911		
Frc consts --	0.4459			0.7264			0.2325		
IR Inten --	15.5711			15.5169			1.7778		
Raman Activ --	3.5435			6.0948			0.4521		
Depolar --	0.3391			0.3841			0.4698		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.07	0.08	-0.06	-0.07	-0.04	-0.03	-0.02	-0.02	0.05
2 6	0.03	0.06	-0.03	-0.09	-0.05	-0.02	-0.01	-0.02	0.06
3 6	0.12	-0.02	-0.01	-0.08	-0.07	-0.01	0.01	0.01	0.02
4 6	0.16	-0.03	-0.05	-0.02	-0.05	-0.01	-0.03	-0.03	0.06
5 6	0.12	-0.05	-0.01	-0.05	-0.04	0.01	-0.02	-0.02	0.00
6 6	-0.02	-0.04	0.02	-0.08	-0.05	-0.03	-0.03	-0.01	0.07
7 6	-0.03	-0.09	0.05	-0.08	-0.06	0.00	-0.02	-0.03	0.07
8 6	0.09	-0.11	0.02	0.01	-0.04	0.00	0.00	-0.05	0.07

9	6	0.02	-0.02	0.00	0.08	0.08	0.00	0.01	0.00	-0.01
10	6	0.06	-0.07	0.01	-0.04	-0.06	-0.01	0.00	0.02	0.02
11	6	-0.05	0.02	0.02	-0.14	-0.09	0.09	0.05	0.08	-0.19
12	8	0.05	-0.11	0.08	0.08	0.04	0.00	0.02	0.00	0.01
13	6	-0.08	0.19	-0.03	0.22	0.18	-0.03	0.03	0.03	-0.02
14	7	-0.13	0.20	-0.04	0.47	-0.10	-0.03	0.07	-0.01	0.00
15	8	0.07	-0.04	-0.01	-0.07	0.01	0.09	-0.03	-0.04	-0.12
16	1	0.09	0.18	-0.09	-0.06	0.01	-0.05	-0.02	-0.03	0.06
17	1	-0.02	0.10	-0.07	-0.10	-0.06	-0.04	-0.01	0.02	0.08
18	1	0.13	0.02	-0.03	-0.08	-0.09	0.00	0.02	0.03	0.01
19	1	0.22	0.00	-0.05	0.00	-0.05	-0.02	-0.02	-0.07	0.04
20	1	-0.09	-0.02	0.06	-0.09	-0.05	-0.02	-0.02	0.02	0.10
21	1	-0.10	-0.16	0.06	-0.13	-0.10	0.00	-0.03	-0.04	0.09
22	1	0.14	-0.18	0.05	-0.02	-0.08	-0.01	-0.05	-0.08	0.05
23	1	0.09	-0.12	-0.01	-0.12	-0.10	0.05	0.00	0.02	0.02
24	1	-0.04	-0.02	0.02	-0.26	-0.30	0.13	0.30	0.50	-0.27
25	1	-0.14	0.09	0.05	-0.09	0.01	0.31	-0.07	-0.12	-0.63
26	1	0.06	-0.18	0.04	0.06	0.18	-0.04	0.01	0.04	0.01
27	8	-0.38	0.08	0.02	-0.09	0.28	-0.05	-0.02	0.05	-0.01
28	1	-0.43	-0.26	0.07	-0.14	0.01	-0.13	-0.03	0.00	0.03

	10			11			12		
	?A			?A			?A		
Frequencies --	500.0181			507.8717			540.7945		
Red. masses --	1.4962			7.1303			2.3923		
Frc consts --	0.2204			1.0836			0.4122		
IR Inten --	71.7220			131.9705			48.4971		
Raman Activ --	4.1664			9.4318			1.0853		
Depolar --	0.7498			0.7500			0.6236		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.01	0.02	-0.04	-0.01	0.02	-0.04	-0.06	-0.02
2 6	0.03	-0.02	0.00	-0.02	-0.03	0.01	-0.08	0.08	0.01

3	6	0.00	0.00	-0.01	-0.04	-0.01	-0.02	0.06	0.03	0.02
4	6	0.00	-0.01	-0.01	-0.02	-0.03	0.01	-0.05	0.03	0.03
5	6	0.00	-0.01	-0.03	-0.07	0.01	-0.02	0.04	0.00	0.05
6	6	0.04	-0.01	-0.02	-0.01	-0.01	-0.02	-0.10	0.04	0.01
7	6	0.00	0.00	-0.04	-0.03	-0.02	-0.02	0.01	0.05	0.04
8	6	0.03	0.00	0.01	0.04	-0.02	0.02	-0.07	0.03	-0.06
9	6	0.00	0.01	0.05	0.06	0.03	0.03	0.00	-0.03	-0.09
10	6	-0.01	0.02	0.02	0.00	0.00	0.00	0.02	-0.06	-0.06
11	6	-0.04	0.02	0.00	-0.07	0.00	0.00	0.12	-0.07	-0.01
12	8	0.00	0.00	0.02	-0.02	0.07	0.01	0.01	-0.04	-0.03
13	6	-0.01	-0.02	0.12	0.12	0.35	-0.01	0.01	0.01	-0.07
14	7	-0.03	-0.03	-0.01	0.12	0.22	-0.08	0.02	0.03	0.04
15	8	0.00	-0.01	-0.07	-0.07	0.03	-0.03	0.04	0.00	0.08
16	1	0.00	0.04	0.05	-0.03	0.03	0.03	-0.05	-0.18	-0.11
17	1	0.05	-0.04	0.01	0.00	-0.04	0.02	-0.08	0.15	0.03
18	1	-0.04	0.02	-0.04	-0.04	-0.02	-0.01	0.16	0.03	0.06
19	1	0.00	-0.05	-0.02	-0.01	-0.08	-0.02	-0.08	0.11	0.07
20	1	0.06	-0.01	-0.03	0.04	0.00	-0.02	-0.15	0.02	0.00
21	1	-0.04	-0.04	-0.07	-0.05	-0.04	0.00	0.12	0.13	0.14
22	1	0.06	0.06	0.02	0.03	-0.01	0.02	-0.17	-0.04	-0.10
23	1	-0.03	0.02	0.04	-0.06	-0.02	0.05	0.09	-0.11	-0.11
24	1	-0.08	0.02	0.01	-0.10	0.01	0.00	0.19	-0.04	-0.02
25	1	-0.02	0.02	0.02	-0.05	0.00	0.00	0.16	-0.12	-0.06
26	1	0.00	0.00	0.02	-0.03	0.15	-0.01	0.02	-0.09	-0.01
27	8	0.00	0.05	0.04	0.06	-0.45	0.12	-0.01	0.01	0.07
28	1	-0.06	-0.15	-0.94	0.02	-0.60	-0.33	-0.07	-0.21	-0.68

	13	14	15
	?A	?A	?A

Frequencies --	555.9577			578.1734			610.5062		
Red. masses --	4.4992			4.3918			5.0641		
Frc consts --	0.8194			0.8650			1.1121		
IR Inten --	24.6765			3.7282			55.3931		
Raman Activ --	2.7436			2.1933			5.8336		
Depolar --	0.3740			0.3667			0.0506		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.07	-0.02	0.02	0.08	0.07	-0.13	0.06	0.13	-0.09
2 6	-0.11	0.04	0.01	0.00	-0.02	-0.08	-0.02	-0.05	-0.03
3 6	-0.01	0.02	0.09	0.05	-0.04	0.19	-0.13	-0.06	0.10
4 6	-0.05	0.00	0.09	0.06	0.10	0.11	0.08	0.02	-0.01
5 6	0.06	-0.09	0.04	-0.04	0.11	0.15	-0.05	-0.15	0.11
6 6	-0.08	0.06	-0.10	-0.03	-0.09	0.00	0.08	0.10	0.04
7 6	0.05	0.17	-0.13	0.02	-0.07	0.04	0.01	0.04	0.08
8 6	0.02	0.12	0.00	0.00	-0.03	0.08	0.01	-0.03	-0.06
9 6	0.03	0.01	0.09	-0.03	-0.02	-0.02	-0.06	0.04	-0.13
10 6	-0.06	-0.01	0.11	0.04	-0.11	0.03	-0.01	0.13	-0.03
11 6	0.06	0.00	0.05	0.04	-0.04	0.03	-0.02	0.13	0.04
12 8	0.10	-0.17	0.00	-0.10	0.15	-0.09	0.18	-0.18	0.01
13 6	0.04	0.04	0.08	-0.03	0.01	-0.03	-0.08	0.02	-0.15
14 7	0.01	0.03	-0.05	0.01	-0.03	0.02	0.02	-0.05	0.06
15 8	0.01	-0.10	-0.22	-0.06	-0.01	-0.22	-0.16	-0.04	0.01
16 1	-0.06	-0.08	-0.09	0.09	0.05	-0.17	0.08	0.21	-0.11
17 1	-0.05	0.00	0.06	-0.09	-0.09	-0.20	-0.08	-0.23	-0.17
18 1	-0.06	0.09	0.03	0.05	-0.25	0.36	-0.21	-0.08	0.09
19 1	-0.06	0.10	0.13	0.22	0.26	0.12	0.13	0.23	0.06
20 1	-0.14	-0.07	-0.23	-0.14	-0.08	0.03	0.17	0.17	0.10
21 1	0.11	0.21	-0.07	0.04	-0.05	0.01	-0.05	-0.01	0.07
22 1	0.04	0.31	-0.01	-0.05	-0.03	0.05	-0.02	-0.15	-0.07
23 1	-0.10	-0.16	0.16	0.14	-0.22	-0.02	0.09	0.24	-0.12

24	1	-0.13	-0.14	0.08	0.02	-0.28	0.07	0.06	0.04	0.04
25	1	0.27	-0.01	0.24	-0.04	0.12	0.23	-0.13	0.22	0.07
26	1	0.11	-0.15	0.04	-0.10	0.13	-0.06	0.14	0.05	-0.06
27	8	-0.02	-0.01	-0.04	0.01	0.01	0.01	0.05	-0.03	0.05
28	1	-0.01	-0.01	0.37	0.01	0.05	-0.12	0.07	0.12	-0.29

	16			17			18		
	?A			?A			?A		
Frequencies --	638.4093			662.2393			674.8984		
Red. masses --	6.2293			4.1776			6.0179		
Frc consts --	1.4958			1.0795			1.6150		
IR Inten --	1.7985			86.6671			28.4014		
Raman Activ --	3.0459			5.9642			5.1888		
Depolar --	0.5953			0.1379			0.6603		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.08	-0.06	0.12	-0.05	-0.04	-0.04	0.11	0.12	0.14
2 6	-0.13	0.04	0.12	-0.01	-0.14	-0.06	-0.09	-0.08	0.12
3 6	-0.10	0.14	0.13	-0.16	0.00	0.01	-0.13	-0.09	-0.08
4 6	0.20	-0.14	0.16	0.00	0.06	0.10	0.04	0.04	-0.05
5 6	0.01	0.05	0.13	0.09	0.06	0.07	-0.06	0.00	-0.09
6 6	-0.09	0.12	-0.14	0.09	0.05	0.02	-0.04	-0.10	0.06
7 6	0.04	-0.13	-0.12	-0.04	-0.03	0.00	0.10	0.13	0.01
8 6	0.21	-0.13	-0.15	-0.08	0.00	0.03	0.10	0.02	-0.08
9 6	0.01	0.01	-0.11	0.08	-0.04	-0.02	0.02	-0.14	-0.07
10 6	-0.15	0.07	-0.19	-0.06	0.16	0.03	-0.13	-0.11	-0.06
11 6	-0.01	-0.07	-0.03	-0.08	-0.06	-0.04	0.15	0.24	0.15
12 8	-0.02	0.06	0.03	-0.04	-0.01	0.00	-0.10	0.11	0.01
13 6	-0.01	-0.02	0.10	0.15	-0.15	-0.11	0.10	-0.09	-0.10
14 7	-0.04	-0.02	-0.03	-0.01	0.14	0.01	0.02	0.08	0.01
15 8	0.01	0.06	0.01	0.19	0.00	-0.04	0.01	-0.18	-0.01
16 1	0.15	0.10	-0.09	-0.05	-0.02	0.01	0.12	0.09	0.08
17 1	-0.08	-0.09	0.12	0.03	-0.27	-0.07	-0.20	-0.03	0.02

18	1	0.08	0.12	0.21	-0.35	-0.11	0.04	-0.02	-0.05	-0.08
19	1	0.08	-0.14	0.20	0.05	0.16	0.12	-0.11	-0.11	-0.06
20	1	0.06	0.21	-0.07	0.18	0.11	0.07	0.09	-0.19	-0.06
21	1	-0.05	-0.26	0.12	-0.04	-0.02	-0.07	0.04	0.08	0.01
22	1	0.14	-0.06	-0.19	-0.18	0.01	-0.02	0.09	-0.04	-0.09
23	1	-0.09	-0.05	-0.23	-0.13	0.29	0.07	-0.21	0.02	-0.02
24	1	-0.18	0.09	-0.04	-0.02	-0.12	-0.03	0.02	0.21	0.16
25	1	0.06	-0.14	-0.08	-0.12	-0.02	-0.01	0.22	0.25	0.22
26	1	-0.02	0.05	-0.02	-0.01	-0.21	0.02	-0.10	0.06	-0.01
27	8	0.00	0.00	-0.02	-0.05	0.02	0.03	-0.04	0.04	0.02
28	1	0.02	0.05	0.04	-0.13	-0.42	0.00	-0.10	-0.30	-0.03

	19			20			21		
	?A			?A			?A		
Frequencies --	707.9668			717.7624			749.3816		
Red. masses --	7.9089			5.1584			5.6512		
Frc consts --	2.3356			1.5658			1.8698		
IR Inten --	9.6104			21.4376			157.4572		
Raman Activ --	3.5668			1.6509			5.9735		
Depolar --	0.6370			0.7490			0.1666		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	-0.01	0.07	-0.02	0.04	-0.07	0.05	0.01	0.05
2	6	-0.16	-0.20	0.08	0.00	-0.04	-0.02	0.05	-0.03	-0.02
3	6	-0.01	-0.19	-0.13	0.02	-0.07	0.00	-0.09	0.08	-0.01
4	6	0.07	0.04	0.06	-0.08	0.12	-0.02	-0.02	0.09	0.01
5	6	0.14	0.05	-0.06	-0.01	-0.01	0.06	0.12	0.09	0.00
6	6	-0.08	-0.21	0.09	0.06	0.03	0.07	0.05	-0.01	0.02
7	6	-0.03	0.02	0.11	-0.03	0.01	0.12	0.02	-0.05	-0.03
8	6	-0.01	0.09	0.06	-0.07	-0.03	-0.11	-0.10	-0.06	-0.09
9	6	0.00	0.19	-0.08	0.02	-0.04	-0.08	-0.12	-0.11	0.00
10	6	-0.12	-0.09	-0.14	0.01	0.01	-0.16	-0.11	0.03	0.06
11	6	0.00	0.03	0.05	0.05	0.03	0.03	0.04	-0.02	0.00

12	8	0.09	-0.10	0.01	0.00	-0.02	-0.02	-0.06	0.00	0.01
13	6	-0.11	0.06	0.02	0.11	0.03	0.45	-0.22	0.34	0.00
14	7	-0.04	-0.06	0.01	-0.02	0.02	-0.14	0.10	-0.14	0.01
15	8	0.14	0.37	-0.14	-0.01	-0.05	0.01	0.21	-0.16	0.01
16	1	0.01	0.03	0.01	-0.05	-0.07	-0.01	0.03	-0.04	0.13
17	1	-0.26	-0.02	0.05	-0.05	-0.05	-0.07	0.05	-0.07	-0.03
18	1	0.15	-0.23	-0.05	0.12	-0.16	0.10	-0.23	0.06	-0.04
19	1	0.02	-0.04	0.04	-0.10	0.31	0.05	-0.12	0.14	0.06
20	1	0.14	-0.19	0.07	0.17	0.12	0.15	0.08	0.00	0.02
21	1	0.01	0.07	0.05	-0.02	0.02	0.10	0.08	0.01	-0.07
22	1	-0.08	-0.06	0.04	-0.21	-0.24	-0.16	-0.10	-0.04	-0.09
23	1	-0.21	0.00	-0.08	0.08	0.14	-0.23	-0.08	0.12	0.02
24	1	0.01	-0.01	0.06	0.25	0.00	0.02	0.03	0.03	0.00
25	1	0.01	0.05	0.09	-0.08	0.07	-0.04	-0.02	0.00	-0.03
26	1	0.11	-0.18	0.00	0.00	-0.01	-0.03	0.00	-0.30	0.05
27	8	0.03	-0.04	0.00	-0.02	-0.01	-0.08	0.03	-0.02	-0.01
28	1	0.09	0.30	-0.07	-0.04	-0.15	0.26	0.13	0.55	-0.12

	22			23			24		
	?A			?A			?A		
Frequencies --	821.6335			829.3208			842.2823		
Red. masses --	6.0932			4.4423			2.6913		
Frc consts --	2.4236			1.8001			1.1250		
IR Inten --	5.3004			4.4075			12.4839		
Raman Activ --	16.2243			1.3886			1.2159		
Depolar --	0.0100			0.1576			0.6583		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.19	0.04	0.01	0.21	0.06	0.09	-0.04	0.02	0.08
2 6	-0.02	0.03	-0.20	0.12	0.14	-0.09	0.09	-0.02	-0.12
3 6	0.02	-0.05	-0.21	-0.04	0.09	-0.10	-0.06	-0.03	0.10
4 6	-0.05	-0.05	0.27	-0.05	0.07	0.11	-0.08	-0.04	-0.08
5 6	-0.03	0.00	0.03	-0.01	0.00	0.02	0.04	0.02	-0.01

```
   6   6     0.07   0.07  -0.21    -0.06  -0.14   0.02    -0.07   0.06  -
0.11
   7   6     0.10  -0.04   0.05     0.08  -0.20  -0.06     0.03  -0.02
0.08
   8   6     0.03  -0.07   0.28    -0.13   0.01   0.00     0.01  -0.09  -
0.08
   9   6     0.03  -0.01   0.03    -0.04  -0.01  -0.01     0.00   0.04  -
0.02
  10   6     0.01   0.01  -0.22    -0.13  -0.01   0.00     0.02  -0.06
0.09
  11   6     0.07   0.16   0.10     0.06  -0.01   0.01     0.04   0.08
0.09
  12   8    -0.01   0.00   0.00     0.07  -0.10   0.01     0.00   0.00
0.00
  13   6    -0.06   0.04  -0.02     0.08  -0.05   0.02     0.01  -0.02
0.01
  14   7    -0.01  -0.04   0.01     0.03   0.05  -0.02    -0.01   0.01
0.00
  15   8     0.02  -0.08   0.05    -0.11   0.07   0.00     0.04   0.10  -
0.02
  16   1    -0.19  -0.10  -0.11     0.18   0.01   0.21    -0.08  -0.08
0.20
  17   1     0.20   0.00   0.01     0.01   0.29  -0.16     0.22  -0.30  -
0.09
  18   1     0.10  -0.19  -0.08    -0.13   0.10  -0.14    -0.36  -0.10
0.07
  19   1     0.26  -0.17   0.14    -0.15   0.09   0.15    -0.20  -0.09  -
0.06
  20   1    -0.01   0.21  -0.05    -0.28  -0.07   0.14    -0.38   0.03  -
0.09
  21   1    -0.03  -0.15  -0.02     0.13  -0.13  -0.19    -0.03  -0.10
0.18
  22   1    -0.20   0.08   0.16    -0.28   0.15  -0.08     0.03  -0.21  -
0.06
  23   1    -0.13  -0.01  -0.12    -0.21   0.08   0.06     0.11  -0.31
0.05
  24   1     0.08   0.11   0.11    -0.09   0.07   0.01     0.13   0.25
0.06
  25   1     0.11   0.15   0.11    -0.10   0.08   0.01     0.00   0.00  -
0.08
  26   1    -0.01   0.01   0.01     0.06  -0.01   0.00     0.01  -0.05
0.01
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.02   0.15  -0.04    -0.04  -0.22   0.05     0.00  -0.03
0.01
                      25                    26                    27
                      ?A                    ?A                    ?A
 Frequencies --    880.8260              907.4612              929.6663
 Red. masses --      3.6676                2.4819                2.6015
 Frc consts  --      1.6765                1.2042                1.3247
 IR Inten    --      2.8975                4.8342                8.0335
 Raman Activ --     19.4746                0.9696                1.3758
 Depolar     --      0.0211                0.5105                0.6522
```

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.16	-0.01	0.08	0.02	0.06	-0.04	-0.07	-0.04	0.04
2	6	0.16	-0.09	-0.05	0.01	-0.08	0.11	0.08	0.00	0.03
3	6	-0.03	-0.02	-0.08	0.02	0.13	0.06	0.00	-0.02	-0.07
4	6	0.11	-0.01	0.06	0.00	0.05	-0.07	-0.03	0.22	-0.05
5	6	-0.03	-0.01	-0.01	0.00	0.00	-0.07	-0.02	0.00	0.06
6	6	-0.16	0.12	-0.04	0.05	0.03	-0.13	-0.04	0.02	-0.01
7	6	-0.10	0.17	0.09	-0.05	-0.03	0.04	-0.03	-0.06	0.04
8	6	-0.04	0.10	0.07	-0.10	-0.04	0.09	0.19	0.01	-0.03
9	6	0.01	-0.01	-0.02	-0.03	0.00	0.07	0.02	0.01	0.06
10	6	0.02	-0.04	-0.09	-0.11	-0.06	-0.06	-0.06	-0.01	-0.05
11	6	-0.08	-0.12	-0.06	0.07	-0.02	0.01	0.00	-0.06	0.01
12	8	-0.01	0.00	0.01	0.02	-0.03	0.01	0.01	-0.03	-0.02
13	6	-0.01	0.01	0.02	0.02	-0.02	-0.03	-0.02	-0.01	-0.06
14	7	0.00	-0.01	0.00	0.02	0.02	0.00	-0.01	0.00	0.02
15	8	-0.01	-0.07	0.00	-0.02	0.02	0.00	-0.03	-0.03	-0.02
16	1	0.19	0.33	0.32	0.01	0.01	-0.04	-0.14	-0.20	0.25
17	1	0.19	-0.21	-0.08	0.08	-0.41	0.04	0.20	0.06	0.18
18	1	-0.08	-0.09	-0.05	0.29	0.40	-0.06	0.07	-0.10	0.00
19	1	0.07	-0.11	0.04	0.10	0.02	-0.11	-0.02	0.56	0.07
20	1	-0.25	0.07	-0.08	0.31	0.12	-0.09	-0.03	0.08	0.05
21	1	0.15	0.36	0.32	0.00	0.02	0.01	-0.12	-0.17	0.18
22	1	-0.09	0.00	0.06	-0.07	-0.12	0.11	0.40	0.04	0.07
23	1	0.01	-0.11	-0.08	-0.17	-0.41	0.03	-0.21	0.01	0.06
24	1	-0.06	-0.11	-0.05	0.21	-0.11	0.01	0.05	-0.02	0.00
25	1	-0.05	-0.11	-0.02	-0.03	0.04	0.01	0.01	-0.11	-0.06
26	1	-0.01	0.03	0.00	0.02	-0.04	0.01	0.01	-0.01	-0.01

```
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.01
  28   1     0.00   0.03   0.00    -0.01  -0.09   0.02     0.01   0.05  -
0.02
                     28                     29                     30
                     ?A                     ?A                     ?A
 Frequencies --    942.9403               976.2424               989.7131
 Red. masses --      2.1095                 2.1836                 2.8378
 Frc consts  --      1.1051                 1.2262                 1.6377
 IR Inten    --      4.1856                 5.1801                 5.9698
 Raman Activ --      4.5712                 4.0209                10.3608
 Depolar     --      0.7456                 0.0640                 0.0312
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.09   0.01   0.00     0.04   0.01   0.05    -0.16   0.19
0.04
   2   6     0.08   0.06   0.06    -0.03   0.12  -0.06    -0.02  -0.01
0.01
   3   6    -0.06   0.01  -0.04     0.04  -0.13   0.02     0.02  -0.02
0.01
   4   6     0.12   0.01   0.01     0.04  -0.05  -0.06    -0.01   0.01  -
0.01
   5   6     0.01   0.01   0.03     0.02   0.03   0.05     0.01   0.00  -
0.03
   6   6     0.02  -0.10  -0.05     0.10   0.03  -0.07     0.01  -0.04
0.01
   7   6    -0.07   0.10  -0.02    -0.03   0.04   0.03     0.25  -0.01
0.05
   8   6    -0.04  -0.11   0.01    -0.07   0.00  -0.02     0.02  -0.03  -
0.02
   9   6    -0.01  -0.03  -0.06    -0.02   0.01   0.07    -0.01   0.00  -
0.04
  10   6    -0.01   0.01   0.05    -0.11   0.01  -0.01    -0.05   0.00
0.02
  11   6     0.07  -0.02   0.00    -0.02  -0.08   0.07    -0.07  -0.12  -
0.09
  12   8     0.00   0.01   0.00     0.00   0.01  -0.01     0.00   0.01
0.00
  13   6     0.01   0.00   0.02     0.01  -0.01  -0.03     0.01  -0.01
0.01
  14   7     0.00   0.00  -0.01     0.01   0.01   0.00     0.00   0.00
0.00
  15   8    -0.05   0.04   0.00    -0.01  -0.01  -0.02    -0.02  -0.01
0.01
  16   1    -0.08   0.05  -0.02     0.06   0.12   0.04    -0.13   0.53
0.17
  17   1     0.23   0.22   0.28    -0.13   0.32  -0.08     0.08  -0.10
0.08
  18   1    -0.27  -0.02  -0.08     0.14  -0.39   0.25     0.12   0.04  -
0.01
  19   1     0.34   0.14   0.00    -0.03  -0.06  -0.05     0.05  -0.01  -
0.04
  20   1    -0.02  -0.32  -0.28     0.31   0.05  -0.10    -0.11  -0.03
0.03
```

21	1	-0.08	0.10	-0.09	0.05	0.11	0.01	0.53	0.20	0.19
22	1	-0.13	-0.36	-0.01	0.05	-0.04	0.04	-0.05	-0.03	-0.05
23	1	0.00	0.15	0.03	-0.29	-0.01	0.13	-0.05	0.10	0.01
24	1	0.15	-0.08	0.00	0.19	0.29	0.00	-0.11	-0.18	-0.08
25	1	0.27	-0.13	0.02	-0.09	-0.25	-0.29	-0.07	-0.10	-0.05
26	1	0.00	0.03	0.00	0.00	-0.03	0.00	0.00	-0.01	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	-0.01	0.00	-0.01	-0.06	0.01	-0.01	-0.03	0.00

	31			32			33		
	?A			?A			?A		
Frequencies --	995.7510			1008.9457			1018.1196		
Red. masses --	2.0514			2.8470			4.3202		
Frc consts --	1.1984			1.7076			2.6385		
IR Inten --	1.5923			4.0406			0.4163		
Raman Activ --	8.8801			1.2001			1.7937		
Depolar --	0.5021			0.7340			0.7270		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	-0.02	-0.02	0.00	0.06	0.07	-0.09	-0.16	-0.06
2	6	0.05	-0.08	-0.04	0.01	0.05	0.05	0.13	0.03	-0.10
3	6	0.16	-0.02	0.01	-0.07	-0.08	0.13	-0.01	0.19	0.09
4	6	-0.04	-0.04	0.00	-0.03	0.03	-0.15	0.03	-0.09	-0.09
5	6	0.01	0.01	0.02	-0.02	0.03	-0.03	-0.01	0.05	0.09
6	6	-0.08	-0.01	0.00	-0.09	-0.02	0.00	0.04	-0.13	0.10
7	6	-0.03	0.05	-0.03	-0.02	-0.06	-0.09	0.09	0.11	0.05
8	6	0.00	-0.08	-0.02	-0.03	0.00	0.17	0.06	0.09	0.07
9	6	-0.01	-0.03	0.01	-0.05	0.02	0.00	-0.08	0.00	-0.08
10	6	-0.11	0.12	0.04	0.05	0.10	-0.13	-0.17	-0.10	-0.10
11	6	0.03	0.06	-0.03	0.09	-0.02	-0.04	-0.14	0.09	0.03
12	8	0.00	0.01	-0.01	0.02	-0.03	0.00	0.02	-0.03	0.00
13	6	0.00	0.00	-0.01	0.01	0.00	0.01	0.02	0.00	0.01
14	7	0.01	0.00	0.00	0.01	0.01	0.00	0.02	0.01	-0.01

15	8	-0.01	0.02	0.02	0.06	-0.03	0.00	0.02	-0.02	0.00
16	1	0.00	-0.05	0.06	-0.05	-0.03	0.22	-0.15	-0.30	0.14
17	1	0.06	-0.21	-0.08	-0.06	0.04	-0.03	0.12	0.02	-0.11
18	1	0.54	-0.06	0.16	-0.10	-0.27	0.27	0.06	0.07	0.21
19	1	-0.09	-0.06	0.01	0.11	-0.15	-0.26	0.29	-0.03	-0.14
20	1	-0.23	-0.11	-0.09	-0.17	0.09	0.14	0.02	-0.06	0.18
21	1	-0.07	0.00	0.02	0.01	-0.01	-0.19	0.13	0.20	-0.19
22	1	0.01	-0.18	0.00	0.13	-0.01	0.25	0.15	-0.05	0.13
23	1	-0.28	0.48	0.12	0.24	0.20	-0.29	-0.01	-0.08	-0.23
24	1	-0.08	-0.11	0.01	-0.16	-0.09	-0.01	-0.23	0.24	0.01
25	1	0.13	0.11	0.16	0.31	-0.06	0.12	-0.07	-0.01	-0.06
26	1	0.00	0.00	-0.01	0.03	-0.09	0.01	0.03	-0.08	0.02
27	8	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.00	0.00
28	1	0.00	-0.02	0.00	-0.01	-0.08	0.02	-0.01	-0.13	0.03

	34			35			36		
	?A			?A			?A		
Frequencies --	1041.3813			1046.4035			1054.2941		
Red. masses --	2.0155			2.2030			2.0976		
Frc consts --	1.2878			1.4212			1.3737		
IR Inten --	3.2324			27.6808			8.4790		
Raman Activ --	5.8084			2.2027			9.2446		
Depolar --	0.7498			0.7155			0.4837		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.06	-0.02	0.05	0.00	-0.01	0.10	-0.02	-0.04	-0.04
2 6	-0.06	-0.07	-0.03	-0.08	-0.03	-0.11	0.07	0.01	0.08
3 6	0.04	0.00	-0.02	0.02	0.03	-0.03	0.01	-0.11	-0.02
4 6	0.15	0.05	-0.03	0.00	0.06	0.01	0.05	-0.02	-0.01
5 6	0.02	0.01	-0.03	0.06	0.04	-0.01	0.04	0.02	-0.01
6 6	-0.03	0.02	0.01	0.06	0.07	0.08	-0.03	0.14	0.06
7 6	0.02	-0.06	-0.04	-0.01	0.07	-0.07	0.06	-0.03	-0.04
8 6	-0.07	0.07	-0.02	0.02	-0.11	0.03	-0.07	-0.02	-0.03

```
    9   6    -0.03  -0.06   0.00     0.00  -0.08   0.02    -0.04  -0.08
0.03
   10   6     0.04   0.03   0.02     0.03  -0.06   0.02    -0.06  -0.05
0.02
   11   6     0.00  -0.02   0.13     0.01  -0.01  -0.05     0.00   0.07  -
0.06
   12   8     0.00   0.01   0.00     0.01   0.00   0.00     0.00   0.01
0.00
   13   6     0.00   0.01   0.01     0.00   0.00   0.00     0.00   0.01
0.00
   14   7     0.01   0.00   0.00     0.00  -0.01   0.00     0.01   0.00
0.00
   15   8    -0.06   0.00   0.00    -0.09   0.05   0.00    -0.03   0.05  -
0.01
   16   1    -0.05  -0.07  -0.05    -0.05  -0.01   0.37    -0.02  -0.17  -
0.16
   17   1     0.05  -0.35  -0.03    -0.32  -0.01  -0.35     0.29   0.14
0.37
   18   1     0.18   0.11  -0.06    -0.01   0.06  -0.05    -0.10  -0.27
0.07
   19   1     0.38   0.12  -0.07     0.02   0.09   0.02     0.19  -0.04  -
0.06
   20   1    -0.33   0.05   0.10     0.26   0.18   0.16     0.03   0.36
0.28
   21   1     0.02  -0.04  -0.18    -0.01   0.09  -0.14     0.13   0.02
0.03
   22   1    -0.07   0.26  -0.04     0.06  -0.31   0.07    -0.11   0.10  -
0.05
   23   1     0.10   0.19  -0.04     0.09  -0.21  -0.01    -0.10  -0.23
0.07
   24   1     0.10   0.38   0.06    -0.25  -0.03  -0.03    -0.24  -0.10  -
0.02
   25   1    -0.01  -0.24  -0.25     0.32  -0.11   0.09    -0.02   0.22
0.16
   26   1     0.01  -0.03   0.00     0.04  -0.14   0.02     0.01  -0.06
0.01
   27   8     0.00   0.00   0.00     0.00   0.01   0.00     0.01   0.01
0.00
   28   1    -0.01  -0.06   0.01    -0.01  -0.04   0.01    -0.02  -0.11
0.03
                     37                     38                     39
                     ?A                     ?A                     ?A
 Frequencies --  1060.8375              1086.2978              1109.6340
 Red. masses --     1.7629                 1.9233                 2.4971
 Frc consts  --     1.1689                 1.3372                 1.8116
 IR Inten    --     1.6156                70.0655                39.0842
 Raman Activ --     6.0478                 1.4214                 6.5009
 Depolar     --     0.6913                 0.1259                 0.7467
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.08   0.08  -0.02     0.02  -0.01  -0.02    -0.01  -0.01
0.01
   2   6     0.06  -0.01  -0.04    -0.03  -0.01   0.02     0.00  -0.01
0.00
```

3	6	0.00	0.02	0.01	-0.01	0.01	-0.01	0.02	-0.01	0.02
4	6	0.00	-0.08	0.04	-0.04	0.01	0.03	0.02	-0.01	-0.01
5	6	0.02	0.02	-0.01	0.11	0.12	-0.03	0.12	0.04	-0.03
6	6	0.02	0.00	0.08	0.01	-0.03	-0.06	-0.01	-0.02	0.01
7	6	-0.09	0.00	-0.01	0.00	0.01	0.05	-0.01	-0.03	0.01
8	6	0.04	0.07	-0.05	0.04	0.02	0.01	-0.02	0.03	-0.01
9	6	-0.04	-0.04	0.01	-0.08	-0.10	0.02	0.09	0.22	-0.06
10	6	-0.05	-0.04	-0.02	0.03	0.03	-0.02	-0.03	0.01	0.02
11	6	0.07	-0.03	0.00	-0.03	0.00	0.00	0.02	0.01	-0.02
12	8	0.01	0.00	0.00	0.03	0.00	0.00	0.00	0.06	-0.01
13	6	0.00	0.01	-0.01	0.01	0.01	0.00	0.03	-0.05	0.01
14	7	0.01	0.00	0.00	0.02	0.00	0.00	-0.02	0.02	0.00
15	8	-0.01	0.01	0.00	-0.11	0.01	0.01	-0.10	-0.13	0.03
16	1	-0.03	0.43	0.08	0.04	-0.07	-0.19	-0.03	-0.07	0.04
17	1	0.09	-0.03	-0.02	0.04	0.01	0.11	0.01	0.02	0.02
18	1	-0.03	-0.05	0.06	-0.09	-0.09	0.05	-0.03	-0.02	0.01
19	1	-0.10	-0.20	0.03	-0.20	-0.17	0.00	0.07	-0.07	-0.05
20	1	0.01	0.12	0.22	0.03	-0.21	-0.26	-0.01	0.09	0.13
21	1	-0.37	-0.23	-0.15	0.04	0.01	0.23	-0.09	-0.08	-0.09
22	1	0.08	0.31	-0.05	0.22	0.14	0.09	-0.23	-0.11	-0.10
23	1	0.00	-0.05	-0.06	0.23	0.16	-0.18	-0.16	-0.15	0.14
24	1	0.38	-0.23	0.01	0.05	-0.03	0.00	-0.04	-0.07	-0.01
25	1	0.25	-0.12	0.02	-0.20	0.09	-0.01	0.07	0.03	0.06
26	1	0.02	-0.05	0.01	0.13	-0.54	0.08	0.12	-0.67	0.10
27	8	0.01	0.00	0.00	0.02	0.01	-0.01	-0.03	-0.04	0.01
28	1	-0.01	-0.06	0.02	-0.03	-0.23	0.05	0.05	0.41	-0.10

	40	41	42
	?A	?A	?A

Frequencies --	1158.9530			1177.9192			1188.1503		
Red. masses --	1.3783			1.7558			3.7004		
Frc consts --	1.0907			1.4354			3.0778		
IR Inten --	8.8669			14.7862			26.6454		
Raman Activ --	1.5605			2.2214			2.2411		
Depolar --	0.7499			0.6077			0.6715		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.02	-0.02	0.04	0.00	0.01	-0.02	-0.06	0.00	0.00
2 6	0.00	0.00	-0.02	0.02	0.02	0.02	0.02	-0.06	0.01
3 6	0.05	-0.02	0.04	-0.07	0.03	0.02	-0.07	0.10	-0.06
4 6	0.03	0.03	0.01	-0.03	-0.01	-0.02	0.06	-0.13	-0.07
5 6	-0.02	-0.01	-0.06	-0.01	0.03	0.00	0.03	-0.01	0.14
6 6	0.00	0.01	-0.04	-0.01	0.00	0.01	-0.08	-0.06	0.01
7 6	-0.01	-0.04	0.05	0.01	0.01	-0.01	0.03	-0.03	0.02
8 6	0.01	0.04	-0.01	0.01	0.01	0.00	-0.14	-0.03	-0.14
9 6	-0.03	-0.01	-0.07	0.11	-0.15	0.03	0.02	0.07	0.25
10 6	-0.04	0.03	0.06	0.04	-0.01	-0.03	0.14	0.02	-0.12
11 6	0.01	0.02	-0.05	0.00	0.00	0.01	0.04	0.08	-0.03
12 8	0.00	-0.01	0.00	0.02	-0.03	0.00	0.00	0.03	-0.01
13 6	0.00	0.01	0.01	0.04	-0.02	0.01	-0.02	0.00	-0.04
14 7	0.00	0.00	0.00	0.01	0.04	-0.01	-0.01	-0.02	0.01
15 8	0.01	-0.01	0.01	-0.02	0.05	-0.01	-0.01	-0.01	-0.04
16 1	-0.11	-0.19	0.36	-0.04	-0.07	0.09	-0.12	0.04	0.41
17 1	-0.20	0.17	-0.16	-0.05	-0.05	-0.09	-0.24	0.19	-0.16
18 1	-0.06	0.00	0.00	0.12	-0.12	0.20	0.10	0.00	0.07
19 1	0.38	-0.08	-0.13	0.14	-0.16	-0.13	0.12	0.22	0.05
20 1	0.23	-0.12	-0.22	0.05	-0.07	-0.08	0.20	-0.11	-0.09
21 1	-0.12	-0.20	0.35	0.05	0.03	0.08	0.14	0.01	0.34
22 1	-0.20	0.32	-0.13	-0.12	0.16	-0.08	0.03	0.16	-0.07
23 1	0.04	-0.04	0.00	-0.14	0.12	0.09	-0.03	0.07	0.01

```
  24   1    -0.02  -0.15  -0.02     0.05   0.02   0.00     0.00  -0.11
0.01
  25   1     0.00   0.11   0.09    -0.08   0.01  -0.04     0.04   0.19
0.14
  26   1    -0.02   0.11  -0.01     0.01  -0.01   0.00     0.02  -0.13
0.02
  27   8     0.01   0.01   0.00    -0.07  -0.04   0.01     0.02   0.02
0.00
  28   1    -0.01  -0.10   0.03     0.08   0.79  -0.19    -0.03  -0.24
0.06
                     43                     44                     45
                     ?A                     ?A                     ?A
 Frequencies --  1215.8635              1218.9827              1226.8247
 Red. masses --     2.9626                 1.7409                 3.5939
 Frc consts  --     2.5805                 1.5241                 3.1870
 IR Inten    --   126.0789                 5.5334                22.3576
 Raman Activ --     4.6482                 4.2769                 2.6583
 Depolar     --     0.3858                 0.7005                 0.7242
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.01  -0.03   0.09    -0.02  -0.01   0.02     0.04   0.03  -
0.02
   2   6    -0.11  -0.03  -0.05    -0.01  -0.06  -0.03    -0.02  -0.06
0.04
   3   6     0.00   0.08  -0.08     0.10  -0.01   0.00     0.01   0.01  -
0.11
   4   6     0.09   0.05  -0.06     0.04  -0.02   0.01    -0.07  -0.08  -
0.14
   5   6    -0.11   0.21   0.06     0.03  -0.03   0.00     0.06  -0.04
0.28
   6   6     0.08   0.02  -0.01    -0.03  -0.02  -0.01    -0.02   0.08  -
0.03
   7   6    -0.01  -0.04   0.05     0.01  -0.01   0.01     0.01  -0.06  -
0.03
   8   6    -0.05   0.02  -0.03    -0.04  -0.01  -0.01    -0.03   0.05
0.13
   9   6    -0.06   0.06  -0.02    -0.11   0.00   0.04    -0.02  -0.05  -
0.21
  10   6     0.06  -0.06   0.06    -0.06   0.06  -0.01     0.02  -0.03
0.07
  11   6     0.02   0.03  -0.07     0.01   0.02   0.00     0.01   0.01
0.02
  12   8     0.03  -0.12   0.01    -0.02   0.01   0.00    -0.01   0.05  -
0.03
  13   6     0.03  -0.03   0.01     0.07  -0.06   0.00     0.01   0.01
0.05
  14   7     0.01   0.02  -0.01     0.05   0.07  -0.02     0.00   0.00  -
0.01
  15   8     0.01  -0.06  -0.01     0.01  -0.01   0.00     0.00   0.02  -
0.01
  16   1     0.05   0.07  -0.18     0.01   0.07  -0.05     0.05   0.23
0.12
  17   1     0.20  -0.08   0.27     0.00   0.18   0.07    -0.06   0.09
0.06
```

18	1	0.13	-0.26	0.23	-0.30	0.08	-0.19	-0.04	0.22	-0.30
19	1	-0.21	-0.34	-0.12	-0.14	0.18	0.13	-0.01	0.01	-0.12
20	1	-0.15	-0.05	-0.04	0.15	0.03	0.01	0.15	-0.03	-0.18
21	1	-0.09	-0.13	0.11	0.05	0.03	0.06	-0.05	-0.15	0.10
22	1	0.09	-0.14	0.05	0.26	0.02	0.14	0.32	0.24	0.29
23	1	-0.07	0.05	0.15	0.34	-0.13	-0.30	-0.24	0.05	0.27
24	1	-0.15	-0.16	-0.03	-0.02	0.01	0.01	-0.02	0.07	0.01
25	1	0.13	0.09	0.14	0.02	0.03	0.03	0.12	-0.06	-0.01
26	1	-0.04	0.35	-0.05	-0.05	0.21	-0.03	0.02	-0.17	0.03
27	8	-0.01	-0.01	0.00	-0.05	-0.04	0.01	0.00	0.00	0.00
28	1	0.01	0.12	-0.03	0.06	0.53	-0.13	0.00	0.04	-0.01

	46	47	48
	?A	?A	?A
Frequencies --	1232.5503	1257.5787	1264.8637
Red. masses --	2.9158	1.0717	2.4480
Frc consts --	2.6098	0.9987	2.3076
IR Inten --	40.6438	1.4111	8.4570
Raman Activ --	3.9306	14.8508	4.2997
Depolar --	0.7010	0.7493	0.5033

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	-0.05	0.10	0.00	-0.02	0.02	-0.04	0.01	0.04
2	6	-0.07	0.14	-0.04	-0.03	-0.02	0.01	-0.01	-0.06	-0.04
3	6	-0.07	-0.06	0.05	0.01	0.00	-0.01	0.09	0.05	0.04
4	6	0.07	-0.04	-0.03	0.02	-0.01	0.00	0.03	0.00	-0.04
5	6	0.07	-0.14	0.01	0.00	0.01	0.02	0.01	0.01	0.03
6	6	0.13	-0.05	-0.07	-0.01	0.03	-0.02	-0.07	-0.10	-0.06
7	6	-0.05	-0.03	0.12	0.02	0.01	-0.02	-0.04	-0.05	0.04
8	6	-0.04	0.11	-0.01	0.01	-0.01	0.00	0.02	0.10	-0.01
9	6	0.01	-0.09	0.00	0.00	0.00	-0.02	0.16	-0.11	-0.02
10	6	-0.01	-0.02	-0.02	0.00	0.00	0.01	0.00	0.13	-0.01
11	6	0.02	0.03	-0.12	-0.01	0.01	0.00	0.03	0.01	0.01

12	8	-0.03	0.07	-0.01	0.00	-0.01	0.00	-0.01	-0.02	0.00
13	6	0.00	0.01	0.00	0.00	0.00	0.00	-0.04	0.05	0.00
14	7	0.01	0.00	0.00	0.00	0.00	0.00	-0.04	-0.05	0.01
15	8	-0.01	0.04	-0.02	0.00	0.00	0.00	-0.05	0.00	0.01
16	1	-0.01	-0.11	0.09	-0.07	-0.10	0.35	0.00	0.00	-0.17
17	1	0.20	-0.32	0.05	-0.06	0.13	0.05	0.04	0.15	0.10
18	1	0.20	0.25	-0.11	0.01	-0.02	0.00	-0.40	-0.07	-0.01
19	1	-0.19	0.21	0.14	0.03	-0.08	-0.03	-0.23	-0.20	-0.05
20	1	-0.33	0.08	0.16	-0.16	0.04	0.02	0.29	0.23	0.25
21	1	-0.05	0.01	-0.02	0.07	0.13	-0.40	0.20	0.20	-0.12
22	1	0.14	-0.07	0.10	0.12	-0.09	0.05	-0.07	-0.24	-0.03
23	1	-0.05	0.23	-0.02	0.03	-0.04	-0.01	-0.15	-0.25	0.16
24	1	-0.13	-0.30	-0.06	0.49	-0.28	0.01	-0.07	0.03	0.01
25	1	0.06	0.21	0.22	-0.44	0.26	0.00	-0.01	0.05	0.04
26	1	-0.02	-0.05	0.00	-0.01	0.04	0.00	-0.04	0.21	-0.02
27	8	-0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.02	-0.01
28	1	0.01	0.09	-0.02	0.00	0.00	0.00	-0.02	-0.15	0.04

	49			50			51		
	?A			?A			?A		
Frequencies --	1288.3088			1312.4127			1342.5828		
Red. masses --	1.7692			1.6385			1.9749		
Frc consts --	1.7300			1.6628			2.0974		
IR Inten --	0.7041			8.2588			13.7949		
Raman Activ --	0.8732			2.7490			1.7609		
Depolar --	0.7440			0.7488			0.6592		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.04	-0.12	-0.04	0.05	0.04	0.01	0.02	0.00	0.05
2 6	-0.02	-0.01	0.04	-0.04	0.01	0.00	-0.06	-0.06	-0.07
3 6	-0.01	-0.01	0.01	0.04	-0.04	-0.02	0.05	0.11	0.03
4 6	-0.01	0.04	-0.03	-0.05	0.03	-0.04	-0.01	0.00	-0.07
5 6	0.00	0.01	-0.02	0.01	0.01	0.14	0.00	-0.11	-0.03

6	6	-0.02	0.00	-0.06	0.03	-0.02	0.00	0.02	0.08	0.06
7	6	0.13	0.02	0.06	0.00	0.05	0.01	0.00	-0.02	-0.04
8	6	-0.03	0.02	0.02	0.04	-0.01	-0.02	-0.01	0.01	0.06
9	6	0.02	-0.05	0.03	0.02	0.01	0.10	0.09	0.01	0.02
10	6	0.01	0.06	0.00	-0.05	-0.01	-0.02	-0.06	-0.09	-0.02
11	6	-0.09	0.05	0.00	-0.01	-0.03	-0.01	0.03	-0.01	0.00
12	8	0.00	0.00	0.00	0.00	0.00	-0.02	-0.01	0.03	0.00
13	6	-0.01	0.01	0.00	0.00	0.00	-0.02	-0.01	0.01	-0.01
14	7	0.00	0.00	0.00	0.00	0.00	0.00	-0.02	-0.02	0.01
15	8	0.00	0.01	0.00	0.00	0.00	-0.02	-0.01	0.02	0.00
16	1	0.12	0.49	0.16	0.01	-0.14	0.02	0.08	0.17	-0.08
17	1	-0.06	0.19	0.08	0.13	-0.08	0.14	0.21	0.16	0.31
18	1	0.09	-0.03	0.06	-0.15	0.27	-0.32	-0.22	-0.32	0.27
19	1	-0.08	0.13	0.02	0.21	-0.41	-0.28	-0.06	0.23	0.04
20	1	-0.12	0.02	-0.02	-0.13	0.04	0.08	0.01	-0.23	-0.28
21	1	-0.32	-0.34	-0.22	-0.15	-0.09	0.00	-0.05	-0.09	0.04
22	1	-0.23	-0.11	-0.06	-0.38	-0.06	-0.23	-0.23	0.01	-0.04
23	1	0.08	-0.18	-0.03	0.24	0.09	-0.26	0.13	0.34	-0.22
24	1	0.15	-0.08	0.00	-0.03	-0.01	-0.02	0.02	-0.02	0.00
25	1	0.33	-0.18	0.01	-0.02	-0.04	-0.03	-0.16	0.11	0.01
26	1	0.01	-0.04	0.00	0.00	0.01	0.02	0.01	-0.08	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
28	1	0.00	0.01	0.00	0.00	0.00	0.00	0.00	-0.03	0.01

	52	53	54
	?A	?A	?A
Frequencies --	1346.4759	1359.1457	1369.1409
Red. masses --	1.4200	1.5022	1.8506
Frc consts --	1.5168	1.6349	2.0439
IR Inten --	8.6781	1.1926	4.3541
Raman Activ --	0.1337	1.4833	0.2862
Depolar --	0.5660	0.7482	0.5756

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	0.02	0.01	-0.03	-0.04	-0.04	-0.02	-0.05	0.00
2	6	0.04	-0.09	-0.06	0.03	0.02	-0.02	0.02	0.00	-0.04
3	6	-0.09	-0.01	0.02	-0.04	-0.03	0.02	0.00	-0.04	0.11
4	6	0.02	0.03	0.00	0.04	0.03	0.02	0.07	0.11	0.00
5	6	-0.03	-0.04	0.02	-0.01	0.00	0.00	0.05	-0.01	0.00
6	6	0.05	0.02	0.01	-0.08	0.02	-0.05	0.00	0.02	0.05
7	6	-0.04	-0.02	-0.01	0.00	-0.05	-0.03	0.03	0.02	-0.03
8	6	0.01	0.01	0.00	0.03	0.06	0.01	-0.07	-0.10	0.01
9	6	0.01	-0.01	-0.01	-0.04	0.01	0.01	0.05	0.02	-0.01
10	6	-0.02	0.05	0.03	0.02	-0.09	0.06	0.01	-0.04	-0.09
11	6	0.03	-0.01	0.01	0.01	0.02	0.03	-0.05	0.03	0.01
12	8	0.01	0.02	0.00	0.00	0.00	0.00	-0.01	-0.01	0.00
13	6	0.00	0.00	0.00	0.01	-0.01	0.00	-0.01	0.01	0.00
14	7	0.00	0.00	0.00	0.01	0.01	0.00	-0.01	-0.01	0.00
15	8	0.01	0.01	-0.01	0.01	0.00	-0.01	-0.02	-0.01	0.00
16	1	0.00	0.01	-0.10	-0.03	0.13	0.13	-0.01	0.01	-0.06
17	1	-0.03	0.57	0.13	0.04	0.07	0.01	0.02	0.14	0.01
18	1	0.52	0.20	0.04	0.19	0.18	-0.06	-0.16	0.33	-0.21
19	1	-0.10	-0.17	-0.04	-0.18	-0.15	0.01	-0.35	-0.39	-0.07
20	1	-0.25	-0.05	-0.01	0.49	0.22	0.06	-0.02	-0.11	-0.08
21	1	0.10	0.08	0.11	0.11	0.04	0.04	0.02	-0.03	0.13
22	1	-0.03	-0.01	-0.02	-0.16	-0.37	-0.05	0.17	0.35	0.10
23	1	0.18	-0.29	-0.09	0.14	0.53	-0.10	-0.30	0.19	0.12
24	1	-0.10	0.07	0.01	0.05	0.02	0.03	0.22	-0.11	0.01
25	1	-0.02	0.02	0.00	0.00	0.01	-0.01	0.10	-0.06	-0.01
26	1	0.03	-0.15	0.02	0.01	-0.05	0.01	-0.04	0.18	-0.02

```
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.01   0.00     0.00   0.02   0.00     0.00  -0.03
0.01
                     55                     56                     57
                     ?A                     ?A                     ?A
 Frequencies --  1371.7237              1380.1672              1396.6342
 Red. masses --     1.5360                 1.8807                 1.6633
 Frc consts  --     1.7029                 2.1108                 1.9116
 IR Inten    --    16.0381                39.5222                 2.7539
 Raman Activ --     2.7301                 1.8968                 8.4681
 Depolar     --     0.6961                 0.3195                 0.6379
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.01  -0.02    -0.03   0.03  -0.04    -0.01  -0.10  -
0.05
   2   6     0.00   0.07  -0.03     0.06  -0.04   0.09    -0.03   0.06
0.03
   3   6    -0.07  -0.04  -0.04    -0.01  -0.01  -0.01     0.03  -0.02  -
0.03
   4   6     0.03  -0.02  -0.02     0.00  -0.05   0.00     0.00   0.01  -
0.01
   5   6     0.09   0.03   0.02     0.12   0.08  -0.01    -0.04   0.03
0.02
   6   6    -0.06   0.00   0.07     0.07   0.07  -0.02     0.06  -0.01
0.02
   7   6     0.02   0.00  -0.01     0.00  -0.04  -0.02    -0.09  -0.08  -
0.05
   8   6    -0.01  -0.01   0.03    -0.01   0.08   0.02     0.03  -0.03
0.01
   9   6     0.06   0.02  -0.02     0.07   0.01   0.01     0.04   0.01
0.00
  10   6    -0.03   0.05   0.03    -0.06  -0.05  -0.01    -0.05   0.02
0.01
  11   6     0.01  -0.02   0.00     0.00   0.00   0.00     0.00   0.08
0.03
  12   8    -0.02  -0.02   0.00    -0.03  -0.04   0.01     0.01   0.00
0.00
  13   6    -0.01   0.01   0.00    -0.01   0.01  -0.01     0.00   0.00
0.00
  14   7    -0.01  -0.01   0.00    -0.01  -0.01   0.00    -0.01  -0.01
0.00
  15   8    -0.03  -0.02   0.00    -0.05  -0.03   0.00     0.00   0.00
0.00
  16   1    -0.05  -0.09   0.13    -0.07  -0.12   0.02     0.03   0.42
0.25
  17   1     0.25  -0.30   0.08    -0.38   0.16  -0.29     0.02  -0.26  -
0.04
  18   1     0.34  -0.01   0.05    -0.09   0.02  -0.05    -0.09  -0.04  -
0.05
  19   1    -0.24   0.03   0.07    -0.13   0.09   0.09    -0.06   0.00  -
0.01
  20   1     0.35  -0.21  -0.22    -0.42  -0.06  -0.08    -0.16  -0.09  -
0.02
```

21	1	-0.08	-0.08	-0.09	0.00	-0.07	0.12	0.47	0.37	0.27
22	1	-0.07	0.11	-0.01	-0.05	-0.30	0.04	-0.10	0.14	-0.07
23	1	0.28	-0.31	-0.16	0.10	0.18	-0.16	0.14	-0.15	-0.12
24	1	-0.02	0.01	0.00	-0.08	0.04	0.00	0.13	0.00	0.04
25	1	-0.10	0.03	-0.02	0.07	-0.06	-0.03	0.17	0.00	0.04
26	1	-0.08	0.33	-0.05	-0.10	0.45	-0.06	0.03	-0.11	0.02
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	-0.04	0.01	0.00	-0.03	0.01	0.00	-0.01	0.00

	58	59	60
	?A	?A	?A
Frequencies --	1406.0205	1409.9994	1426.3504
Red. masses --	1.4573	1.6735	1.4638
Frc consts --	1.6974	1.9603	1.7546
IR Inten --	1.2077	15.3609	14.1518
Raman Activ --	1.9440	5.3320	0.5024
Depolar --	0.5902	0.7484	0.7437

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	0.05	0.03	0.06	-0.03	-0.05	-0.02	-0.05	0.10
2	6	0.00	-0.02	0.01	-0.06	-0.03	-0.04	0.05	0.03	0.00
3	6	-0.02	0.04	-0.03	-0.04	0.01	0.04	-0.02	0.01	-0.03
4	6	0.03	-0.02	-0.05	-0.10	-0.02	0.03	-0.06	0.04	0.01
5	6	0.03	-0.01	0.01	0.12	0.03	-0.05	0.02	-0.03	0.02
6	6	0.00	-0.05	-0.06	0.01	-0.05	-0.04	-0.02	-0.03	0.00
7	6	-0.01	0.03	-0.01	-0.04	0.03	0.00	0.02	0.01	-0.06
8	6	0.04	-0.06	0.05	-0.01	-0.03	-0.02	-0.05	0.01	-0.02
9	6	-0.02	0.01	-0.02	0.02	0.03	-0.02	0.06	0.01	-0.01
10	6	0.00	-0.02	0.05	0.03	-0.02	0.01	-0.03	0.00	0.04
11	6	-0.09	0.03	-0.01	0.02	0.00	0.02	-0.03	0.02	-0.01
12	8	-0.01	0.00	0.00	-0.03	-0.03	0.01	-0.01	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.01	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	-0.01	0.00

15	8	-0.01	0.00	0.00	-0.03	-0.01	0.01	0.00	0.00	0.00
16	1	-0.01	-0.33	-0.14	0.06	0.23	0.26	0.13	0.18	-0.48
17	1	-0.05	0.06	-0.01	0.23	0.18	0.37	-0.11	-0.11	-0.22
18	1	0.10	-0.13	0.13	0.12	0.06	0.06	0.12	-0.08	0.07
19	1	-0.23	0.17	0.09	0.40	0.08	-0.08	0.35	-0.10	-0.16
20	1	0.01	0.27	0.28	-0.02	0.21	0.26	0.09	0.08	0.10
21	1	0.11	0.12	0.11	0.04	0.08	0.13	-0.02	-0.10	0.28
22	1	-0.29	0.38	-0.15	0.19	0.14	0.06	0.27	-0.16	0.14
23	1	0.11	0.11	-0.04	-0.03	0.16	0.04	0.20	-0.03	-0.13
24	1	0.33	-0.16	-0.01	-0.09	0.16	0.01	0.29	-0.20	0.00
25	1	0.24	-0.15	0.01	0.00	0.03	0.03	-0.07	0.07	0.02
26	1	-0.02	0.08	-0.02	-0.08	0.36	-0.05	-0.02	0.05	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	-0.02	0.00	0.00	-0.02	0.00

	61	62	63
	?A	?A	?A
Frequencies --	1440.4583	1447.8104	1459.7658
Red. masses --	1.5840	1.6259	1.7455
Frc consts --	1.9365	2.0081	2.1915
IR Inten --	15.1862	1.1179	6.6471
Raman Activ --	2.0399	1.3413	4.8204
Depolar --	0.7097	0.7475	0.7491

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.05	0.06	-0.05	0.02	0.04	-0.07	-0.04	-0.04	-0.02
2	6	-0.02	-0.01	0.01	-0.04	0.01	0.00	0.04	0.00	0.06
3	6	0.01	0.03	-0.03	0.02	0.00	-0.01	0.01	0.01	-0.03
4	6	-0.01	0.03	0.06	0.05	-0.02	0.03	0.04	0.03	-0.01
5	6	-0.02	-0.05	0.00	-0.09	0.01	-0.02	-0.05	0.01	0.02
6	6	-0.01	0.04	-0.01	0.03	-0.06	-0.01	0.00	-0.01	-0.08
7	6	-0.01	-0.07	0.08	0.04	0.06	-0.10	0.00	0.05	0.08
8	6	-0.05	0.01	-0.07	-0.08	0.02	0.01	-0.04	-0.09	-0.01

```
    9   6     0.07   0.01   0.00     0.07  -0.02  -0.02     0.10   0.01  -
0.02
   10   6    -0.04  -0.02   0.03    -0.03   0.01   0.02    -0.05  -0.04
0.06
   11   6    -0.07   0.03  -0.01    -0.01  -0.02   0.03     0.08  -0.04  -
0.01
   12   8     0.00   0.01   0.00     0.02   0.01   0.00     0.01   0.00
0.00
   13   6    -0.01   0.01   0.00    -0.01   0.01   0.00    -0.01   0.01
0.00
   14   7    -0.01  -0.01   0.00    -0.01  -0.01   0.00    -0.01  -0.01
0.00
   15   8     0.00   0.00   0.00     0.01   0.01   0.00     0.00   0.00
0.00
   16   1    -0.06  -0.31   0.14    -0.11  -0.21   0.35    -0.01   0.19
0.01
   17   1     0.06   0.00   0.09     0.10  -0.05   0.14    -0.19   0.00  -
0.19
   18   1     0.01  -0.15   0.11    -0.05  -0.04   0.00    -0.01  -0.07
0.02
   19   1     0.13  -0.27  -0.08    -0.19  -0.02   0.10    -0.16  -0.08
0.00
   20   1     0.08  -0.08  -0.16    -0.08   0.15   0.24    -0.01   0.20
0.15
   21   1     0.14   0.13  -0.28    -0.19  -0.28   0.55    -0.14   0.01  -
0.27
   22   1     0.39  -0.02   0.14     0.20  -0.18   0.17     0.15   0.45
0.04
   23   1     0.18   0.07  -0.15     0.09  -0.05  -0.07     0.25   0.21  -
0.20
   24   1     0.03  -0.03  -0.01     0.07   0.06   0.00    -0.36   0.18  -
0.01
   25   1     0.47  -0.28   0.01    -0.07  -0.03  -0.06    -0.23   0.16
0.02
   26   1     0.01  -0.06   0.01     0.05  -0.19   0.02     0.02  -0.08
0.01
   27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   28   1     0.00  -0.01   0.00     0.00   0.00   0.00     0.00  -0.01
0.00
                     64                    65                    66
                     ?A                    ?A                    ?A
 Frequencies --  1468.2544             1635.0509             1975.0440
 Red. masses --     2.2661                1.1028               11.6750
 Frc consts  --     2.8782                1.7370               26.8325
 IR Inten    --    64.0961                2.9438              235.2060
 Raman Activ --     4.0685                9.2081              105.6994
 Depolar     --     0.5772                0.6824                0.1914
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.03   0.02   0.07    -0.01   0.00   0.00     0.00   0.00
0.00
   2   6     0.01  -0.01  -0.06     0.00   0.00   0.00     0.00   0.00
0.00
```

3	6	0.00	-0.10	0.07	0.00	0.00	0.00	0.00	0.00	0.00
4	6	-0.03	-0.12	-0.02	0.00	0.00	0.00	0.00	0.00	0.00
5	6	-0.13	0.18	-0.03	0.00	0.00	0.00	0.00	-0.01	0.00
6	6	-0.02	0.03	0.01	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	-0.01	0.02	0.01	-0.01	0.00	0.00	0.00	0.00
8	6	-0.03	-0.01	-0.01	0.00	0.01	0.00	0.00	0.00	0.00
9	6	0.12	-0.02	0.00	0.00	0.00	0.00	-0.13	0.01	0.01
10	6	-0.03	-0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	-0.03	0.02	-0.02	-0.04	-0.07	-0.04	0.00	0.00	0.00
12	8	0.03	-0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	-0.01	0.02	0.00	0.00	0.00	0.00	0.67	0.33	-0.14
14	7	-0.02	-0.02	0.01	0.00	0.00	0.00	-0.44	-0.33	0.12
15	8	0.01	-0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.00
16	1	0.06	-0.07	-0.19	-0.02	-0.01	-0.01	0.00	0.00	0.00
17	1	0.10	0.15	0.10	-0.01	-0.01	-0.02	0.00	0.00	0.00
18	1	0.04	0.43	-0.31	0.00	-0.01	0.00	0.01	-0.01	0.00
19	1	0.19	0.53	0.15	-0.02	-0.02	-0.01	0.01	-0.01	0.00
20	1	0.11	-0.03	-0.08	-0.01	-0.02	-0.02	0.00	0.00	0.00
21	1	0.04	0.05	-0.12	0.00	-0.02	-0.01	-0.01	0.00	0.00
22	1	0.11	0.12	0.05	-0.01	-0.02	-0.01	0.01	0.01	0.00
23	1	0.08	0.12	-0.10	0.00	-0.01	0.00	0.00	0.01	0.00
24	1	0.14	-0.09	-0.02	0.33	0.61	-0.14	0.00	0.00	0.00
25	1	0.10	0.00	0.06	0.13	0.28	0.63	0.00	0.00	0.00
26	1	0.06	-0.16	0.02	0.00	0.00	0.00	0.00	0.00	0.00
27	8	0.00	0.01	0.00	0.00	0.00	0.00	-0.03	0.03	0.00
28	1	0.00	-0.01	0.00	0.00	0.00	0.00	0.04	0.28	-0.07

	67	68	69
	?A	?A	?A

Frequencies --		3178.2008			3212.1761			3220.1672		
Red. masses --		1.0592			1.0866			1.1035		
Frc consts --		6.3039			6.6056			6.7421		
IR Inten --		71.1561			59.1322			51.3882		
Raman Activ --		137.7754			120.2749			104.4084		
Depolar --		0.2869			0.3544			0.6921		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	0.00	0.00	-0.07	0.01	-0.01	0.01	0.00	0.00
2	6	0.00	0.00	0.00	0.02	0.01	-0.02	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	-0.03	-0.06	-0.02	-0.01	-0.02	0.01	-0.01	-0.02	0.09
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	-0.24	0.04	-0.05	0.87	-0.16	0.16	-0.15	0.03	-0.03
17	1	0.00	0.00	0.00	-0.20	-0.08	0.18	0.04	0.01	-0.04
18	1	0.00	0.00	0.00	0.01	-0.01	-0.02	0.00	0.00	0.00
19	1	0.00	0.00	0.00	-0.04	0.05	-0.14	0.01	-0.02	0.05
20	1	0.00	-0.01	0.01	0.00	0.01	-0.01	0.00	-0.01	0.01
21	1	0.03	-0.03	-0.01	0.02	-0.02	0.00	-0.01	0.01	0.00
22	1	0.01	0.00	-0.01	0.00	0.00	0.01	0.00	0.00	0.01
23	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

24	1	0.03	0.06	0.56	0.00	0.00	0.00	-0.06	-0.12	-0.81
25	1	0.34	0.59	-0.39	0.13	0.22	-0.14	0.24	0.41	-0.24
26	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	70			71			72		
	?A			?A			?A		
Frequencies --	3244.0332			3263.3710			3273.1601		
Red. masses --	1.0881			1.0882			1.0886		
Frc consts --	6.7466			6.8277			6.8713		
IR Inten --	66.5237			50.8192			58.8862		
Raman Activ --	128.9818			89.6393			137.8856		
Depolar --	0.4675			0.3389			0.4230		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	0.00	0.00	-0.01	0.00	0.00	-0.01	0.00	0.00
2	6	-0.05	-0.02	0.05	0.00	0.00	0.00	-0.01	0.00	0.01
3	6	0.00	-0.01	-0.01	0.00	0.00	-0.01	0.01	-0.01	-0.02
4	6	0.00	0.00	0.01	-0.02	0.03	-0.07	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.02	-0.02	0.00	0.01	-0.01	0.01	-0.06	0.05
7	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.01	0.00
8	6	0.00	0.00	0.00	-0.01	0.00	0.02	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	-0.01
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	0.24	-0.04	0.05	0.17	-0.03	0.03	0.06	-0.01	0.01
17	1	0.62	0.24	-0.59	0.03	0.01	-0.03	0.17	0.06	-0.16

18	1	-0.05	0.11	0.15	-0.02	0.06	0.07	-0.06	0.15	0.19
19	1	-0.04	0.05	-0.14	0.24	-0.31	0.84	0.02	-0.02	0.06
20	1	0.03	-0.21	0.19	0.01	-0.09	0.08	-0.11	0.67	-0.61
21	1	0.00	0.00	0.00	-0.01	0.01	0.00	0.08	-0.09	-0.01
22	1	-0.01	0.00	0.01	0.12	-0.02	-0.25	0.02	0.00	-0.04
23	1	-0.02	0.00	-0.02	-0.01	0.00	-0.02	0.07	0.01	0.09
24	1	0.00	0.01	0.04	0.00	0.01	0.04	0.00	0.00	0.01
25	1	0.02	0.03	-0.02	0.01	0.01	-0.01	0.01	0.02	-0.01
26	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	73			74			75		
	?A			?A			?A		
Frequencies --	3285.3685			3292.6537			3328.8824		
Red. masses --	1.0896			1.0883			1.0901		
Frc consts --	6.9290			6.9518			7.1172		
IR Inten --	68.2437			23.6691			34.1521		
Raman Activ --	133.9525			136.1248			82.2762		
Depolar --	0.1719			0.2218			0.4839		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6	0.02	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.02	-0.05	-0.06	0.00	0.01	0.01	0.00	-0.01	-0.01
4	6	0.00	0.00	0.00	-0.01	0.01	-0.02	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.01	-0.01	0.00	0.00	0.00	0.00	0.01	0.00
7	6	0.00	0.00	0.00	-0.01	0.01	0.00	0.03	-0.03	-0.01
8	6	0.01	0.00	-0.01	0.03	-0.01	-0.07	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	0.01	0.00	0.01	0.00	0.00	0.00	-0.05	-0.01	-0.06
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1    -0.05   0.01  -0.01     0.05  -0.01   0.01     0.00   0.00
0.00
  17   1    -0.18  -0.07   0.16     0.04   0.01  -0.03    -0.02  -0.01
0.02
  18   1    -0.21   0.54   0.71     0.03  -0.08  -0.10    -0.04   0.08
0.11
  19   1    -0.01   0.01  -0.04     0.08  -0.10   0.25     0.00   0.00
0.00
  20   1     0.02  -0.11   0.10     0.00   0.01  -0.01     0.01  -0.05
0.04
  21   1    -0.01   0.01   0.00     0.12  -0.13  -0.03    -0.31   0.34
0.07
  22   1    -0.08   0.01   0.16    -0.41   0.07   0.83    -0.02   0.00
0.04
  23   1    -0.11  -0.02  -0.15     0.04   0.01   0.06     0.52   0.08
0.68
  24   1     0.00   0.00  -0.01     0.00   0.00   0.02     0.00   0.00
0.02
  25   1    -0.01  -0.01   0.01     0.00   0.00   0.00     0.01   0.01  -
0.01
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     76                     77                     78
                     ?A                     ?A                     ?A
 Frequencies --  3334.2003              3874.5436              3881.8853
 Red. masses --     1.0905                 1.0660                 1.0669
 Frc consts  --     7.1424                 9.4287                 9.4721
 IR Inten    --    18.3868                 8.2600                36.8579
 Raman Activ --   210.5387               168.3575                85.3634
 Depolar     --     0.0519                 0.2498                 0.2470
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   2   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   3   6     0.00   0.00   0.01     0.00   0.00   0.00     0.00   0.00
0.00
   4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

```
   6   6     0.00  -0.01   0.01     0.00   0.00   0.00     0.00   0.00
0.00
   7   6     0.05  -0.05  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
   8   6     0.01   0.00  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.02   0.00   0.03     0.00   0.00   0.00     0.00   0.00
0.00
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00    -0.06  -0.01
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.03   0.00   0.01     0.00   0.00   0.00     0.00   0.00
0.00
  17   1     0.03   0.01  -0.03     0.00   0.00   0.00     0.00   0.00
0.00
  18   1     0.02  -0.05  -0.06     0.00   0.00   0.00     0.00   0.00
0.00
  19   1     0.01  -0.01   0.04     0.00   0.00   0.00     0.00   0.00
0.00
  20   1    -0.02   0.13  -0.12     0.00   0.00   0.00     0.00   0.00
0.00
  21   1    -0.57   0.62   0.13     0.00   0.00   0.00     0.00   0.00
0.00
  22   1    -0.07   0.01   0.15     0.00   0.00   0.00     0.00   0.00
0.00
  23   1    -0.27  -0.04  -0.35     0.00   0.00   0.00     0.00   0.00
0.00
  24   1     0.01   0.01   0.04     0.00   0.00   0.00     0.00   0.00
0.00
  25   1     0.02   0.03  -0.02     0.00   0.00   0.00     0.00   0.00
0.00
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.98   0.15  -
0.08
  27   8     0.00   0.00   0.00     0.06  -0.01   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00    -0.98   0.18   0.03     0.00   0.00
0.00

 --------------------
 - Thermochemistry -
 --------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Atom  1 has atomic number  6 and mass  12.00000
 Atom  2 has atomic number  6 and mass  12.00000
 Atom  3 has atomic number  6 and mass  12.00000
```

```
Atom  4 has atomic number  6 and mass  12.00000
Atom  5 has atomic number  6 and mass  12.00000
Atom  6 has atomic number  6 and mass  12.00000
Atom  7 has atomic number  6 and mass  12.00000
Atom  8 has atomic number  6 and mass  12.00000
Atom  9 has atomic number  6 and mass  12.00000
Atom 10 has atomic number  6 and mass  12.00000
Atom 11 has atomic number  6 and mass  12.00000
Atom 12 has atomic number  8 and mass  15.99491
Atom 13 has atomic number  6 and mass  12.00000
Atom 14 has atomic number  7 and mass  14.00307
Atom 15 has atomic number  8 and mass  15.99491
Atom 16 has atomic number  1 and mass   1.00783
Atom 17 has atomic number  1 and mass   1.00783
Atom 18 has atomic number  1 and mass   1.00783
Atom 19 has atomic number  1 and mass   1.00783
Atom 20 has atomic number  1 and mass   1.00783
Atom 21 has atomic number  1 and mass   1.00783
Atom 22 has atomic number  1 and mass   1.00783
Atom 23 has atomic number  1 and mass   1.00783
Atom 24 has atomic number  1 and mass   1.00783
Atom 25 has atomic number  1 and mass   1.00783
Atom 26 has atomic number  1 and mass   1.00783
Atom 27 has atomic number  8 and mass  15.99491
Atom 28 has atomic number  1 and mass   1.00783
Molecular mass:   218.08172 amu.
Principal axes and moments of inertia in atomic units:
                          1         2         3
    EIGENVALUES --  1923.88612 2766.80176 3673.79955
          X            0.99996  -0.00716   0.00619
          Y            0.00708   0.99988   0.01392
          Z           -0.00629  -0.01387   0.99988
THIS MOLECULE IS AN ASYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER  1.
WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
          MAY CAUSE SIGNIFICANT ERROR
ROTATIONAL TEMPERATURES (KELVIN)      0.04502     0.03130     0.02358
ROTATIONAL CONSTANTS (GHZ)            0.93807     0.65228     0.49125
   1 IMAGINARY FREQUENCIES IGNORED.
Zero-point vibrational energy     623816.6 (Joules/Mol)
                                  149.09574 (Kcal/Mol)
WARNING-- EXPLICIT CONSIDERATION OF  14 DEGREES OF FREEDOM AS
          VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
VIBRATIONAL TEMPERATURES:     96.32   222.80   253.42   383.63   457.94
         (KELVIN)            501.81   569.59   597.15   719.41   730.71
                             778.08   799.89   831.86   878.38   918.52
                             952.81   971.02  1018.60  1032.69  1078.19
                            1182.14  1193.20  1211.85  1267.30  1305.63
                            1337.57  1356.67  1404.59  1423.97  1432.66
                            1451.64  1464.84  1498.31  1505.53  1516.89
                            1526.30  1562.93  1596.51  1667.47  1694.75
                            1709.47  1749.35  1753.83  1765.12  1773.35
                            1809.36  1819.85  1853.58  1888.26  1931.67
                            1937.27  1955.50  1969.88  1973.59  1985.74
```

2009.43	2022.94	2028.66	2052.19	2072.49
2083.06	2100.27	2112.48	2352.46	2841.63
4572.70	4621.58	4633.08	4667.41	4695.24
4709.32	4726.89	4737.37	4789.49	4797.14
5574.57	5585.13			

Zero-point correction=	0.237599
(Hartree/Particle)	
Thermal correction to Energy=	0.247195
Thermal correction to Enthalpy=	0.248140
Thermal correction to Gibbs Free Energy=	0.202296
Sum of electronic and zero-point Energies=	-736.140253
Sum of electronic and thermal Energies=	-736.130657
Sum of electronic and thermal Enthalpies=	-736.129713
Sum of electronic and thermal Free Energies=	-736.175556

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	155.118	42.597	96.486
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	42.042
ROTATIONAL	0.889	2.981	31.348
VIBRATIONAL	153.340	36.635	23.095
VIBRATION 1	0.598	1.970	4.241
VIBRATION 2	0.620	1.897	2.612
VIBRATION 3	0.628	1.872	2.369
VIBRATION 4	0.672	1.734	1.618
VIBRATION 5	0.705	1.639	1.319
VIBRATION 6	0.726	1.578	1.172
VIBRATION 7	0.763	1.479	0.978
VIBRATION 8	0.778	1.438	0.909
VIBRATION 9	0.855	1.250	0.658
VIBRATION 10	0.863	1.233	0.639
VIBRATION 11	0.896	1.160	0.564
VIBRATION 12	0.911	1.127	0.532
VIBRATION 13	0.935	1.078	0.489
VIBRATION 14	0.970	1.010	0.432

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.892966D-93	-93.049165	-214.253621
TOTAL V=0	0.173036D+17	16.238135	37.389688
VIB (BOT)	0.445615-107	-107.351040	-247.184905
VIB (BOT) 1	0.308202D+01	0.488835	1.125585
VIB (BOT) 2	0.130755D+01	0.116457	0.268153
VIB (BOT) 3	0.114183D+01	0.057600	0.132629
VIB (BOT) 4	0.726053D+00	-0.139032	-0.320132
VIB (BOT) 5	0.591215D+00	-0.228255	-0.525576
VIB (BOT) 6	0.529411D+00	-0.276207	-0.635991
VIB (BOT) 7	0.451572D+00	-0.345273	-0.795021
VIB (BOT) 8	0.424660D+00	-0.371959	-0.856467
VIB (BOT) 9	0.328691D+00	-0.483212	-1.112636
VIB (BOT) 10	0.321346D+00	-0.493027	-1.135237
VIB (BOT) 11	0.292749D+00	-0.533505	-1.228440
VIB (BOT) 12	0.280660D+00	-0.551820	-1.270613
VIB (BOT) 13	0.264042D+00	-0.578327	-1.331648

VIB (BOT) 14	0.241939D+00	-0.616294	-1.419070
VIB (V=0)	0.863496D+02	1.936260	4.458404
VIB (V=0) 1	0.362231D+01	0.558986	1.287113
VIB (V=0) 2	0.189989D+01	0.278728	0.641794
VIB (V=0) 3	0.174650D+01	0.242169	0.557615
VIB (V=0) 4	0.138156D+01	0.140371	0.323215
VIB (V=0) 5	0.127430D+01	0.105271	0.242394
VIB (V=0) 6	0.122820D+01	0.089269	0.205550
VIB (V=0) 7	0.117373D+01	0.069570	0.160190
VIB (V=0) 8	0.115600D+01	0.062958	0.144966
VIB (V=0) 9	0.109836D+01	0.040746	0.093821
VIB (V=0) 10	0.109436D+01	0.039160	0.090169
VIB (V=0) 11	0.107940D+01	0.033182	0.076403
VIB (V=0) 12	0.107338D+01	0.030755	0.070817
VIB (V=0) 13	0.106544D+01	0.027527	0.063384
VIB (V=0) 14	0.105546D+01	0.023441	0.053975
ELECTRONIC	0.100000D+01	0.000000	0.000000
TRANSLATIONAL	0.126587D+09	8.102389	18.656441
ROTATIONAL	0.158302D+07	6.199486	14.274844

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000896	0.000001283	-0.000000780
2	6	0.000002163	-0.000004378	-0.000003555
3	6	-0.000001631	0.000002832	-0.000000357
4	6	0.000001627	0.000003592	-0.000001931
5	6	0.000002865	-0.000003983	0.000006551
6	6	0.000002261	0.000002553	-0.000002654
7	6	0.000003604	-0.000006482	0.000001284
8	6	-0.000002436	-0.000000428	0.000002004
9	6	-0.000006547	0.000001120	-0.000009488
10	6	0.000012241	-0.000001497	0.000000896
11	6	-0.000002903	0.000003162	-0.000000858
12	8	-0.000005459	0.000002873	-0.000010929
13	6	0.000012448	0.000000846	0.000004692
14	7	-0.000003626	-0.000001129	-0.000002867
15	8	-0.000000764	0.000000862	0.000001997
16	1	0.000000585	-0.000000275	0.000001263
17	1	-0.000000035	0.000001090	0.000001531
18	1	0.000001354	0.000000102	0.000000190
19	1	-0.000001049	-0.000000854	0.000000390
20	1	-0.000000513	-0.000000919	0.000001064
21	1	-0.000000905	0.000001971	-0.000001371
22	1	0.000002742	-0.000000780	-0.000000488
23	1	-0.000003875	0.000000546	-0.000000599
24	1	0.000001018	-0.000000276	0.000000228
25	1	-0.000000911	-0.000000912	-0.000000128
26	1	0.000003035	-0.000000481	0.000002226
27	8	-0.000009889	-0.000009802	0.000013670
28	1	-0.000004503	0.000009362	-0.000001984

Cartesian Forces: Max 0.000013670 RMS 0.000004145

```
--------------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
--------------------------------------------------------------------------------
  1  C        -0.000001(   1)      0.000001(  29)     -0.000001(  57)
  2  C         0.000002(   2)     -0.000004(  30)     -0.000004(  58)
  3  C        -0.000002(   3)      0.000003(  31)      0.000000(  59)
  4  C         0.000002(   4)      0.000004(  32)     -0.000002(  60)
  5  C         0.000003(   5)     -0.000004(  33)      0.000007(  61)
  6  C         0.000002(   6)      0.000003(  34)     -0.000003(  62)
  7  C         0.000004(   7)     -0.000006(  35)      0.000001(  63)
  8  C        -0.000002(   8)      0.000000(  36)      0.000002(  64)
  9  C        -0.000007(   9)      0.000001(  37)     -0.000009(  65)
 10  C         0.000012(  10)     -0.000001(  38)      0.000001(  66)
 11  C        -0.000003(  11)      0.000003(  39)     -0.000001(  67)
 12  O        -0.000005(  12)      0.000003(  40)     -0.000011(  68)
 13  C         0.000012(  13)      0.000001(  41)      0.000005(  69)
 14  N        -0.000004(  14)     -0.000001(  42)     -0.000003(  70)
 15  O        -0.000001(  15)      0.000001(  43)      0.000002(  71)
 16  H         0.000001(  16)      0.000000(  44)      0.000001(  72)
 17  H         0.000000(  17)      0.000001(  45)      0.000002(  73)
 18  H         0.000001(  18)      0.000000(  46)      0.000000(  74)
 19  H        -0.000001(  19)     -0.000001(  47)      0.000000(  75)
 20  H        -0.000001(  20)     -0.000001(  48)      0.000001(  76)
 21  H        -0.000001(  21)      0.000002(  49)     -0.000001(  77)
 22  H         0.000003(  22)     -0.000001(  50)      0.000000(  78)
 23  H        -0.000004(  23)      0.000001(  51)     -0.000001(  79)
 24  H         0.000001(  24)      0.000000(  52)      0.000000(  80)
 25  H        -0.000001(  25)     -0.000001(  53)      0.000000(  81)
 26  H         0.000003(  26)      0.000000(  54)      0.000002(  82)
 27  O        -0.000010(  27)     -0.000010(  55)      0.000014(  83)
 28  H        -0.000005(  28)      0.000009(  56)     -0.000002(  84)
--------------------------------------------------------------------------------
Internal  Forces:  Max     0.000013670 RMS     0.000004145

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   1 out of a maximum of  94
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
    Eigenvalues ---   -0.00079   0.00169   0.00583   0.00635   0.01197
    Eigenvalues ---    0.01269   0.02053   0.02736   0.02898   0.03339
    Eigenvalues ---    0.03993   0.04263   0.04407   0.04526   0.04591
    Eigenvalues ---    0.04678   0.04931   0.04972   0.05069   0.05117
    Eigenvalues ---    0.05274   0.05400   0.05532   0.05820   0.05960
    Eigenvalues ---    0.06641   0.07569   0.09015   0.09560   0.11023
    Eigenvalues ---    0.11716   0.14280   0.15024   0.15636   0.15971
    Eigenvalues ---    0.17613   0.17957   0.19303   0.20226   0.21186
    Eigenvalues ---    0.24869   0.25289   0.29071   0.29651   0.34278
    Eigenvalues ---    0.36008   0.36233   0.36951   0.39697   0.40124
    Eigenvalues ---    0.47897   0.48468   0.49920   0.51437   0.52435
    Eigenvalues ---    0.56334   0.58786   0.62231   0.62407   0.65355
    Eigenvalues ---    0.67528   0.71834   0.75915   0.77985   0.85060
```

```
    Eigenvalues ---    0.86287   0.93897   0.94207   0.95118   0.97561
    Eigenvalues ---    0.97990   1.02288   1.04855   1.07698   1.09125
    Eigenvalues ---    1.10365   1.14057   1.88017
Eigenvalue   1 out of range, new value =    0.000793 Eigenvector:
                           1
          X1           0.01276
          Y1           0.03126
          Z1          -0.00540
          X2          -0.01030
          Y2           0.02753
          Z2           0.01092
          X3          -0.01771
          Y3           0.04022
          Z3           0.01697
          X4           0.02545
          Y4           0.03510
          Z4          -0.01189
          X5           0.00794
          Y5           0.05711
          Z5           0.00285
          X6          -0.01556
          Y6           0.00090
          Z6           0.00849
          X7           0.01137
          Y7          -0.00891
          Z7          -0.00432
          X8           0.02321
          Y8           0.01071
          Z8          -0.00822
          X9           0.00246
          Y9           0.01739
          Z9           0.00166
          X10         -0.02077
          Y10          0.01765
          Z10          0.01238
          X11          0.01996
          Y11          0.00117
          Z11         -0.00772
          X12          0.01851
          Y12          0.12553
          Z12          0.00442
          X13         -0.00086
          Y13         -0.00624
          Z13          0.00002
          X14         -0.00025
          Y14         -0.01403
          Z14         -0.00209
          X15          0.00558
          Y15          0.03840
          Z15          0.00214
          X16          0.01056
          Y16          0.04879
          Z16         -0.01087
          X17         -0.01795
```

Y17	0.03050
Z17	0.01549
X18	-0.01835
Y18	0.03548
Z18	0.01211
X19	0.02527
Y19	0.03157
Z19	-0.01162
X20	-0.02973
Y20	-0.01401
Z20	0.01127
X21	0.01437
Y21	-0.03124
Z21	-0.00446
X22	0.04225
Y22	0.00246
Z22	-0.01786
X23	-0.04115
Y23	0.01210
Z23	0.02081
X24	0.03692
Y24	-0.00116
Z24	-0.01639
X25	0.01202
Y25	-0.00580
Z25	-0.00367
X26	-0.16885
Y26	-0.95884
Z26	-0.05258
X27	-0.00664
Y27	-0.02995
Z27	0.00165
X28	-0.00702
Y28	-0.04011
Z28	0.00151

Angle between quadratic step and forces= 64.90 degrees.
Linear search not attempted -- first point.
TrRot= -0.000001 -0.000011 0.000001 0.000002 0.000001 0.000002

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
X1	-0.72749	0.00000	0.00000	0.00002	0.00002	-0.72747
Y1	-0.86533	0.00000	0.00000	0.00003	0.00002	-0.86531
Z1	-4.16914	0.00000	0.00000	-0.00003	-0.00002	-4.16917
X2	-0.64304	0.00000	0.00000	0.00006	0.00004	-0.64300
Y2	1.96922	0.00000	0.00000	0.00002	0.00000	1.96922
Z2	-3.42031	0.00000	0.00000	-0.00001	-0.00001	-3.42032
X3	1.67476	0.00000	0.00000	0.00004	0.00002	1.67478
Y3	2.37215	0.00000	0.00000	-0.00001	-0.00002	2.37214
Z3	-1.63455	0.00000	0.00000	0.00003	0.00003	-1.63452
X4	0.83902	0.00000	0.00000	-0.00002	-0.00001	0.83901
Y4	-2.09227	0.00000	0.00000	0.00001	0.00000	-2.09228
Z4	-2.02937	0.00000	0.00000	-0.00001	-0.00001	-2.02937
X5	2.92793	0.00000	0.00000	-0.00001	-0.00001	2.92792
Y5	-0.22506	0.00000	0.00000	-0.00004	-0.00004	-0.22510

Z5	-1.23230	0.00001	0.00000	0.00002	0.00001	-1.23228
X6	-2.45948	0.00000	0.00000	0.00004	0.00003	-2.45945
Y6	2.09787	0.00000	0.00000	0.00001	-0.00002	2.09785
Z6	-1.05695	0.00000	0.00000	-0.00003	-0.00002	-1.05698
X7	-3.35987	0.00000	0.00000	0.00000	0.00000	-3.35987
Y7	-0.66674	-0.00001	0.00000	0.00001	-0.00002	-0.66676
Z7	-0.74933	0.00000	0.00000	-0.00004	-0.00003	-0.74936
X8	-0.97722	0.00000	0.00000	-0.00004	-0.00003	-0.97725
Y8	-1.95411	0.00000	0.00000	-0.00001	-0.00003	-1.95414
Z8	0.32212	0.00000	0.00000	-0.00001	-0.00001	0.32211
X9	0.40993	-0.00001	0.00000	-0.00005	-0.00005	0.40988
Y9	-0.03591	0.00000	0.00000	-0.00002	-0.00003	-0.03595
Z9	2.05017	-0.00001	0.00000	0.00000	0.00000	2.05017
X10	-0.13543	0.00001	0.00000	0.00003	0.00002	-0.13541
Y10	2.50465	0.00000	0.00000	-0.00002	-0.00003	2.50462
Z10	0.69984	0.00000	0.00000	0.00001	0.00001	0.69985
X11	-3.46625	0.00000	0.00000	0.00001	0.00001	-3.46624
Y11	-1.62484	0.00000	0.00000	0.00004	0.00001	-1.62483
Z11	-3.50519	0.00000	0.00000	-0.00005	-0.00004	-3.50523
X12	5.36803	-0.00001	0.00000	-0.00005	-0.00005	5.36798
Y12	-0.59387	0.00000	0.00000	-0.00002	-0.00001	-0.59388
Z12	-2.31920	-0.00001	0.00000	-0.00009	-0.00009	-2.31929
X13	-0.14415	0.00001	0.00000	0.00004	0.00005	-0.14410
Y13	-0.16518	0.00000	0.00000	0.00001	0.00000	-0.16518
Z13	4.82628	0.00000	0.00000	0.00005	0.00005	4.82633
X14	0.94949	0.00000	0.00000	0.00017	0.00018	0.94967
Y14	-0.63365	0.00000	0.00000	0.00038	0.00038	-0.63328
Z14	6.77118	0.00000	0.00000	0.00005	0.00005	6.77123
X15	3.08853	0.00000	0.00000	-0.00002	-0.00002	3.08851
Y15	-0.48932	0.00000	0.00000	-0.00006	-0.00006	-0.48938
Z15	1.45329	0.00000	0.00000	0.00002	0.00001	1.45330
X16	-0.09762	0.00000	0.00000	0.00005	0.00005	-0.09757
Y16	-1.28947	0.00000	0.00000	0.00001	0.00000	-1.28947
Z16	-6.07278	0.00000	0.00000	-0.00001	-0.00001	-6.07279
X17	-0.94703	0.00000	0.00000	0.00008	0.00006	-0.94697
Y17	3.29126	0.00000	0.00000	0.00006	0.00004	3.29130
Z17	-4.94932	0.00000	0.00000	0.00002	0.00003	-4.94929
X18	2.98159	0.00000	0.00000	0.00008	0.00006	2.98166
Y18	3.90104	0.00000	0.00000	-0.00004	-0.00004	3.90100
Z18	-1.97114	0.00000	0.00000	0.00006	0.00006	-1.97108
X19	1.55706	0.00000	0.00000	-0.00006	-0.00004	1.55702
Y19	-3.96498	0.00000	0.00000	-0.00001	-0.00001	-3.96499
Z19	-2.42026	0.00000	0.00000	-0.00001	-0.00001	-2.42027
X20	-3.93760	0.00000	0.00000	0.00004	0.00002	-3.93758
Y20	3.50439	0.00000	0.00000	0.00000	-0.00003	3.50436
Z20	-1.04856	0.00000	0.00000	-0.00002	-0.00001	-1.04857
X21	-5.02057	0.00000	0.00000	-0.00003	-0.00003	-5.02060
Y21	-0.89789	0.00000	0.00000	0.00007	0.00003	-0.89786
Z21	0.40184	0.00000	0.00000	-0.00007	-0.00007	0.40177
X22	-1.29466	0.00000	0.00000	-0.00001	0.00001	-1.29465
Y22	-3.75224	0.00000	0.00000	-0.00003	-0.00004	-3.75229
Z22	1.23048	0.00000	0.00000	-0.00003	-0.00003	1.23045
X23	-0.06932	0.00000	0.00000	-0.00005	-0.00007	-0.06938
Y23	4.13403	0.00000	0.00000	-0.00001	-0.00003	4.13400

```
  Z23        1.91385   0.00000   0.00000   0.00001   0.00001   1.91386
  X24       -3.78783   0.00000   0.00000   0.00003   0.00004  -3.78779
  Y24       -3.64759   0.00000   0.00000   0.00004   0.00001  -3.64758
  Z24       -3.63976   0.00000   0.00000  -0.00006  -0.00006  -3.63982
  X25       -4.86147   0.00000   0.00000   0.00000  -0.00001  -4.86148
  Y25       -0.63633   0.00000   0.00000   0.00003  -0.00001  -0.63633
  Z25       -4.64378   0.00000   0.00000  -0.00005  -0.00004  -4.64382
  X26        5.31378   0.00000   0.00000  -0.00008  -0.00008   5.31370
  Y26       -0.48875   0.00000   0.00000   0.00003   0.00004  -0.48871
  Z26       -4.14037   0.00000   0.00000  -0.00008  -0.00008  -4.14045
  X27       -3.02415  -0.00001   0.00000  -0.00019  -0.00019  -3.02434
  Y27        0.56249  -0.00001   0.00000  -0.00048  -0.00051   0.56198
  Z27        4.72452   0.00001   0.00000   0.00011   0.00012   4.72464
  X28       -3.57427   0.00000   0.00000  -0.00003  -0.00003  -3.57429
  Y28        0.56108   0.00001   0.00000   0.00041   0.00038   0.56146
  Z28        6.46501   0.00000   0.00000   0.00016   0.00017   6.46517
         Item               Value     Threshold  Converged?
Maximum Force            0.000014     0.000450     YES
RMS     Force            0.000004     0.000300     YES
Maximum Displacement     0.000510     0.001800     YES
RMS     Displacement     0.000095     0.001200     YES
Predicted change in Energy=-7.068925D-09
Optimization completed.
   -- Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1|1|UNPC-UNK|Freq|RHF|3-21+G*|C12H12N1O3(1-)|PCUSER|24-Apr-2002|0||#N
RHF/3-21+G* FREQ||Freq calc of output str of mech1st8ts||-1,1|C,-0.384
972,-0.457912,-2.2062159043|C,-0.340283,1.042067,-1.8099499043|C,0.886
244,1.255289,-0.8649649043|C,0.443991,-1.107184,-1.0738939043|C,1.5493
92,-0.119096,-0.6521029043|C,-1.3015,1.110144,-0.5593159043|C,-1.77796
9,-0.352824,-0.3965289043|C,-0.517124,-1.03407,0.1704590957|C,0.216923
,-0.019004,1.0849040957|C,-0.071666,1.325402,0.3703380957|C,-1.834259,
-0.85983,-1.8548649043|O,2.84064,-0.314264,-1.2272679043|C,-0.076279,-
0.087411,2.5539560957|N,0.502447,-0.335314,3.5831530957|O,1.634382,-0.
258939,0.7690470957|H,-0.05166,-0.682356,-3.2135789043|H,-0.501147,1.7
41658,-2.6190649043|H,1.577792,2.064343,-1.0430819043|H,0.823961,-2.09
8175,-1.2807479043|H,-2.083688,1.854443,-0.5548759043|H,-2.656772,-0.4
75145,0.2126420957|H,-0.685106,-1.985602,0.6511430957|H,-0.036681,2.18
7632,1.0127650957|H,-2.004436,-1.930221,-1.9260779043|H,-2.572581,-0.3
36729,-2.4573839043|H,2.811933,-0.258637,-2.1909879043|O,-1.600311,0.2
97659,2.5001110957|H,-1.89142,0.296913,3.4211340957||Version=x86-Win32
-G98RevA.7|HF=-736.3778526|RMSD=8.126e-009|RMSF=4.145e-006|Dipole=-1.5
725667,0.585003,-5.681399|DipoleDeriv=0.0234524,0.0021635,-0.0829061,-
0.0105611,-0.010658,0.0519112,-0.0660792,0.062009,0.1652083,-0.0065199
,-0.0301367,0.0790945,0.0132819,0.0870256,-0.0973883,0.0419256,-0.0955
13,0.0427603,-0.0814282,0.1100617,0.0566604,0.1474675,-0.0477629,-0.00
44036,0.1190829,-0.0298188,-0.1228936,-0.1469586,-0.0808688,0.0352674,
-0.1622659,0.0503782,0.0081838,0.0942754,0.0205319,-0.1293753,1.120582
2,-0.0724868,-0.2709893,-0.0750448,0.5830009,0.0524304,-0.4478751,0.06
90017,0.8375044,0.0965248,-0.1148907,-0.0156899,-0.0899115,0.0854341,0
.0387984,-0.0224781,-0.010156,0.0645123,0.0456504,0.0391971,0.0002146,
0.0268348,0.0159927,0.0117165,-0.0400174,0.0316895,0.1180648,0.003083,
0.0109009,0.0147325,-0.0150498,0.060959,-0.0984052,-0.0808798,-0.06478
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31,-0.005973,0.4281206,0.0402764,-0.2471584,0.0209347,0.3913845,0.0346
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8225,-0.00170898,0.00046601,-0.04026573,0.01038956,0.01187004,-0.00253
849,0.00164637,0.00087933,0.00143682,0.00026616,0.00073176,-0.00040275
,0.00004968,0.00216534,0.00976950,-0.01510811,0.01880090,-0.07587628,0
.02977096,-0.06133930,0.00138492,-0.00081193,0.01067269,0.00037570,-0.
00008647,0.00008326,0.00034115,-0.00007458,0.00008644,-0.00004539,-0.0
0007439,0.00043577,-0.00006468,0.00006968,0.00025270,0.00071155,-0.000
86839,0.00098389,0.00223026,0.00114292,0.00108042,-0.00036533,0.000746
61,-0.00004504,-0.00063626,-0.00035974,0.00014551,-0.00007230,0.000049
92,-0.00003208,0.00018543,-0.00006686,0.00034602,-0.00017797,-0.000025
05,0.00002605,0.18878727,0.00001107,-0.00019132,-0.00014860,-0.0000181
0,0.00027962,-0.00006397,-0.00007246,0.00135503,-0.00024977,0.00001999
,0.00067124,0.00009519,0.00013374,-0.00098367,0.00110662,-0.00024364,-
0.00074085,-0.00088755,-0.00078074,-0.00104486,-0.00049273,-0.00001425
,-0.00057479,0.00101644,0.00903357,0.00399852,-0.00143930,-0.00085716,
-0.00217689,-0.00115067,0.00024632,0.00050279,0.00003198,0.00004988,0.
00050876,-0.00034230,-0.01515895,-0.03549330,-0.00082848,0.02887191,0.
00980063,0.01722640,-0.00062744,0.00118144,-0.00168641,0.00001346,0.00
019125,-0.00009518,-0.00000993,0.00006109,-0.00001053,0.00004204,0.000
03792,-0.00011446,0.00000403,0.00004062,-0.00004795,-0.00041076,0.0005
0900,-0.00073707,0.00103054,-0.00081954,0.00005332,-0.00032882,0.00089
797,0.00011072,0.00083777,0.00155746,0.00063035,-0.00000401,0.00012167
,0.00015871,-0.00009986,0.00001233,-0.00019997,-0.00000036,-0.00015941
,-0.00003039,-0.03002490,0.03350426,-0.00015424,-0.00031848,-0.0007796
5,0.00015740,0.00027409,0.00014302,0.00008923,-0.00011637,-0.00021426,
-0.00015968,0.00028145,0.00057755,0.00166973,-0.00043245,0.00247749,0.
00087571,-0.00053405,0.00044734,-0.00206181,-0.00161528,-0.00213313,0.
00009439,-0.00006061,0.00078844,0.03241731,-0.00642886,-0.00617446,0.0
0148968,-0.00005166,-0.00044849,0.00111033,0.00062518,0.00005790,0.001
11943,-0.00013062,-0.00160335,0.03819422,-0.00554041,-0.08304668,-0.05
437245,0.01565477,-0.00114580,0.00450561,-0.00024598,-0.00912186,0.000
28557,0.00003139,-0.00019963,0.00005462,0.00005203,-0.00023393,0.00019
833,0.00005438,-0.00020420,0.00011103,-0.00008277,-0.00016184,-0.00010

592,-0.00003667,0.00016654,0.00185784,-0.00000862,-0.00196216,-0.00031
583,-0.00026572,-0.00005184,-0.00003448,-0.00003207,-0.00030762,-0.000
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002692,0.00003838,-0.00005580,-0.13914458,-0.01069875,0.59180317,0.000
02297,-0.00003078,-0.00012178,0.00001496,0.00000198,-0.00000464,0.0000
6398,0.00009891,-0.00022428,-0.00010673,-0.00014632,-0.00002231,-0.000
75621,0.00030795,-0.00064761,0.00028700,-0.00015461,0.00026222,-0.0001
8178,-0.00012237,-0.00012492,0.00037548,0.00015743,-0.00041859,-0.0099
3092,0.00278395,-0.00217808,0.00004917,0.00008068,-0.00067725,0.000204
48,0.00001116,-0.00008645,0.00003442,-0.00005653,0.00037500,-0.0109506
5,-0.00065841,0.04719049,0.00666130,-0.00200506,-0.00641428,-0.0005709
3,0.00007341,0.00279646,0.00002562,0.00001523,-0.00004766,0.00002542,0
.00001183,-0.00004010,0.00004892,-0.00000201,-0.00005129,0.00004297,-0
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2969,-0.00004898,-0.00010256,0.00001751,0.00006280,-0.07825692,0.00835
705,0.11231371,0.09251137,-0.00000123,-0.00002120,0.00000276,-0.000085
26,-0.00008748,0.00003042,-0.00001521,-0.00013292,0.00007686,-0.000058
64,-0.00008223,0.00012024,0.00022766,0.00008350,0.00017240,-0.00021389
,0.00018608,-0.00005917,0.00011430,-0.00011889,-0.00028170,0.00012404,
0.00028338,0.00024423,0.00271582,0.00073382,0.00073706,-0.00032440,0.0
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0002350,-0.00009243,0.00341577,0.00242722,-0.01122470,-0.00248837,-0.0
0282585,0.00119817,0.00021838,0.00057771,-0.00066095,-0.00000362,-0.00
000893,0.00001463,-0.00002188,-0.00000406,0.00003325,-0.00004919,0.000
00831,0.00006166,0.00001196,0.00001637,-0.00002083,0.00004914,-0.00002
025,0.00008267,-0.00003770,0.00009328,-0.00028348,0.00001891,-0.000117
89,-0.00008291,-0.00009363,0.00003346,0.00002386,0.00000564,-0.0000285
6,-0.00002463,0.00001571,-0.00001292,0.00000799,0.00003790,0.00001140,
-0.00001516,0.00513245,-0.01304697,0.00975096,-0.00862207,0.01152567,0
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0.00004574,-0.00000938,0.00000849,0.00005680,-0.00007337,0.00002281,0.
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10682,0.00021889,0.00098130,-0.00057208,-0.00040063,0.00014192,0.00002
283,0.00001893,-0.00005453,0.00004428,-0.00003782,-0.00001059,-0.00136
635,0.00095365,-0.00261961,-0.00125116,-0.00014059,0.00134979,-0.00056
489,0.00008033,0.00023530,0.00001726,-0.00001426,-0.00000887,0.0000216
5,0.00000676,-0.00004188,0.00001898,-0.00000292,-0.00001529,0.00001779
,-0.00000469,-0.00001681,0.00002595,0.00001348,0.00000775,0.00031233,0
.00012654,-0.00003839,0.00004399,-0.00006554,-0.00006606,-0.00003041,0
.00003287,-0.00004446,0.00000127,-0.00003536,-0.00003437,-0.00000456,0
.00000950,-0.00005825,-0.00001155,0.00000550,0.00001706,0.15523776,-0.
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00648,-0.00000128,0.00000244,0.00000043,-0.00000200,0.00000655,-0.0000
0112,0.00000949,-0.00001224,0.00000150,-0.00000090,0.00000290,-0.00000
316,0.00000086,0.00000546,-0.00000287,0.00001093,-0.00001245,-0.000000
85,-0.00000469,0.00000363,0.00000113,0.00000287,0.00000076,-0.00000086
,-0.00000200,-0.00000058,0.00000027,-0.00000126,0.00000003,-0.00000109
,-0.00000153,-0.00000135,-0.00000010,-0.00000019,0.00000105,0.00000085

```
 ,-0.00000039,0.00000051,0.00000092,-0.00000106,0.00000090,-0.00000197,
 0.00000137,-0.00000274,0.00000078,0.00000049,0.00000388,-0.00000055,0.
 00000060,-0.00000102,0.00000028,-0.00000023,0.00000091,0.00000091,0.00
 000013,-0.00000304,0.00000048,-0.00000223,0.00000989,0.00000980,-0.000
 01367,0.00000450,-0.00000936,0.00000198|||@


 WHEN YOU REACH FOR THE STARS, YOU MAY NOT QUITE GET ONE,
 BUT YOU WON'T COME UP WITH A HANDFUL OF MUD, EITHER.

                                          -- LEO BURNETT (AD AGENCY HEAD)
 Job cpu time:  0 days 18 hours 43 minutes  8.0 seconds.
 File lengths (MBytes):  RWF=  307 Int=    0 D2E=    0 Chk=    5 Scr=
1
 Normal termination of Gaussian 98.
```

```
%nproc=2
%chk=mech1st8ts
%nosave

#N RHF/3-21+G* OPT=(TS,NOEIGENTEST,GDIIS) OPTCYC=100

TS search for mech1str5 using input@1.65A from mech1str8S2

-1  1
 C                 -0.452220   -0.415838   -2.166229
 C                 -0.432061    1.075434   -1.732337
 C                  0.806764    1.292315   -0.810820
 C                  0.411440   -1.062523   -1.059250
 C                  1.504971   -0.057058   -0.663260
 C                 -1.365897    1.091460   -0.459154
 C                 -1.809226   -0.392497   -0.336992
 C                 -0.520433   -1.049127    0.207735
 C                  0.125551   -0.020130    1.188427
 C                 -0.113255    1.321274    0.449688
 C                 -1.879582   -0.864801   -1.805425
 O                  2.717515   -0.124522   -1.426228
 C                  0.164550   -0.171751    2.626828
 N                  0.573571   -0.360071    3.724620
 O                  1.676073   -0.241704    0.719619
 H                 -0.119095   -0.605478   -3.178823
 H                 -0.627097    1.789505   -2.520585
 H                  1.480868    2.112802   -0.994843
 H                  0.794818   -2.048915   -1.297693
 H                 -2.166789    1.816742   -0.423689
 H                 -2.686611   -0.565452    0.259807
 H                 -0.651952   -2.019235    0.662956
 H                 -0.076601    2.179340    1.098835
 H                 -2.027198   -1.937798   -1.902267
 H                 -2.643730   -0.344739   -2.378478
 H                  2.962477   -1.031095   -1.646888
 O                 -1.251856    0.161276    2.078566
 H                 -2.031567    0.333869    2.638406
```

```
%chk=mech1st8ts2
# opt=(calcfc,gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity
optcyc=100

TS search for mech1str5 using input@1.65A from mech1str8S2 & calcfc

-1  1
 C                  0.000000    0.000000    0.000000
 C                  0.000000    0.000000    1.556235
 C                  1.488457    0.000000    2.020051
 C                  1.410608   -0.549783   -0.307765
 C                  2.351654    0.011805    0.756438
 C                 -0.098820   -1.533576    1.907056
 C                 -0.166055   -2.216508    0.516525
 C                  1.305293   -2.087776    0.043267
 C                  2.148864   -2.308850    1.318283
 C                  1.390516   -1.519925    2.390038
 C                 -0.920294   -1.183223   -0.343346
 O                  2.847289    1.329924    0.421108
 C                  3.323100   -3.124496    1.462117
 N                  4.250922   -3.782717    1.585234
 O                  3.374628   -0.907122    0.938125
 H                 -0.216092    0.955186   -0.459845
 H                 -0.695736    0.685622    2.019961
 H                  1.820805    0.684541    2.784082
 H                  1.768647   -0.366547   -1.310521
 H                 -0.842659   -1.867642    2.613014
 H                 -0.530312   -3.224329    0.535229
 H                  1.583601   -2.749838   -0.761082
 H                  1.609582   -1.827444    3.396344
 H                 -0.917857   -1.429073   -1.402130
 H                 -1.945782   -1.037196   -0.012859
 H                  3.812814    1.278217    0.395955
 O                  1.155641   -3.948007    1.815346
 H                  1.696198   -4.674894    2.160023

 1  2 1.0  4 1.0  11 1.0  16 1.0
 2  3 1.0  6 1.0  17 1.0
 3  5 1.0  10 1.0  18 1.0
 4  5 1.0  8 1.0  19 1.0
 5  12 1.0  15 1.0
 6  7 1.0  10 1.0  20 1.0
 7  8 1.0  11 1.0  21 1.0
 8  9 1.0  22 1.0
 9  10 1.0  13 1.5
 10  23 1.0
 11  24 1.0  25 1.0
 12  26 1.0
 13  14 3.0
 14
 15
 16
 17
 18
```

```
19
20
21
22
23
24
25
26
27  28 1.0
28
```

Entering Link 1 = C:\G98W\l1.exe PID=   88.

Gaussian, Inc. access to this program. By using this program,
the user acknowledges that Gaussian, Inc. is engaged in the
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Cite this work as:
Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

****
Gaussian 98: x86-Win32-G98RevA.7 11-Apr-1999
07-May-2002
****
%chk=mech1st8ts2F
Default route: MaxDisk=2000MB

#N RHF/3-21+G* FREQ

1/10=4,30=1,38=1/1,3;
2/17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11,27=262144000/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Freq calc of output str of mech1st8ts2

Symbolic Z-matrix:
Charge = -1 Multiplicity = 1
C -0.45407 -0.4233 -2.14386

C	-0.4169	1.07523	-1.72566
C	0.8128	1.26422	-0.78612
C	0.37807	-1.07758	-1.01857
C	1.49612	-0.09951	-0.66245
C	-1.36924	1.11281	-0.47014
C	-1.84929	-0.35585	-0.33939
C	-0.58212	-1.0396	0.23695
C	0.01215	-0.00362	1.21662
C	-0.13052	1.32292	0.46422
C	-1.89454	-0.83947	-1.80227
O	2.6501	-0.23544	-1.52581
C	0.50902	-0.23715	2.54454
N	0.89397	-0.4154	3.60723
O	1.8108	-0.29179	0.67469
H	-0.09398	-0.63103	-3.14271
H	-0.5821	1.78407	-2.52531
H	1.49587	2.08405	-0.94135
H	0.75238	-2.06722	-1.23723
H	-2.15303	1.85221	-0.42293
H	-2.72525	-0.48334	0.2649
H	-0.75329	-1.9993	0.69786
H	-0.10356	2.19036	1.09828
H	-2.05887	-1.91029	-1.89061
H	-2.64246	-0.31352	-2.39062
H	3.41032	-0.43748	-0.96298
O	-1.73263	0.30829	2.10702
H	-1.69885	0.39621	3.07165

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 94 maximum allowed number of steps= 168.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C	0	-0.454065		-0.423299		-2.143856	
2	2	C	0	-0.416901		1.075234		-1.725663	
3	3	C	0	0.812804		1.264215		-0.786119	
4	4	C	0	0.378068		-1.077582		-1.018572	
5	5	C	0	1.496116		-0.099513		-0.662446	
6	6	C	0	-1.369238		1.112805		-0.470139	
7	7	C	0	-1.849288		-0.355850		-0.339393	
8	8	C	0	-0.582116		-1.039598		0.236952	
9	9	C	0	0.012151		-0.003618		1.216618	
10	10	C	0	-0.130524		1.322915		0.464218	
11	11	C	0	-1.894539		-0.839467		-1.802267	
12	12	O	0	2.650095		-0.235437		-1.525808	
13	13	C	0	0.509021		-0.237150		2.544542	
14	14	N	0	0.893967		-0.415402		3.607232	
15	15	O	0	1.810797		-0.291785		0.674685	

16	16	H	0	-0.093978	-0.631031	-3.142714
17	17	H	0	-0.582099	1.784069	-2.525308
18	18	H	0	1.495869	2.084046	-0.941349
19	19	H	0	0.752376	-2.067215	-1.237227
20	20	H	0	-2.153026	1.852209	-0.422928
21	21	H	0	-2.725250	-0.483342	0.264902
22	22	H	0	-0.753292	-1.999297	0.697857
23	23	H	0	-0.103562	2.190356	1.098276
24	24	H	0	-2.058872	-1.910290	-1.890615
25	25	H	0	-2.642458	-0.313515	-2.390623
26	26	H	0	3.410324	-0.437480	-0.962980
27	27	O	0	-1.732627	0.308291	2.107022
28	28	H	0	-1.698845	0.396206	3.071646

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.454065	-0.423299	-2.143856
2	6	0	-0.416901	1.075234	-1.725663
3	6	0	0.812804	1.264215	-0.786119
4	6	0	0.378068	-1.077582	-1.018572
5	6	0	1.496116	-0.099513	-0.662446
6	6	0	-1.369238	1.112805	-0.470139
7	6	0	-1.849288	-0.355850	-0.339393
8	6	0	-0.582116	-1.039598	0.236952
9	6	0	0.012151	-0.003618	1.216618
10	6	0	-0.130524	1.322915	0.464218
11	6	0	-1.894539	-0.839467	-1.802267
12	8	0	2.650095	-0.235437	-1.525808
13	6	0	0.509021	-0.237150	2.544542
14	7	0	0.893967	-0.415402	3.607232
15	8	0	1.810797	-0.291785	0.674685
16	1	0	-0.093978	-0.631031	-3.142714
17	1	0	-0.582099	1.784069	-2.525308
18	1	0	1.495869	2.084046	-0.941349
19	1	0	0.752376	-2.067215	-1.237227
20	1	0	-2.153026	1.852209	-0.422928
21	1	0	-2.725250	-0.483342	0.264902
22	1	0	-0.753292	-1.999297	0.697857
23	1	0	-0.103562	2.190356	1.098276
24	1	0	-2.058872	-1.910290	-1.890615
25	1	0	-2.642458	-0.313515	-2.390623
26	1	0	3.410324	-0.437480	-0.962980
27	8	0	-1.732627	0.308291	2.107022
28	1	0	-1.698845	0.396206	3.071646

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.556235	0.000000			
3	C	2.509205	1.559048	0.000000		
4	C	1.544926	2.401368	2.393124	0.000000	

5	C	2.470348	2.483968	1.530348	1.527572	0.000000
6	C	2.449181	1.576292	2.209994	2.855110	3.117202
7	C	2.281947	2.453870	3.148160	2.437888	3.370727
8	C	2.462614	2.889925	2.880977	1.581056	2.451882
9	C	3.418519	3.163072	2.501880	2.506665	2.396295
10	C	3.155312	2.222372	1.567372	2.867005	2.436931
11	C	1.537805	2.419786	3.575995	2.415703	3.652843
12	O	3.170660	3.341297	2.484298	2.475602	1.447597
13	C	4.789913	4.562273	3.666017	3.663230	3.358284
14	N	5.906968	5.690355	4.704172	4.701351	4.323485
15	O	3.618158	3.548669	2.356072	2.353149	1.387052
16	H	1.081912	2.241351	3.157175	2.221309	2.993767
17	H	2.243741	1.081281	2.289275	3.373606	3.367063
18	H	3.396328	2.300335	1.078331	3.354301	2.201299
19	H	2.231577	3.388328	3.362377	1.080412	2.180682
20	H	3.320542	2.305415	3.045290	3.917257	4.145217
21	H	3.311193	3.423446	4.083678	3.410427	4.339036
22	H	3.263225	3.929294	3.912206	2.252923	3.243369
23	H	4.179170	3.052263	2.290940	3.923319	3.301910
24	H	2.202426	3.411251	4.420850	2.718922	4.174356
25	H	2.204997	2.706270	4.123409	3.404394	4.490010
26	H	4.040813	4.185408	3.110331	3.099580	1.966910
27	O	4.498879	4.124174	3.970299	4.018086	4.273294
28	H	5.424254	5.011849	4.684461	4.818247	4.939328

		6	7	8	9	10
6	C	0.000000				
7	C	1.550642	0.000000			
8	C	2.398411	1.550938	0.000000		
9	C	2.449446	2.451569	1.544718	0.000000	
10	C	1.565753	2.533415	2.415999	1.531715	0.000000
11	C	2.421130	1.541406	2.433294	3.667121	3.595080
12	O	4.368894	4.654732	3.768446	3.812268	3.757726
13	C	3.799807	3.727304	2.675719	1.436941	2.677792
14	N	4.907389	4.806750	3.731920	2.581124	3.734952
15	O	3.660071	3.798510	2.544969	1.900489	2.533827
16	H	3.436555	3.318953	3.439091	4.405529	4.102341
17	H	2.300848	3.311079	3.950086	4.189388	3.058406
18	H	3.061729	4.183960	3.932374	3.349117	2.280371
19	H	3.899000	3.240915	2.238318	3.290550	3.894536
20	H	1.078550	2.230417	3.356449	3.289407	2.271056
21	H	2.219626	1.071791	2.214323	2.937561	3.167790
22	H	3.380648	2.231146	1.078312	2.199489	3.388144
23	H	2.285383	3.405527	3.376906	2.200208	1.074807
24	H	3.410638	2.206014	2.732298	4.192783	4.440426
25	H	2.709933	2.199649	3.417068	4.489451	4.139787
26	H	5.048811	5.297079	4.212121	4.060353	4.203985
27	O	2.724161	2.537644	2.576362	1.983521	2.508984
28	H	3.628553	3.496199	3.368101	2.555092	3.180739

		11	12	13	14	15
11	C	0.000000				
12	O	4.592927	0.000000			
13	C	5.003462	4.599125	0.000000		
14	N	6.100678	5.428119	1.144232	0.000000	
15	O	4.490519	2.355794	2.279029	3.075011	0.000000

16	H	2.254388	3.209488	5.732681	6.825269	4.279695
17	H	3.021296	3.940112	5.565900	6.680156	4.502785
18	H	4.558835	2.655905	4.302703	5.224856	2.890557
19	H	2.972002	2.653305	4.208341	5.120285	2.815637
20	H	3.035541	5.352063	4.500866	5.537907	4.638249
21	H	2.256124	5.671193	3.964578	4.926918	4.558546
22	H	2.982997	4.431583	2.847603	3.699547	3.080696
23	H	4.560765	4.511421	2.891320	3.752319	3.163103
24	H	1.086956	5.011246	5.391112	6.417186	4.916773
25	H	1.087277	5.363312	5.856066	6.963544	5.406299
26	H	5.385867	0.967236	4.556358	5.217219	2.293831
27	O	4.077512	5.718509	2.348173	3.110202	3.868790
28	H	5.031919	6.359940	2.356618	2.769158	4.305385

		16	17	18	19	20
16	H	0.000000				
17	H	2.540110	0.000000			
18	H	3.839956	2.629993	0.000000		
19	H	2.531762	4.274619	4.227682	0.000000	
20	H	4.219407	2.625349	3.692823	4.946345	0.000000
21	H	4.307813	4.185633	5.085702	4.105962	2.501070
22	H	4.129992	4.973124	4.941600	2.452794	4.248472
23	H	5.093752	3.677557	2.594138	4.930934	2.574628
24	H	2.658019	4.028893	5.430655	2.890442	4.039724
25	H	2.676043	2.943311	4.997444	3.991326	2.966771
26	H	4.131445	4.828622	3.166023	3.129846	6.040298
27	O	5.579178	4.996010	4.782160	4.796068	2.993504
28	H	6.499930	5.873600	5.399919	5.535640	3.812909

		21	22	23	24	25
21	H	0.000000				
22	H	2.524715	0.000000			
23	H	3.836199	4.258600	0.000000		
24	H	2.669549	2.900457	5.438015	0.000000	
25	H	2.662238	3.993685	4.988765	1.772081	0.000000
26	H	6.257401	4.746931	4.847854	5.739493	6.220105
27	O	2.237273	2.875727	2.685813	4.583627	4.630685
28	H	3.115273	3.502482	3.107747	5.483938	5.588425

		26	27	28
26	H	0.000000		
27	O	6.035812	0.000000	
28	H	6.563295	0.969211	0.000000

Interatomic angles:

C1-C2-C3=107.3075	C2-C1-C4=101.4907	C1-C4-C3= 75.7694
C2-C3-C4= 71.3106	C2-C1-C5= 72.1692	C1-C5-C3= 73.4918
C2-C3-C5=107.0297	C1-C4-C5=107.03	C2-C4-C5= 74.7483
C3-C5-C4=102.9982	C1-C2-C6=102.8595	C1-C6-C3= 64.9331
C3-C2-C6= 89.6357	C4-C1-C6= 88.2309	C4-C2-C6= 89.2461
C4-C3-C6= 76.5547	C5-C1-C6= 78.6368	C5-C2-C6= 97.7954
C5-C3-C6=111.6079	C5-C4-C6= 84.9477	C2-C1-C7= 76.9175
C3-C1-C7= 82.0065	C3-C2-C7=100.9912	C4-C1-C7= 76.46
C2-C4-C7= 60.933	C3-C4-C7= 81.3275	C5-C1-C7= 90.2637
C5-C2-C7= 86.0971	C5-C4-C7=114.4692	C1-C7-C6= 76.8228
C2-C6-C7=103.3926	C3-C6-C7=112.4955	C4-C7-C6= 88.5135
C2-C1-C8= 88.9933	C3-C1-C8= 70.8183	C2-C3-C8= 74.6433
C1-C4-C8=103.9528	C2-C4-C8= 90.6441	C3-C4-C8= 90.5546

C1-C8-C5= 60.3525 C2-C5-C8= 71.6729 C3-C5-C8= 89.5903
C5-C4-C8=104.1216 C1-C6-C8= 61.0518 C2-C6-C8= 90.8684
C3-C6-C8= 77.2676 C4-C8-C6= 89.241 C5-C8-C6= 79.9761
C1-C7-C8= 77.3657 C2-C7-C8= 89.4338 C3-C8-C7= 84.8991
C4-C8-C7=102.2211 C5-C8-C7=112.7791 C6-C7-C8=101.3
C1-C3-C9= 86.0301 C2-C3-C9= 99.7044 C1-C4-C9=112.9181
C2-C4-C9= 80.2203 C4-C3-C9= 61.5583 C1-C5-C9= 89.2326
C2-C5-C9= 80.7806 C3-C5-C9= 75.5934 C4-C5-C9= 75.8288
C1-C6-C9= 88.5099 C2-C6-C9=101.3562 C3-C6-C9= 64.7137
C4-C9-C6= 70.3396 C5-C9-C6= 80.0665 C1-C7-C9= 92.4014
C2-C7-C9= 80.3027 C3-C9-C7= 78.9142 C4-C7-C9= 61.6826
C5-C9-C7= 88.0948 C7-C6-C9= 71.6296 C1-C8-C9=115.1691
C2-C8-C9= 85.2921 C3-C9-C8= 87.4379 C4-C8-C9=106.6246
C5-C9-C8= 73.3867 C6-C8-C9= 73.2235 C7-C8-C9=104.7339
C1-C2-C10=112.0358 C1-C3-C10= 98.7991 C2-C3-C10= 90.6055
C1-C4-C10= 85.7888 C4-C2-C10= 76.5325 C4-C3-C10= 90.2751
C1-C5-C10= 80.0265 C2-C10-C5= 64.2396 C5-C3-C10=103.7472
C4-C5-C10= 89.5968 C1-C6-C10=101.3236 C2-C6-C10= 90.0308
C3-C10-C6= 89.7179 C4-C6-C10= 74.5386 C5-C10-C6=100.0121
C1-C7-C10= 81.698 C7-C2-C10= 65.3889 C3-C10-C7= 97.4962
C4-C7-C10= 70.4091 C5-C10-C7= 85.3778 C7-C6-C10=108.7657
C1-C8-C10= 80.59 C2-C10-C8= 76.9524 C3-C10-C8= 90.0478
C4-C8-C10= 89.122 C5-C10-C8= 60.6924 C8-C6-C10= 71.6307
C7-C8-C10= 75.9111 C2-C10-C9=113.5479 C3-C10-C9=107.6595
C4-C9-C10= 86.9409 C5-C9-C10= 72.9716 C6-C10-C9=104.5134
C7-C9-C10= 75.0445 C8-C9-C10=103.5007 C2-C1-C11=102.9011
C3-C1-C11=122.3264 C3-C2-C11=126.6299 C4-C1-C11=103.187
C2-C4-C11= 60.3084 C3-C4-C11= 96.0822 C5-C1-C11=129.9214
C5-C2-C11= 96.2935 C5-C4-C11=134.5135 C1-C11-C6= 72.5884
C6-C2-C11= 71.0432 C3-C6-C11=100.9993 C4-C11-C6= 72.3544
C1-C11-C7= 95.6472 C2-C11-C7= 72.7686 C4-C11-C7= 72.2671
C6-C7-C11=103.0751 C1-C11-C8= 72.7338 C2-C11-C8= 73.0935
C3-C8-C11= 84.1328 C8-C4-C11= 71.5741 C5-C8-C11= 96.7893
C8-C6-C11= 60.6447 C8-C7-C11=103.7888 C9-C4-C11= 96.2992
C9-C6-C11= 97.685 C9-C7-C11=132.0464 C9-C8-C11=133.1437
C10-C2-C11=101.4241 C10-C4-C11= 85.3176 C10-C6-C11=127.4586
C10-C7-C11=121.9289 C10-C8-C11= 95.6944 C1-C3-O12= 78.8319
C2-C3-O12=109.3129 C1-C4-O12=101.5969 C2-C4-O12= 86.4756
C3-C4-O12= 61.3341 C1-C5-O12=105.0317 C2-C5-O12=113.7696
C3-C5-O12=113.0427 C4-C5-O12=112.6 C6-C3-O12=137.0057
C6-C4-O12=109.8797 C7-C4-O12=142.6443 C8-C3-O12= 88.9169
C8-C4-O12=135.3897 C8-C5-O12=149.1441 C9-C3-O12= 99.7364
C9-C4-O12= 99.8419 C9-C5-O12=164.8186 C10-C3-O12=134.8485
C10-C4-O12= 89.0804 C10-C5-O12=149.6156 C11-C4-O12=139.7649
C1-C8-C13=137.5199 C2-C8-C13=110.0543 C3-C8-C13= 82.4721
C4-C8-C13=116.385 C5-C8-C13= 81.7043 C6-C8-C13= 96.8314
C7-C8-C13=121.4296 C3-C9-C13=135.3539 C4-C9-C13=134.744
C5-C9-C13=120.2666 C6-C9-C13=154.8861 C7-C9-C13=145.664
C8-C9-C13=127.5981 C2-C10-C13=137.0013 C3-C10-C13=117.0121
C4-C10-C13= 82.6247 C5-C10-C13= 81.9346 C6-C10-C13=125.0555
C7-C10-C13= 91.284 C10-C8-C13= 63.2172 C10-C9-C13=128.8222
C11-C8-C13=156.6397 C3-C9-N14=135.4732 C4-C9-N14=135.0448
C5-C9-N14=120.5522 C6-C9-N14=154.5802 C7-C9-N14=145.521
C8-C9-N14=127.722 C10-C9-N14=128.6783 C8-C13-N14=153.0536

C9-C13-N14=179.2885 C10-C13-N14=153.2049 C1-C3-O15= 96.0388
C2-C3-O15=128.8804 C1-C4-O15=135.2869 C2-C4-O15= 96.55
C3-O15-C4= 61.0851 C1-C5-O15=137.6484 C2-C5-O15=130.7612
C3-C5-O15=107.6217 C4-C5-O15=107.5799 C6-C3-O15=106.5189
C6-C4-O15= 88.7512 C7-C4-O15=104.8891 C1-C8-O15= 92.5137
C2-C8-O15= 81.2586 C3-O15-C8= 71.8889 C8-C4-O15= 77.8967
C8-C5-O15= 77.6156 C6-C8-O15= 95.485 C7-C8-O15=134.6355
C3-O15-C9= 71.0815 C4-O15-C9= 71.3125 C5-O15-C9= 92.2443
C6-C9-O15=113.9841 C7-C9-O15=121.0525 C8-C9-O15= 94.678
C2-C10-O15= 96.2897 C10-C3-O15= 77.5882 C4-O15-C10= 71.7327
C10-C5-O15= 77.6817 C6-C10-O15=124.7632 C7-C10-O15= 97.1151
C8-C10-O15= 61.8275 C10-C9-O15= 94.5541 C11-C4-O15=140.6525
C11-C8-O15=128.8373 C3-O15-O12= 63.6387 C4-O15-O12= 63.4339
O12-C5-O15=112.4003 C8-O15-O12=100.4485 C9-O15-O12=126.8633
C10-O15-O12=100.3774 C3-O15-C13=104.5319 C4-O15-C13=104.5135
C5-O15-C13=131.1492 C8-O15-C13= 67.1135 C13-C9-O15= 84.9298
C10-O15-C13= 67.3714 O12-O15-C13=165.7666 N14-C9-O15= 85.2151
N14-C13-O15=124.4783 C2-C1-H16=115.1526 C3-C1-H16=117.4293
C3-C2-H16=111.0784 C4-C1-H16=114.3229 C2-H16-C4= 65.1073
C3-C4-H16= 86.26 C5-C1-H16=108.4251 C5-C2-H16= 78.4413
C3-C5-H16= 81.6108 C5-C4-H16=104.4631 C6-C1-H16=151.1288
C6-C2-H16=127.5002 C6-C4-H16= 84.2266 C7-C1-H16=159.9215
C7-C2-H16= 89.8454 C7-C4-H16= 90.7297 C8-C1-H16=149.5216
C8-C2-H16= 83.1372 C8-C4-H16=128.7175 C8-C5-H16= 77.6218
C9-C4-H16=137.353 C9-C5-H16=109.1377 C10-C2-H16=133.5719
C10-C4-H16=106.7712 C10-C5-H16= 97.5927 C11-C1-H16=117.7021
C2-H16-C11= 65.127 C4-H16-C11= 65.3267 C5-H16-C11= 87.0204
C6-C11-H16= 94.5489 C7-C11-H16=120.7868 C8-C11-H16= 94.3082
O12-C4-H16= 86.0271 O12-C5-H16= 84.9872 O15-C4-H16=138.6207
O15-C5-H16=153.4505 C1-C2-H17=115.3957 C1-H17-C3= 67.2117
C3-C2-H17=119.1249 C4-C1-H17=124.8342 C4-C2-H17=148.8742
C4-C3-H17= 92.1622 C5-C1-H17= 91.0344 C5-C2-H17=138.0937
C5-C3-H17=122.3995 C1-H17-C6= 65.2065 C6-C2-H17=118.7582
C6-C3-H17= 61.482 C4-C6-H17= 80.9601 C7-C1-H17= 94.0408
C7-C2-H17=135.3097 C7-C6-H17=117.2288 C8-C1-H17=114.054
C8-C2-H17=166.7126 C8-C3-H17= 98.9951 C8-C6-H17=114.3861
C9-C3-H17=121.8855 C9-C6-H17=123.7201 C10-C2-H17=132.4813
C10-C3-H17=103.3452 C10-C6-H17=102.8985 C11-C1-H17=104.5101
C11-C2-H17=113.7039 C11-C6-H17= 79.5146 O12-C3-H17=111.1928
O15-C3-H17=151.5342 H16-C1-H17= 92.9192 H16-C2-H17= 93.067
C3-H17-H16= 81.4693 C4-H16-H17= 89.9738 C5-H16-H17= 74.4482
C6-H17-H16= 90.313 C11-H16-H17= 77.872 C1-C2-H18=122.2605
C1-C3-H18=138.8714 C2-C3-H18=120.3339 C4-C2-H18= 91.0021
C4-C3-H18=147.6785 C1-C5-H18= 93.0924 C2-H18-C5= 66.9382
C5-C3-H18=113.9724 C4-C5-H18=127.2646 C6-C2-H18=102.7294
C6-C3-H18=134.2751 C7-C2-H18=123.2656 C8-C2-H18= 97.8693
C8-C3-H18=164.9701 C8-C5-H18=115.2586 C9-C3-H18=134.6861
C9-C5-H18= 93.4161 C2-C10-H18= 61.4281 C10-C3-H18=117.8789
C4-C10-H18= 80.4539 C5-H18-C10= 65.8517 C6-C10-H18=103.9582
C7-C10-H18=120.6325 C8-C10-H18=113.6856 C9-C10-H18=121.6954
C11-C2-H18=149.9479 C2-H18-O12= 84.453 O12-C3-H18= 86.9968
C4-O12-H18= 81.5554 O12-C5-H18= 91.0121 C10-H18-O12= 98.8645
C13-C10-H18=120.1965 C2-H18-O15= 85.455 O15-C3-H18=108.8469
C4-O15-H18= 78.8044 O15-C5-H18=105.0503 C8-O15-H18= 92.4595

C9-O15-H18= 86.0827 O15-C10-H18= 73.5882 O15-O12-H18= 70.1539
C13-O15-H18=112.1333 H16-C2-H18=115.4432 H16-C5-H18= 94.0762
C1-H17-H18= 87.9791 H17-C2-H18= 95.2612 H17-C3-H18= 95.9674
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O12-H18-H17= 96.3858 O15-H18-H17=109.2108 H16-H17-H18= 95.9122
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C2-C4-H19=151.1956 C3-C4-H19=148.5454 C1-H19-C5= 68.0841
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C3-C8-H19= 81.0586 C8-C4-H19=113.1487 C5-H19-C8= 67.3861
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C9-C5-H19= 91.8101 C9-C8-H19=119.7509 C10-C4-H19=158.9171
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C2-C11-H19= 77.115 C11-C4-H19=110.5215 C5-H19-C11= 88.9174
C6-C11-H19= 92.0211 C7-C11-H19= 85.5857 C11-C8-H19= 78.8943
C1-H19-O12= 80.4393 C3-O12-H19= 81.6863 O12-C4-H19= 87.2584
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O15-C4-H19=103.92 O15-C5-H19=101.9107 O15-C8-H19= 71.7962
C9-O15-H19= 86.1856 C10-O15-H19= 93.2918 C11-H19-O15=101.7359
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C8-H19-H16= 92.0603 C11-H16-H19= 76.5285 O12-H19-H16= 76.4444
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H18-C5-H19=149.4999 H18-O12-H19=105.5549 H18-O15-H19= 95.6062
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C3-C6-H20=132.5944 C4-C6-H20=168.2626 C1-C7-H20= 94.7558
C2-H20-C7= 65.4787 C4-C7-H20=114.0207 C7-C6-H20=114.8751
C8-C2-H20= 79.6199 C8-C6-H20=147.2272 C8-C7-H20=124.1681
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C1-C7-H21=160.3954 C2-C7-H21=149.8785 C4-C7-H21=150.2927
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C9-C7-H21=106.2477 C9-C8-H21=101.295 C10-C6-H21=112.4699
C10-C7-H21=117.03 C10-C8-H21= 86.22 C10-C9-H21= 84.0009
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N14-C9-H21=126.3259 O15-C8-H21=146.5158 O15-C9-H21=139.8873
H16-C11-H21=145.5158 H17-C6-H21=135.6098 H19-C8-H21=134.4815
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H20-C7-H21= 91.5803 C8-H21-H20= 90.5544 C9-H21-H20= 73.9425
C10-H20-H21= 83.032 C11-H21-H20= 79.116 H17-H20-H21=109.4447
C1-C4-H22=117.2392 C2-C4-H22=115.1421 C3-C4-H22=114.6811
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C2-C7-H22=113.9206 C4-H22-C7= 65.8666 C6-C7-H22=125.7869
C1-C8-H22=130.1073 C2-C8-H22=161.9252 C3-C8-H22=160.1103
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C5-C9-H22= 89.6709 C6-C9-H22= 93.1455 C7-H22-C9= 67.1861
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C10-C8-H22=149.29 C10-C9-H22=129.6074 C1-C11-H22= 86.1597
C2-C11-H22= 92.7225 C11-C4-H22= 79.3425 C6-C11-H22= 76.6657
C11-C7-H22=102.9749 C11-C8-H22=110.2299 C9-H22-C11= 88.7413
O12-C4-H22=139.1264 C4-H22-C13= 91.0483 C7-H22-C13= 93.6365
C13-C8-H22= 87.8808 C13-C9-H22=101.0016 C10-C13-H22= 75.572
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O15-C13-H22= 72.9202 H16-C4-H22=134.7545 H16-C11-H22=103.2221
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C7-H22-H19= 87.4305 H19-C8-H22= 88.1406 C9-H22-H19= 89.8607
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C8-C3-H23= 80.6484 C8-C6-H23= 92.2382 C3-H23-C9= 67.6718
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H21-C9-H23= 95.5325 H21-H20-H23= 98.1798 H22-C9-H23=150.9007
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C4-C1-H24= 91.3057 C2-C4-H24= 83.3046 C3-C4-H24=119.582
C5-C1-H24=126.4959 C5-C4-H24=157.9522 C6-C1-H24= 94.1636
C6-C4-H24= 75.4069 C1-H24-C7= 62.347 C2-C7-H24= 93.9652
C4-C7-H24= 71.4757 C6-C7-H24=129.6059 C8-C1-H24= 71.4568
C2-C8-H24= 74.6498 C3-C8-H24=103.8866 C8-C4-H24= 73.6043
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O12-C4-H24=149.4351 C13-C8-H24=170.9364 O15-C4-H24=151.4946
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C4-H16-H24= 67.0381 C5-H16-H24= 95.0378 C7-H24-H16= 85.5196
C8-H24-H16= 79.2745 H16-C11-H24= 99.4106 H17-C1-H24=129.9549
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C8-H21-H24= 67.29 C9-H21-H24= 96.6773 H21-C11-H24=100.0386
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C1-H24-H22= 78.1907 H22-C4-H24= 70.6683 H22-C7-H24= 81.6362
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C5-C1-H25=147.5732 C5-C2-H25=119.7243 C6-C1-H25= 70.9981
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C1-H25-C7= 62.4066 C2-C7-H25= 70.8797 C4-C7-H25= 94.3214
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C9-C7-H25=149.6437 C10-C2-H25=113.9087 C10-C6-H25=149.9093
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C4-H16-H25= 87.563 C5-H16-H25=104.5906 C6-H25-H16= 79.2913
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C7-H25-H17= 78.6951 C11-H25-H17= 83.5678 H17-H16-H25= 68.646
H18-C2-H25=173.0438 H18-H17-H25=127.3592 H19-C1-H25=128.221
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C6-H21-H25= 66.7221 H21-C7-H25=103.4949 C8-H21-H25= 88.4721
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H17-H25-H24=115.1216 H19-H24-H25=115.6582 H20-H25-H24=114.6018
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H19-C5-H26= 97.8513 H19-O12-H26=110.7724 H19-O15-H26= 74.7688

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     C4-C6-O27= 92.1085      C1-C7-O27=137.8982      C2-C7-O27=111.4172
     C4-C7-O27=107.7014      C6-C7-O27= 79.5822      C1-C8-O27=126.4438
     C2-C8-O27= 97.7944      C3-C8-O27= 93.1882      C4-C8-O27=149.3364
     C5-C8-O27=116.3707      C6-C8-O27= 66.2921      C8-C7-O27= 73.714
     C3-C9-O27=124.1358      C4-C9-O27=126.5885      C5-C9-O27=154.5602
     C6-C9-O27= 75.0114      C7-C9-O27= 68.8762      C8-C9-O27= 92.9665
    C2-C10-O27=121.1877     C3-C10-O27=153.0615     C4-C10-O27= 96.5068
    C5-C10-O27=119.5314     C6-C10-O27= 80.2872     C7-C10-O27= 60.4297
    C8-C10-O27= 63.0504     C10-C9-O27= 90.1367     C11-C6-O27=104.6813
    C11-C7-O27=176.7541     C11-C8-O27=108.9301     C6-O27-C13= 96.7493
    C7-O27-C13= 99.3648     C8-O27-C13= 65.6326     C13-C9-O27= 85.1169
   C10-O27-C13= 66.8185     N14-C9-O27= 84.8271    N14-C13-O27=122.032
    O15-C8-O27= 98.1234     O15-C9-O27=169.8495    O15-C10-O27=100.2031
   O15-C13-O27=113.4521     H17-C6-O27=167.639     H18-C10-O27=173.7108
    H19-C8-O27=169.8958     C2-H20-O27=101.4196     H20-C6-O27= 93.6759
    H20-C7-O27= 77.4832     C8-O27-H20= 73.6854     C9-O27-H20= 79.9359
   H20-C10-O27= 77.3709    C13-O27-H20=114.2889    H17-H20-O27=125.4065
    C6-H21-O27= 75.3549     C7-H21-O27= 93.4131     C8-H21-O27= 70.7232
    C9-O27-H21= 87.9952    C10-O27-H21= 83.5277    C11-H21-O27=130.3089
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    C6-O27-H22= 74.2151     H22-C7-O27= 73.8599     H22-C8-O27= 94.8463
    H22-C9-O27= 86.6998    C10-O27-H22= 77.6545    C11-H22-O27= 88.1897
   H22-C13-O27= 66.4049    H19-H22-O27=128.1602    H20-O27-H22= 92.7254
   H22-H21-O27= 74.0216     C3-H23-O27=105.561      C6-H23-O27= 65.8859
    C7-O27-H23= 81.3266     C8-O27-H23= 79.8126     H23-C9-O27= 79.6931
   H23-C10-O27= 87.4855    C13-O27-H23= 69.7402    H18-H23-O27=129.833
   H20-H23-O27= 69.3323    H21-O27-H23=101.9942    H22-O27-H23= 99.8866
    H24-C7-O27=150.0752     H24-C8-O27=119.3777    H24-H21-O27=138.0063
   H24-H22-O27=105.0342     H25-C6-O27=116.8932     H25-C7-O27=155.5803
   H25-H20-O27=101.9588    H25-H21-O27=141.7144      C3-C9-H28=135.7391
     C4-C9-H28=144.3095      C5-C9-H28=171.9965      C6-C9-H28= 92.9222
     C7-C9-H28= 88.5579      C8-C9-H28=107.9248     C10-C9-H28= 99.1333
    C8-C13-H28= 83.768      C9-C13-H28= 80.7388    C10-C13-H28= 78.0787
    N14-C9-H28= 65.2484    N14-C13-H28= 98.5878     O15-C9-H28=149.8267
   O15-C13-H28=136.477      H21-C9-H28= 68.7004     H22-C9-H28= 94.5985
   H22-C13-H28= 84.0335     H23-C9-H28= 81.2452    H23-C13-H28= 71.8046
    C6-O27-H28=155.5224     C7-O27-H28=170.007      C8-O27-H28=138.9653
    C9-O27-H28=115.4917    C10-O27-H28=126.3511    C13-O27-H28= 78.6007
   N14-H28-O27=101.4519    H20-O27-H28=143.0594    H21-O27-H28=150.1166
   H22-O27-H28=123.2723    H23-O27-H28=106.8042
Stoichiometry    C12H12NO3(1-)
Framework group  C1[X(C12H12NO3)]
Deg. of freedom   78
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0       -2.164405   -0.327381   -0.435484
   2          6             0       -1.742337   -0.381352    1.061451
```

3	6	0	-0.742808	0.790276	1.304060
4	6	0	-1.000460	0.478067	-1.054580
5	6	0	-0.587814	1.529989	-0.026641
6	6	0	-0.535385	-1.395165	1.049311
7	6	0	-0.431039	-1.811530	-0.440737
8	6	0	0.206105	-0.543595	-1.066675
9	6	0	1.215722	-0.047711	-0.007937
10	6	0	0.459445	-0.215286	1.313469
11	6	0	-1.895181	-1.761799	-0.920056
12	8	0	-1.393279	2.730256	-0.104875
13	6	0	2.566195	0.393485	-0.223271
14	7	0	3.646317	0.733501	-0.387564
15	8	0	0.762915	1.787027	-0.209334
16	1	0	-3.144585	0.090895	-0.622098
17	1	0	-2.547967	-0.540039	1.764977
18	1	0	-0.862672	1.440882	2.155612
19	1	0	-1.202020	0.908797	-2.024701
20	1	0	-0.525736	-2.214209	1.750985
21	1	0	0.128978	-2.709269	-0.611559
22	1	0	0.656347	-0.692004	-2.035186
23	1	0	1.095535	-0.260424	2.178664
24	1	0	-1.993370	-1.871070	-1.997038
25	1	0	-2.518910	-2.503679	-0.427362
26	1	0	-0.793887	3.470455	-0.273339
27	8	0	2.019278	-1.847009	0.218298
28	1	0	2.984541	-1.865013	0.303819

Rotational constants (GHZ): 0.8957508 0.6837219 0.4967974
Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,O-16,C-12,N-14,
O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,O-16,H-1
Standard basis: 3-21+G* (6D, 7F)
There are 232 symmetry adapted basis functions of A symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be 262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
232 basis functions 340 primitive gaussians
58 alpha electrons 58 beta electrons
nuclear repulsion energy 1206.6205108529 Hartrees.
One-electron integrals computed using PRISM.
NBasis= 232 RedAO= T NBF= 232
NBsUse= 232 1.00D-04 NBFU= 232
Projected INDO Guess.
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done: E(RHF) = -736.360938120 A.U. after 19 cycles
Convg = 0.9837D-08 -V/T = 2.0022
S**2 = 0.0000
Range of M.O.s used for correlation: 1 232
NBasis= 232 NAE= 58 NBE= 58 NFC= 0 NFV= 0
NROrb= 232 NOA= 58 NOB= 58 NVA= 174 NVB= 174

**** Warning!!: The largest alpha MO coefficient is 0.10274505D+03

```
          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   3 vectors were produced by pass 12.
   2 vectors were produced by pass 13.
   1 vectors were produced by pass 14.
 Inv2:  IOpt= 1 Iter= 1 AM= 7.36D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  42 with in-core refinement.
 G2DrvN: will do   28 atoms at a time, making    1 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  87 IRICut=      82 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
          There are  87 degrees of freedom in the 1st order CPHF.
  84 vectors were produced by pass  0.
 AX will form  84 AO Fock derivatives at one time.
  84 vectors were produced by pass  1.
  84 vectors were produced by pass  2.
  84 vectors were produced by pass  3.
  84 vectors were produced by pass  4.
  84 vectors were produced by pass  5.
  84 vectors were produced by pass  6.
  48 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   1 vectors were produced by pass  9.
 Inv2:  IOpt= 1 Iter= 1 AM= 4.99D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 640 with in-core refinement.

 ********************************************************************

            Population analysis using the SCF density.
```

```
 **********************************************************************

 Alpha  occ. eigenvalues --  -20.34644 -20.27019 -20.23093 -15.36068 -
11.17572
 Alpha  occ. eigenvalues --  -11.13607 -11.09728 -11.06506 -11.06180 -
11.05624
 Alpha  occ. eigenvalues --  -11.05366 -11.05149 -11.05122 -11.04584 -
11.04437
 Alpha  occ. eigenvalues --  -11.04351  -1.25400  -1.16368  -1.10937  -
1.09377
 Alpha  occ. eigenvalues --   -1.06031  -0.96491  -0.93384  -0.89909  -
0.82298
 Alpha  occ. eigenvalues --   -0.78561  -0.75013  -0.70140  -0.65930  -
0.63025
 Alpha  occ. eigenvalues --   -0.60633  -0.58823  -0.55469  -0.52805  -
0.51206
 Alpha  occ. eigenvalues --   -0.50005  -0.48985  -0.46451  -0.44652  -
0.42060
 Alpha  occ. eigenvalues --   -0.40431  -0.40095  -0.39820  -0.38189  -
0.37423
 Alpha  occ. eigenvalues --   -0.36304  -0.34946  -0.33809  -0.32748  -
0.32253
 Alpha  occ. eigenvalues --   -0.31639  -0.30983  -0.29494  -0.28663  -
0.27103
 Alpha  occ. eigenvalues --   -0.24501  -0.23420  -0.21071
 Alpha virt. eigenvalues --    0.15535   0.17011   0.17523   0.17946
0.19173
 Alpha virt. eigenvalues --    0.19481   0.19517   0.19684   0.20988
0.21616
 Alpha virt. eigenvalues --    0.22425   0.23072   0.23593   0.24556
0.26771
 Alpha virt. eigenvalues --    0.27252   0.27791   0.28342   0.28817
0.29313
 Alpha virt. eigenvalues --    0.29476   0.29636   0.30658   0.31343
0.31764
 Alpha virt. eigenvalues --    0.32411   0.32589   0.33015   0.34445
0.34950
 Alpha virt. eigenvalues --    0.35783   0.35877   0.36070   0.36486
0.37220
 Alpha virt. eigenvalues --    0.37415   0.37908   0.38993   0.39700
0.39825
 Alpha virt. eigenvalues --    0.40623   0.41209   0.41316   0.41690
0.43107
 Alpha virt. eigenvalues --    0.43400   0.43826   0.45117   0.46042
0.46672
 Alpha virt. eigenvalues --    0.47306   0.48469   0.49078   0.49812
0.50717
 Alpha virt. eigenvalues --    0.51241   0.51644   0.52335   0.53033
0.54053
 Alpha virt. eigenvalues --    0.54463   0.54747   0.56640   0.57023
0.57630
 Alpha virt. eigenvalues --    0.58590   0.58827   0.59155   0.60429
0.61513
```

```
 Alpha virt. eigenvalues --    0.61946   0.62558   0.63093   0.63574
0.64788
 Alpha virt. eigenvalues --    0.65850   0.66850   0.67478   0.67767
0.69079
 Alpha virt. eigenvalues --    0.69619   0.71082   0.71835   0.73052
0.73371
 Alpha virt. eigenvalues --    0.74004   0.74683   0.76058   0.76532
0.78363
 Alpha virt. eigenvalues --    0.79017   0.79693   0.81286   0.83793
0.84918
 Alpha virt. eigenvalues --    0.87220   0.91551   1.20287   1.23990
1.26087
 Alpha virt. eigenvalues --    1.27037   1.27731   1.29139   1.29818
1.30628
 Alpha virt. eigenvalues --    1.31546   1.32215   1.33381   1.33531
1.34905
 Alpha virt. eigenvalues --    1.35734   1.36180   1.36946   1.38350
1.38658
 Alpha virt. eigenvalues --    1.40132   1.41989   1.43946   1.44478
1.44784
 Alpha virt. eigenvalues --    1.47010   1.48729   1.51132   1.52937
1.54835
 Alpha virt. eigenvalues --    1.55861   1.58456   1.62765   1.63664
1.65077
 Alpha virt. eigenvalues --    1.66182   1.66906   1.68203   1.69801
1.72143
 Alpha virt. eigenvalues --    1.72338   1.73475   1.75186   1.77525
1.82658
 Alpha virt. eigenvalues --    1.86334   1.86910   1.88571   1.89918
1.92662
 Alpha virt. eigenvalues --    1.94767   2.02666   2.08180   2.13480
2.22718
 Alpha virt. eigenvalues --    2.27105   2.30944   2.35925   2.37681
2.39740
 Alpha virt. eigenvalues --    2.41851   2.48472   2.50935   2.54294
2.59434
 Alpha virt. eigenvalues --    2.63950   2.68040   2.70334   2.75802
3.02524
 Alpha virt. eigenvalues --    3.08572   3.29521   3.35386   3.67293
3.72010
 Alpha virt. eigenvalues --    3.82194   3.94476   4.14573   4.15479
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
  1  C   15.693321  -7.231454   1.653898  -9.310117   3.379178   5.563953
  2  C   -7.231454  20.293062 -11.266205   2.846104   4.066445 -11.611909
  3  C    1.653898 -11.266205  43.520178  18.153365 -45.529798   8.036158
  4  C   -9.310117   2.846104  18.153365  39.734590 -42.089159  -3.697713
  5  C    3.379178   4.066445 -45.529798 -42.089159  88.972178  -1.564302
  6  C    5.563953 -11.611909   8.036158  -3.697713  -1.564302  24.536945
  7  C   -3.726526   5.840818  -3.678219   3.152002   1.898387 -11.008400
  8  C    9.864402  -5.824689 -16.550122 -33.625712  39.443820   8.115021
  9  C   -3.850422  -2.148920  26.416537  24.563911 -44.055954   5.214777
 10  C    0.087936   8.808588 -36.378013 -20.107984  45.601382 -12.894221
 11  C   -3.574811   0.018400   2.768508   4.287858  -5.093662  -1.006668
```

12	O	-0.009594	0.010703	1.010601	0.922238	-2.389749	-0.034393
13	C	-2.443300	1.592132	15.832917	18.369835	-31.864856	-3.175822
14	N	0.040505	-0.042495	-0.463143	-0.525537	1.043487	0.105130
15	O	-0.098087	0.046758	0.994648	1.083973	-2.706210	-0.184591
16	H	0.563261	-0.116209	0.069077	-0.171080	-0.043099	0.053607
17	H	-0.089528	0.586514	-0.159291	0.017855	0.017909	-0.147708
18	H	0.047417	-0.159201	0.668407	0.040854	-0.199354	0.088850
19	H	-0.034582	-0.019362	0.089669	0.604562	-0.205710	0.014679
20	H	0.006666	-0.158897	0.111576	0.012566	-0.015109	0.561475
21	H	-0.039041	0.068126	-0.039175	0.042835	0.035887	-0.143925
22	H	0.012236	0.018358	-0.049106	-0.152733	0.098165	-0.024259
23	H	0.009662	0.028596	-0.136765	-0.031680	0.071978	-0.035572
24	H	-0.072432	0.020848	0.013804	0.043013	-0.034574	0.048910
25	H	-0.052063	-0.021621	0.008392	0.012224	-0.002906	0.044077
26	H	-0.002640	0.000986	-0.003755	0.004243	0.028402	0.001443
27	O	-0.132113	0.120315	0.112689	0.221653	-0.282206	-0.288913
28	H	0.005896	-0.005295	-0.024396	-0.029129	0.040308	0.006484

		7	8	9	10	11	12
1	C	-3.726526	9.864402	-3.850422	0.087936	-3.574811	-0.009594
2	C	5.840818	-5.824689	-2.148920	8.808588	0.018400	0.010703
3	C	-3.678219	-16.550122	26.416537	-36.378013	2.768508	1.010601
4	C	3.152002	-33.625712	24.563911	-20.107984	4.287858	0.922238
5	C	1.898387	39.443820	-44.055954	45.601382	-5.093662	-2.389749
6	C	-11.008400	8.115021	5.214777	-12.894221	-1.006668	-0.034393
7	C	20.168471	-9.524769	-2.214163	7.538821	-1.809318	0.009825
8	C	-9.524769	78.856131	-47.981515	44.412384	-4.701863	-0.840308
9	C	-2.214163	-47.981515	134.453187	-56.983933	4.071111	0.998223
10	C	7.538821	44.412384	-56.983933	89.844175	-3.242999	-0.876388
11	C	-1.809318	-4.701863	4.071111	-3.242999	12.403529	0.092040
12	O	0.009825	-0.840308	0.998223	-0.876388	0.092040	8.862614
13	C	-1.376192	-52.396752	-40.593418	-56.710827	2.073169	0.634498
14	N	-0.022805	1.577117	2.718305	1.603086	-0.035868	-0.015012
15	O	0.261328	-0.497208	0.251880	-0.180111	0.075532	-0.005661
16	H	-0.054880	0.044345	0.035283	-0.043734	0.005811	0.004028
17	H	0.002444	0.024360	-0.039427	0.128978	0.022756	0.001086
18	H	-0.015961	0.033112	0.006880	-0.098512	-0.001936	-0.000443
19	H	0.019732	-0.102700	0.031527	0.001549	0.007861	0.000449
20	H	-0.066811	0.092353	-0.122959	-0.028848	0.024018	0.000044
21	H	0.647436	-0.122171	-0.062060	0.143284	-0.078041	-0.000048
22	H	0.012676	0.745095	-0.230391	0.215789	-0.011206	-0.000179
23	H	-0.009769	0.168269	-0.203964	0.814798	-0.010051	-0.000141
24	H	-0.169867	0.054412	-0.024503	-0.002450	0.440037	0.000188
25	H	-0.158247	0.101333	-0.028489	-0.008509	0.423150	0.000025
26	H	0.002264	-0.012179	0.020297	0.001457	-0.001956	0.188279
27	O	0.025979	0.327410	-1.021328	0.742802	-0.020633	0.004453
28	H	0.053076	0.002120	0.122213	0.045665	0.000748	-0.000029

		13	14	15	16	17	18
1	C	-2.443300	0.040505	-0.098087	0.563261	-0.089528	0.047417
2	C	1.592132	-0.042495	0.046758	-0.116209	0.586514	-0.159201
3	C	15.832917	-0.463143	0.994648	0.069077	-0.159291	0.668407
4	C	18.369835	-0.525537	1.083973	-0.171080	0.017855	0.040854
5	C	-31.864856	1.043487	-2.706210	-0.043099	0.017909	-0.199354
6	C	-3.175822	0.105130	-0.184591	0.053607	-0.147708	0.088850
7	C	-1.376192	-0.022805	0.261328	-0.054880	0.002444	-0.015961

8	C	-52.396752	1.577117	-0.497208	0.044345	0.024360	0.033112
9	C	-40.593418	2.718305	0.251880	0.035283	-0.039427	0.006880
10	C	-56.710827	1.603086	-0.180111	-0.043734	0.128978	-0.098512
11	C	2.073169	-0.035868	0.075532	0.005811	0.022756	-0.001936
12	O	0.634498	-0.015012	-0.005661	0.004028	0.001086	-0.000443
13	C	157.913462	-6.290726	-0.105397	0.006322	-0.003422	-0.052968
14	N	-6.290726	8.445886	-0.093839	-0.000016	0.000019	0.000204
15	O	-0.105397	-0.093839	9.496392	-0.000892	-0.000118	0.006797
16	H	0.006322	-0.000016	-0.000892	0.407138	-0.000435	-0.000031
17	H	-0.003422	0.000019	-0.000118	-0.000435	0.409305	-0.000164
18	H	-0.052968	0.000204	0.006797	-0.000031	-0.000164	0.384956
19	H	-0.058695	0.000230	0.006580	-0.000199	-0.000016	-0.000023
20	H	-0.055038	0.000174	0.000499	-0.000015	-0.000423	-0.000102
21	H	-0.090092	0.000587	-0.000594	-0.000017	-0.000012	0.000001
22	H	-0.288069	0.002894	0.008001	-0.000021	0.000001	0.000000
23	H	-0.305140	0.001576	0.008826	0.000001	-0.000092	-0.000747
24	H	-0.002480	0.000019	-0.000038	-0.000127	-0.000034	0.000000
25	H	-0.000802	0.000000	0.000140	-0.000371	0.000168	0.000000
26	H	-0.024179	0.000390	0.011228	-0.000002	0.000002	0.000388
27	O	-0.429864	-0.083460	0.133024	0.000068	-0.000094	-0.000201
28	H	-0.151283	0.004116	-0.002204	0.000000	0.000000	0.000000

		19	20	21	22	23	24
1	C	-0.034582	0.006666	-0.039041	0.012236	0.009662	-0.072432
2	C	-0.019362	-0.158897	0.068126	0.018358	0.028596	0.020848
3	C	0.089669	0.111576	-0.039175	-0.049106	-0.136765	0.013804
4	C	0.604562	0.012566	0.042835	-0.152733	-0.031680	0.043013
5	C	-0.205710	-0.015109	0.035887	0.098165	0.071978	-0.034574
6	C	0.014679	0.561475	-0.143925	-0.024259	-0.035572	0.048910
7	C	0.019732	-0.066811	0.647436	0.012676	-0.009769	-0.169867
8	C	-0.102700	0.092353	-0.122171	0.745095	0.168269	0.054412
9	C	0.031527	-0.122959	-0.062060	-0.230391	-0.203964	-0.024503
10	C	0.001549	-0.028848	0.143284	0.215789	0.814798	-0.002450
11	C	0.007861	0.024018	-0.078041	-0.011206	-0.010051	0.440037
12	O	0.000449	0.000044	-0.000048	-0.000179	-0.000141	0.000188
13	C	-0.058695	-0.055038	-0.090092	-0.288069	-0.305140	-0.002480
14	N	0.000230	0.000174	0.000587	0.002894	0.001576	0.000019
15	O	0.006580	0.000499	-0.000594	0.008001	0.008826	-0.000038
16	H	-0.000199	-0.000015	-0.000017	-0.000021	0.000001	-0.000127
17	H	-0.000016	-0.000423	-0.000012	0.000001	-0.000092	-0.000034
18	H	-0.000023	-0.000102	0.000001	0.000000	-0.000747	0.000000
19	H	0.388084	0.000001	-0.000018	-0.000847	0.000000	0.000145
20	H	0.000001	0.392859	-0.000108	-0.000012	-0.000227	-0.000043
21	H	-0.000018	-0.000108	0.333704	0.000181	0.000000	-0.000103
22	H	-0.000847	-0.000012	0.000181	0.385097	-0.000015	-0.000049
23	H	0.000000	-0.000227	0.000000	-0.000015	0.378838	0.000000
24	H	0.000145	-0.000043	-0.000103	-0.000049	0.000000	0.468916
25	H	-0.000041	0.000095	-0.000278	-0.000042	0.000001	-0.020315
26	H	0.000427	0.000000	0.000000	-0.000001	-0.000001	0.000000
27	O	-0.000082	0.005268	-0.007772	0.007924	-0.000857	-0.000289
28	H	0.000000	-0.000059	0.000436	0.000046	0.000340	0.000000

		25	26	27	28
1	C	-0.052063	-0.002640	-0.132113	0.005896
2	C	-0.021621	0.000986	0.120315	-0.005295
3	C	0.008392	-0.003755	0.112689	-0.024396

4	C	0.012224	0.004243	0.221653	-0.029129
5	C	-0.002906	0.028402	-0.282206	0.040308
6	C	0.044077	0.001443	-0.288913	0.006484
7	C	-0.158247	0.002264	0.025979	0.053076
8	C	0.101333	-0.012179	0.327410	0.002120
9	C	-0.028489	0.020297	-1.021328	0.122213
10	C	-0.008509	0.001457	0.742802	0.045665
11	C	0.423150	-0.001956	-0.020633	0.000748
12	O	0.000025	0.188279	0.004453	-0.000029
13	C	-0.000802	-0.024179	-0.429864	-0.151283
14	N	0.000000	0.000390	-0.083460	0.004116
15	O	0.000140	0.011228	0.133024	-0.002204
16	H	-0.000371	-0.000002	0.000068	0.000000
17	H	0.000168	0.000002	-0.000094	0.000000
18	H	0.000000	0.000388	-0.000201	0.000000
19	H	-0.000041	0.000427	-0.000082	0.000000
20	H	0.000095	0.000000	0.005268	-0.000059
21	H	-0.000278	0.000000	-0.007772	0.000436
22	H	-0.000042	-0.000001	0.007924	0.000046
23	H	0.000001	-0.000001	-0.000857	0.000340
24	H	-0.020315	0.000000	-0.000289	0.000000
25	H	0.469573	0.000000	-0.000288	0.000000
26	H	0.000000	0.335061	-0.000012	0.000000
27	O	-0.000288	-0.000012	9.566865	0.129513
28	H	0.000000	0.000000	0.129513	0.423381

Total atomic charges:

		1
1	C	-0.261619
2	C	0.239504
3	C	0.817564
4	C	1.627165
5	C	-2.620878
6	C	-0.573112
7	C	0.202667
8	C	-5.681696
9	C	6.657316
10	C	-6.434166
11	C	-1.125518
12	O	-0.567347
13	C	5.996987
14	N	-0.970824
15	O	-0.510657
16	H	0.242186
17	H	0.229371
18	H	0.251777
19	H	0.256779
20	H	0.241055
21	H	0.310979
22	H	0.250466
23	H	0.252134
24	H	0.237011
25	H	0.234794
26	H	0.449858
27	O	-1.129849

```
28  H    0.378055
Sum of Mulliken charges=  -1.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  C   -0.019434
 2  C    0.468875
 3  C    1.069340
 4  C    1.883944
 5  C   -2.620878
 6  C   -0.332056
 7  C    0.513646
 8  C   -5.431231
 9  C    6.657316
10  C   -6.182032
11  C   -0.653714
12  O   -0.117489
13  C    5.996987
14  N   -0.970824
15  O   -0.510657
16  H    0.000000
17  H    0.000000
18  H    0.000000
19  H    0.000000
20  H    0.000000
21  H    0.000000
22  H    0.000000
23  H    0.000000
24  H    0.000000
25  H    0.000000
26  H    0.000000
27  O   -0.751794
28  H    0.000000
Sum of Mulliken charges=  -1.00000
Electronic spatial extent (au):  <R**2>=  2531.9152
Charge=    -1.0000 electrons
Dipole moment (Debye):
   X=    -7.3463    Y=    -1.7731    Z=     0.6828  Tot=     7.5880
Quadrupole moment (Debye-Ang):
  XX=  -136.3033   YY=  -120.8386   ZZ=   -96.8788
  XY=     3.3435   XZ=     3.0001   YZ=     1.8854
Octapole moment (Debye-Ang**2):
 XXX=   -94.7823  YYY=    27.8894  ZZZ=    -0.0859  XYY=   -15.7087
 XXY=   -29.7830  XXZ=    15.6851  XZZ=    -1.0119  YZZ=     4.1435
 YYZ=    -1.7710  XYZ=     7.4012
Hexadecapole moment (Debye-Ang**3):
XXXX= -2216.7045 YYYY= -1220.8941 ZZZZ=  -527.3465 XXXY=  -107.0263
XXXZ=    57.7476 YYYX=    32.9838 YYYZ=   -12.7290 ZZZX=     5.4119
ZZZY=    -0.0910 XXYY=  -611.8188 XXZZ=  -394.4896 YYZZ=  -298.7853
XXYZ=     7.7306 YYXZ=    -0.2469 ZZXY=    -9.4269
N-N= 1.206620510853D+03 E-N=-4.155004625338D+03  KE= 7.347595918838D+02
 Exact polarizability: 150.410  -2.413 140.487  -0.241  -1.828 109.640
Approx polarizability: 130.793  -0.776 127.112  -1.747  -2.875 105.292
Full mass-weighted force constant matrix:
```

```
 Low frequencies --- -650.1169   -0.7612   -0.0013   -0.0002    0.0012
0.1750
 Low frequencies ---    0.9868  123.6896  197.1199
 ******    1 imaginary frequencies (negative Signs) ******
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                      1                      2                      3
                    ?A                     ?A                     ?A
 Frequencies --  -650.1169               123.6896               197.1199
 Red. masses --     8.8572                 9.9991                 8.3622
 Frc consts  --     2.2056                 0.0901                 0.1914
 IR Inten    --  1064.7499                 2.5466                 5.7825
 Raman Activ --     6.2740                 1.4438                 1.6942
 Depolar     --     0.1935                 0.7484                 0.6697
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.02  -0.01   0.00    -0.04  -0.01   0.11    -0.01   0.00  -
0.03
   2   6    -0.01  -0.01   0.00     0.05   0.04   0.08    -0.07   0.00  -
0.02
   3   6    -0.05   0.01   0.03     0.08   0.04  -0.03    -0.04  -0.03
0.01
   4   6    -0.05   0.00  -0.02    -0.07  -0.04   0.00     0.03  -0.04
0.00
   5   6    -0.10  -0.03   0.02     0.00  -0.01  -0.07     0.06  -0.04
0.01
   6   6     0.03   0.02  -0.02     0.04   0.02   0.03    -0.10  -0.04
0.04
   7   6     0.04   0.03   0.01    -0.05  -0.02   0.03    -0.06  -0.06
0.06
   8   6    -0.01   0.05  -0.01    -0.07  -0.04  -0.05     0.00  -0.09
0.06
   9   6    -0.22   0.66  -0.08    -0.01  -0.01  -0.11    -0.01  -0.07
0.06
  10   6    -0.01   0.04  -0.02     0.07   0.01  -0.07    -0.06  -0.08
0.05
  11   6     0.02   0.00   0.00    -0.09  -0.02   0.14    -0.04  -0.02
0.00
  12   8     0.05   0.01  -0.01     0.01  -0.01  -0.08     0.33   0.11  -
0.09
  13   6     0.04  -0.09   0.01     0.02   0.03   0.15    -0.08   0.12
0.00
  14   7     0.02  -0.03   0.00     0.06   0.11   0.57    -0.20   0.46  -
0.12
  15   8     0.03  -0.27   0.03    -0.01  -0.03  -0.17     0.09  -0.18
0.09
  16   1    -0.03  -0.03   0.01    -0.05   0.00   0.16     0.00   0.02  -
0.07
  17   1     0.00  -0.03   0.00     0.10   0.07   0.14    -0.10   0.04  -
0.04
  18   1    -0.08   0.02   0.01     0.15   0.07  -0.04    -0.04  -0.03
0.01
```

19	1	-0.08	0.03	0.00	-0.14	-0.07	0.00	0.08	-0.04	-0.01
20	1	0.07	0.03	-0.01	0.07	0.04	0.05	-0.17	-0.03	0.06
21	1	0.09	0.07	0.01	-0.07	-0.03	0.02	-0.08	-0.08	0.08
22	1	0.02	0.06	0.01	-0.13	-0.08	-0.07	0.02	-0.13	0.07
23	1	0.05	0.03	-0.07	0.12	0.04	-0.11	-0.09	-0.09	0.08
24	1	0.01	0.00	0.00	-0.18	-0.07	0.15	-0.01	-0.03	0.00
25	1	0.03	-0.01	0.00	-0.05	0.00	0.22	-0.09	0.01	-0.01
26	1	0.00	0.05	-0.01	0.01	-0.02	-0.11	0.54	-0.04	-0.02
27	8	0.13	-0.20	0.03	0.00	-0.05	-0.41	0.04	-0.04	-0.10
28	1	0.12	-0.51	0.06	-0.03	-0.02	-0.07	0.02	0.04	0.15

	4			5			6		
	?A			?A			?A		
Frequencies --	211.5432			243.7378			261.9626		
Red. masses --	4.3536			1.3267			3.3432		
Frc consts --	0.1148			0.0464			0.1352		
IR Inten --	87.6968			59.0156			61.7767		
Raman Activ --	0.3373			2.5253			2.0263		
Depolar --	0.7485			0.7385			0.4616		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	-0.01	-0.04	0.00	-0.02	-0.02	0.03	0.11	-0.03
2	6	-0.05	0.02	-0.01	-0.01	0.00	-0.01	-0.01	0.09	-0.01
3	6	-0.07	0.03	0.02	-0.02	0.01	0.00	0.05	0.02	0.00
4	6	0.06	-0.01	0.01	0.00	-0.01	0.00	0.10	0.01	-0.01
5	6	-0.01	0.01	0.02	0.00	0.00	0.01	0.05	-0.02	0.00
6	6	-0.04	0.03	0.07	0.00	0.00	0.00	-0.06	0.02	0.02
7	6	0.04	0.01	0.09	0.01	-0.01	0.00	-0.06	0.00	0.03
8	6	0.05	0.01	0.08	0.00	-0.01	0.00	0.03	-0.04	0.02
9	6	0.00	0.03	0.09	0.00	0.00	0.00	0.01	-0.01	0.02
10	6	-0.04	0.04	0.08	-0.01	0.01	0.00	0.01	-0.03	0.02
11	6	0.08	-0.02	0.01	0.02	-0.02	-0.01	-0.05	0.09	-0.01
12	8	-0.07	-0.03	-0.10	0.03	0.03	0.12	-0.17	-0.16	0.01

13	6	0.01	-0.03	0.01	0.00	0.00	0.00	0.00	0.00	0.02
14	7	0.02	-0.12	-0.11	0.00	-0.01	0.00	-0.04	0.12	-0.03
15	8	0.00	0.04	0.14	-0.01	-0.01	-0.04	0.04	0.04	0.02
16	1	0.04	-0.02	-0.10	0.00	-0.03	-0.02	0.07	0.19	-0.05
17	1	-0.09	0.03	-0.06	-0.01	0.00	-0.02	-0.03	0.13	-0.03
18	1	-0.12	0.04	0.01	-0.03	0.01	-0.01	0.08	0.05	-0.01
19	1	0.11	-0.01	0.00	0.01	-0.01	-0.01	0.14	0.03	-0.01
20	1	-0.08	0.05	0.09	0.00	0.01	0.01	-0.11	0.03	0.03
21	1	0.07	0.02	0.12	0.02	0.00	0.01	-0.10	-0.03	0.05
22	1	0.10	-0.03	0.12	0.01	-0.01	0.00	0.05	-0.09	0.04
23	1	-0.09	0.08	0.12	-0.02	0.03	0.00	0.01	-0.07	0.01
24	1	0.15	-0.04	0.00	0.03	-0.02	-0.01	-0.03	0.09	-0.01
25	1	0.05	-0.01	-0.02	0.02	-0.02	-0.01	-0.11	0.14	-0.02
26	1	-0.08	0.02	0.06	-0.07	-0.13	-0.93	-0.40	-0.08	-0.46
27	8	0.01	-0.02	-0.33	-0.02	0.01	-0.01	0.10	-0.17	0.00
28	1	-0.09	0.10	0.75	-0.04	0.05	0.28	0.14	-0.24	-0.43

	7			8			9		
	?A			?A			?A		
Frequencies --	278.8933			311.7690			330.9336		
Red. masses --	1.4731			3.8949			3.4450		
Frc consts --	0.0675			0.2231			0.2223		
IR Inten --	88.8746			19.6240			25.8771		
Raman Activ --	1.8649			1.1158			1.8674		
Depolar --	0.6654			0.4951			0.7459		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.01	0.02	0.00	-0.02	0.00	-0.11	0.05	-0.06	-0.06
2 6	0.03	0.01	0.00	-0.07	0.08	-0.08	0.02	0.01	-0.04
3 6	0.04	0.00	-0.01	0.00	0.02	-0.07	-0.01	0.03	-0.04
4 6	0.01	0.01	-0.01	-0.01	0.00	-0.07	0.02	0.00	-0.04
5 6	0.02	-0.01	-0.01	0.00	0.01	-0.05	0.00	0.03	-0.03
6 6	0.02	0.01	-0.02	-0.09	0.04	0.05	0.04	0.04	0.04

7	6	0.00	0.00	-0.02	-0.02	-0.03	0.09	0.08	0.00	0.06
8	6	0.01	-0.01	-0.02	-0.01	-0.06	0.03	0.04	0.01	0.02
9	6	0.01	0.00	-0.03	-0.01	-0.02	0.00	0.00	0.01	0.02
10	6	0.02	0.00	-0.02	-0.04	0.01	0.01	0.01	0.06	0.03
11	6	-0.01	0.02	0.00	0.01	-0.06	0.01	0.13	-0.08	0.02
12	8	-0.04	-0.04	0.04	0.01	0.04	0.26	0.00	0.04	0.11
13	6	0.01	0.00	-0.03	-0.02	-0.03	0.00	-0.01	0.01	0.03
14	7	-0.02	0.08	0.01	-0.01	-0.05	0.01	-0.04	0.06	-0.02
15	8	0.01	0.00	-0.05	-0.01	0.00	-0.13	0.00	0.05	-0.04
16	1	0.01	0.03	0.02	-0.02	-0.05	-0.17	0.02	-0.13	-0.09
17	1	0.03	0.02	0.01	-0.10	0.16	-0.10	0.00	0.03	-0.06
18	1	0.05	0.01	-0.01	-0.02	0.05	-0.10	-0.05	0.04	-0.05
19	1	0.00	0.01	0.00	0.07	-0.03	-0.10	0.04	-0.03	-0.06
20	1	0.02	0.00	-0.02	-0.17	0.08	0.10	0.04	0.06	0.07
21	1	-0.01	0.00	-0.02	0.01	-0.02	0.16	0.12	0.03	0.09
22	1	0.00	0.00	-0.03	0.00	-0.13	0.04	0.06	-0.01	0.04
23	1	0.03	-0.01	-0.03	-0.05	0.03	0.02	0.01	0.11	0.03
24	1	-0.02	0.03	0.00	0.05	-0.15	0.02	0.17	-0.15	0.02
25	1	-0.01	0.02	0.00	-0.03	0.00	0.05	0.14	-0.07	0.04
26	1	-0.06	0.04	0.31	0.04	0.11	0.69	0.01	0.06	0.23
27	8	-0.06	-0.08	0.05	0.22	0.03	-0.03	-0.26	-0.16	-0.04
28	1	-0.13	0.00	0.92	0.22	0.15	0.00	-0.21	-0.39	-0.63

	10	11	12
	?A	?A	?A
Frequencies --	368.9643	397.7349	463.0660
Red. masses --	8.3990	2.8119	7.2703
Frc consts --	0.6737	0.2621	0.9185
IR Inten --	5.3551	13.3568	12.7435
Raman Activ --	13.7080	0.8350	9.2055
Depolar --	0.3249	0.4215	0.0972

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z

1	6	-0.01	-0.07	0.07	0.02	0.00	-0.07	-0.12	-0.03	0.03
2	6	0.04	-0.07	0.04	0.00	0.01	-0.07	-0.10	-0.05	0.00
3	6	-0.02	0.02	0.00	-0.03	-0.01	-0.04	-0.10	-0.02	-0.02
4	6	-0.08	0.06	0.07	0.04	0.01	-0.08	-0.09	-0.01	0.04
5	6	-0.06	0.15	0.01	0.01	0.02	0.01	-0.09	0.01	-0.02
6	6	0.06	-0.04	0.00	0.02	0.01	-0.05	-0.07	-0.03	-0.06
7	6	0.06	0.01	-0.04	0.00	-0.01	-0.03	-0.05	0.03	-0.07
8	6	-0.04	0.06	0.00	-0.01	-0.01	-0.09	0.04	0.05	0.05
9	6	-0.05	-0.15	0.01	0.00	0.00	-0.06	0.21	-0.02	0.12
10	6	0.01	-0.01	-0.02	-0.01	0.00	-0.07	-0.06	-0.03	0.05
11	6	0.09	-0.03	-0.05	-0.08	-0.11	0.19	-0.13	-0.03	0.06
12	8	0.03	0.26	-0.12	0.00	0.02	0.02	-0.03	0.10	-0.01
13	6	-0.14	-0.10	0.01	0.00	0.00	-0.04	0.36	0.09	0.13
14	7	-0.17	-0.04	0.04	0.01	0.00	0.03	0.34	0.11	-0.14
15	8	-0.09	0.26	-0.02	0.02	0.07	0.20	-0.09	0.00	-0.11
16	1	-0.05	-0.15	0.12	0.02	0.00	-0.08	-0.11	-0.02	0.02
17	1	0.07	-0.10	0.07	-0.02	-0.01	-0.09	-0.06	-0.08	0.03
18	1	0.01	-0.08	0.09	-0.02	-0.03	-0.03	-0.12	-0.04	0.00
19	1	-0.13	-0.02	0.04	0.04	0.04	-0.07	-0.09	-0.07	0.01
20	1	0.12	-0.06	-0.04	0.02	0.02	-0.05	-0.08	-0.08	-0.12
21	1	0.15	0.07	-0.06	0.00	-0.01	-0.03	-0.07	0.02	-0.08
22	1	-0.07	0.15	-0.03	0.00	-0.03	-0.08	0.02	0.15	0.03
23	1	0.02	0.04	-0.03	0.01	0.02	-0.08	-0.24	-0.09	0.18
24	1	0.12	0.08	-0.06	-0.36	-0.47	0.26	-0.31	-0.14	0.09
25	1	0.11	-0.12	-0.14	0.04	0.07	0.61	0.01	-0.02	0.24
26	1	0.19	0.12	-0.21	0.00	0.01	-0.08	0.06	0.03	0.01
27	8	0.26	-0.36	0.04	0.01	-0.02	0.03	0.03	-0.15	0.00

28	1	0.26	-0.11	0.21	0.01	0.00	0.06	0.03	-0.27	0.03

	13	14	15
	?A	?A	?A
Frequencies --	470.9152	541.7535	565.4796
Red. masses --	4.0032	4.1800	4.1793
Frc consts --	0.5230	0.7228	0.7874
IR Inten --	18.6825	0.9244	5.0344
Raman Activ --	3.2179	0.9292	0.4016
Depolar --	0.2329	0.3630	0.1777

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.04	0.05	0.00	-0.10	-0.05	-0.01	0.08	0.05	-0.13
2	6	0.05	-0.01	-0.03	-0.10	0.12	0.01	-0.05	-0.02	-0.07
3	6	0.04	-0.02	0.03	0.03	0.05	0.05	0.01	-0.06	0.20
4	6	0.03	0.03	-0.01	-0.10	0.08	0.07	0.10	0.05	0.12
5	6	0.04	-0.01	-0.03	0.05	-0.02	0.07	0.00	0.04	0.18
6	6	0.04	-0.04	-0.09	-0.10	0.11	-0.03	-0.07	-0.05	0.00
7	6	0.06	0.07	-0.13	0.09	0.16	-0.04	0.00	-0.05	0.06
8	6	0.05	0.11	0.01	-0.07	0.15	-0.05	-0.01	-0.02	0.06
9	6	-0.06	0.02	0.16	0.03	-0.13	-0.03	-0.02	0.07	-0.07
10	6	-0.02	-0.06	0.10	-0.03	-0.03	0.01	0.01	-0.10	0.03
11	6	-0.03	0.00	0.12	0.16	-0.10	0.03	0.02	-0.04	0.03
12	8	0.02	-0.05	-0.02	-0.02	-0.09	-0.03	0.00	0.04	-0.08
13	6	-0.11	-0.01	0.22	0.03	-0.11	-0.09	-0.01	0.06	-0.19
14	7	-0.15	-0.06	-0.07	0.00	0.05	0.03	0.05	-0.01	0.06
15	8	0.01	-0.03	-0.18	0.07	-0.13	0.01	-0.06	0.06	-0.17
16	1	0.04	0.06	0.02	-0.15	-0.25	-0.14	0.10	0.06	-0.21
17	1	0.05	-0.05	-0.04	-0.06	0.14	0.06	-0.15	-0.07	-0.19
18	1	-0.02	0.00	0.01	0.07	0.06	0.05	-0.02	-0.25	0.34
19	1	0.03	0.05	0.00	-0.12	0.20	0.13	0.28	0.25	0.17
20	1	-0.02	-0.12	-0.18	-0.18	0.03	-0.12	-0.16	-0.03	0.04
21	1	0.06	0.08	-0.20	0.25	0.25	0.06	0.02	-0.04	0.06

22	1	0.21	0.25	0.06	-0.15	0.23	-0.11	-0.09	-0.05
0.03									
23	1	-0.06	-0.13	0.12	-0.02	-0.10	0.01	0.10	-0.23
-0.04									
24	1	-0.35	-0.25	0.18	0.11	-0.17	0.04	-0.02	-0.27
0.06									
25	1	0.13	0.10	0.48	0.33	-0.18	0.11	-0.02	0.12
0.22									
26	1	-0.02	-0.02	0.00	-0.12	-0.02	-0.07	0.07	0.00
0.01									
27	8	0.00	0.03	-0.03	0.03	-0.02	0.01	-0.03	0.01
0.01									
28	1	0.00	0.07	0.04	0.03	0.13	-0.06	-0.03	-0.07
-0.01									

	16	17	18
	?A	?A	?A
Frequencies --	591.2894	612.4195	632.1956
Red. masses --	6.9370	4.8288	6.1567
Frc consts --	1.4290	1.0671	1.4498
IR Inten --	6.1667	4.5932	2.0181
Raman Activ --	0.7899	2.0096	3.3869
Depolar --	0.6729	0.3224	0.6224

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.12	-0.10	0.05	0.04	0.04	0.04	0.05	-0.09	0.09
2	6	-0.09	0.08	0.06	-0.08	-0.05	0.04	-0.07	0.10	0.08
3	6	0.10	-0.01	0.00	-0.21	0.07	0.08	0.02	0.15	0.13
4	6	-0.04	-0.09	0.02	0.10	-0.09	0.06	0.12	-0.12	0.15
5	6	0.11	-0.10	-0.01	-0.04	-0.12	0.06	0.03	0.10	0.11
6	6	-0.14	0.03	-0.04	0.07	0.14	-0.05	-0.09	0.10	-0.13
7	6	-0.03	0.01	-0.01	0.04	0.06	-0.08	0.01	-0.15	-0.11
8	6	-0.04	0.02	-0.04	0.12	-0.04	-0.08	0.12	-0.16	-0.13
9	6	-0.04	0.17	-0.02	0.02	-0.08	-0.03	-0.02	0.02	-0.09
10	6	-0.03	-0.07	-0.03	-0.09	0.22	0.00	-0.09	0.02	-0.18
11	6	0.00	-0.11	-0.05	-0.02	0.11	0.03	0.01	-0.12	-0.04
12	8	0.22	-0.23	0.01	0.12	-0.13	0.04	-0.10	0.13	0.01
13	6	-0.05	0.24	0.07	-0.03	-0.01	-0.11	0.02	-0.05	0.24
14	7	0.04	-0.08	-0.03	-0.01	-0.01	0.04	-0.05	0.01	-0.08
15	8	0.02	0.33	0.00	-0.11	-0.01	-0.04	0.07	-0.02	-0.01

16	1	-0.12	-0.14	-0.06	0.11	0.18	-0.03	0.11	-0.03	-0.09
17	1	-0.02	0.18	0.16	-0.09	-0.27	-0.02	-0.03	0.03	0.11
18	1	0.20	0.09	-0.07	-0.30	0.14	0.02	0.21	0.05	0.24
19	1	-0.12	-0.05	0.06	0.08	-0.01	0.11	0.03	-0.10	0.17
20	1	-0.17	0.02	-0.05	0.24	0.13	-0.07	-0.02	0.17	-0.06
21	1	0.06	0.04	0.10	-0.06	-0.02	-0.02	-0.04	-0.22	0.10
22	1	-0.03	0.02	-0.03	0.13	0.04	-0.08	0.08	-0.06	-0.17
23	1	-0.02	-0.20	-0.05	-0.09	0.26	0.01	-0.05	-0.17	-0.23
24	1	0.04	0.03	-0.07	-0.14	0.11	0.04	-0.10	0.04	-0.05
25	1	0.07	-0.24	-0.17	0.05	0.09	0.09	0.04	-0.19	-0.10
26	1	0.28	-0.29	-0.03	0.28	-0.23	0.16	-0.16	0.21	0.12
27	8	-0.01	-0.05	0.01	0.04	-0.08	-0.01	-0.01	0.06	-0.02
28	1	-0.02	-0.08	0.09	0.05	0.08	-0.12	-0.02	-0.11	0.00

	19			20			21		
	?A			?A			?A		
Frequencies --	651.3155			675.2927			683.0613		
Red. masses --	7.6925			4.5960			5.5262		
Frc consts --	1.9226			1.2349			1.5191		
IR Inten --	18.0621			15.8654			61.1875		
Raman Activ --	11.1714			0.7358			7.7879		
Depolar --	0.6878			0.6191			0.2430		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.06	0.07	-0.02	-0.04	0.03	-0.17	-0.08	-0.07	-0.05
2 6	0.03	0.15	0.04	0.06	-0.01	-0.10	0.08	-0.04	-0.10
3 6	0.11	-0.01	0.02	0.02	-0.02	0.08	-0.04	0.11	0.04
4 6	-0.01	0.00	-0.08	-0.07	0.10	0.00	-0.03	0.02	0.08
5 6	-0.16	-0.07	0.00	-0.04	-0.05	0.13	0.12	0.08	0.05
6 6	-0.04	0.05	0.00	0.12	0.10	0.04	0.10	0.07	-0.04
7 6	0.06	0.06	0.02	-0.06	-0.01	0.10	-0.06	-0.08	-0.07
8 6	0.07	-0.03	-0.09	-0.14	-0.01	-0.06	-0.09	-0.01	0.06
9 6	0.02	-0.11	-0.04	0.01	-0.05	-0.05	0.01	-0.03	0.07

10	6	0.07	-0.11	-0.08	0.13	0.10	-0.06	0.05	0.15	0.11
11	6	0.12	0.08	0.05	-0.04	-0.03	-0.04	-0.14	-0.14	-0.11
12	8	-0.03	0.08	-0.01	0.06	-0.08	-0.03	-0.05	0.00	0.00
13	6	-0.13	0.44	0.08	0.07	-0.08	0.30	-0.10	0.29	-0.06
14	7	0.05	-0.17	-0.03	-0.02	0.02	-0.10	0.03	-0.09	0.02
15	8	-0.22	-0.23	0.08	-0.10	0.01	0.00	0.19	-0.10	-0.01
16	1	0.05	0.02	-0.08	-0.08	-0.03	-0.09	-0.09	-0.06	0.04
17	1	0.00	0.21	0.01	0.05	-0.12	-0.14	0.16	-0.18	-0.04
18	1	0.30	0.03	0.02	-0.04	-0.12	0.14	-0.28	0.07	0.05
19	1	-0.02	0.03	-0.07	0.08	0.37	0.10	0.05	0.07	0.09
20	1	-0.11	0.03	-0.03	0.14	0.20	0.16	0.07	0.13	0.02
21	1	0.03	0.03	0.11	-0.03	0.01	0.07	-0.02	-0.05	-0.10
22	1	0.06	-0.10	-0.09	-0.27	-0.11	-0.10	-0.08	0.11	0.05
23	1	0.11	-0.18	-0.12	0.24	0.15	-0.14	0.02	0.15	0.13
24	1	0.13	0.08	0.05	0.17	-0.14	-0.05	-0.12	-0.14	-0.11
25	1	0.13	0.07	0.05	-0.18	0.06	-0.09	-0.17	-0.12	-0.12
26	1	0.17	-0.08	-0.04	0.17	-0.16	-0.02	-0.29	0.19	0.03
27	8	0.00	-0.13	0.03	0.02	0.01	0.00	0.02	-0.11	0.00
28	1	0.00	0.31	0.05	0.01	0.00	0.09	0.03	0.35	-0.04

	22	23	24
	?A	?A	?A
Frequencies --	699.2843	814.8511	825.5440
Red. masses --	5.1260	3.3916	2.9474
Frc consts --	1.4768	1.3268	1.1835
IR Inten --	27.5063	16.0034	25.0190
Raman Activ --	3.6026	9.7023	4.4394
Depolar --	0.7249	0.0239	0.0778

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.05	-0.05	-0.06	-0.13	0.01	-0.04	0.08	-0.06	-0.07
2	6	0.13	0.17	-0.05	-0.08	-0.01	-0.04	-0.07	0.00	0.17
3	6	0.16	0.10	0.08	0.05	-0.07	-0.16	0.06	0.00	-0.03

```
    4   6    -0.02  -0.12  -0.02     0.04  -0.03   0.18     0.11   0.01  -
0.01
    5   6    -0.11  -0.06   0.01    -0.02   0.01   0.02    -0.03  -0.01
0.01
    6   6     0.00   0.11  -0.11     0.05   0.02  -0.05     0.00  -0.08
0.16
    7   6    -0.02  -0.03  -0.12     0.01   0.05   0.03    -0.07   0.05  -
0.05
    8   6     0.06  -0.02   0.09     0.06   0.03   0.21     0.03   0.14
0.00
    9   6     0.02   0.02   0.12     0.06  -0.02   0.02    -0.01   0.01  -
0.01
   10   6     0.16   0.00   0.15     0.04   0.04  -0.19     0.00   0.04  -
0.04
   11   6    -0.11  -0.09  -0.10    -0.01   0.03   0.00    -0.11  -0.12  -
0.11
   12   8     0.02   0.03   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   13   6     0.00  -0.14  -0.13    -0.06   0.04  -0.01     0.01  -0.02
0.00
   14   7    -0.03   0.03   0.05    -0.05  -0.03   0.01     0.00   0.01
0.00
   15   8    -0.19   0.01   0.07     0.00  -0.04   0.01    -0.03  -0.03  -
0.01
   16   1    -0.03   0.00  -0.08    -0.09   0.03  -0.16     0.16   0.11  -
0.12
   17   1     0.22   0.12   0.05     0.02   0.07   0.09    -0.19   0.29
0.09
   18   1     0.12   0.21  -0.02     0.24  -0.20  -0.04     0.29   0.04  -
0.02
   19   1     0.09  -0.17  -0.07     0.27  -0.13   0.10     0.13   0.07
0.01
   20   1    -0.24   0.11  -0.10     0.20   0.06  -0.01     0.27  -0.14
0.09
   21   1    -0.03  -0.06  -0.05    -0.04   0.03  -0.01     0.06   0.14  -
0.09
   22   1     0.22   0.15   0.14    -0.05   0.15   0.15     0.07   0.17
0.01
   23   1     0.14  -0.21   0.15    -0.06   0.19  -0.12     0.01   0.26  -
0.04
   24   1    -0.18  -0.04  -0.10    -0.03  -0.09   0.02    -0.19  -0.21  -
0.10
   25   1    -0.04  -0.14  -0.09     0.08   0.01   0.10    -0.08  -0.06
0.01
   26   1     0.23  -0.13  -0.02     0.02  -0.02   0.00     0.04  -0.03
0.01
   27   8    -0.01   0.04  -0.01     0.01   0.04   0.00    -0.01  -0.03
0.00
   28   1    -0.01  -0.23  -0.01    -0.01  -0.60   0.08     0.00   0.44  -
0.06
                     25                    26                    27
                     ?A                    ?A                    ?A
 Frequencies --    829.2167              844.2981              881.1379
 Red. masses --      2.8604                1.7162                3.2916
```

Frc consts	--	1.1588			0.7208			1.5057		
IR Inten	--	55.6916			48.9410			0.5048		
Raman Activ	--	6.0177			4.1124			15.5488		
Depolar	--	0.0838			0.3721			0.0385		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.10	0.03	0.05	-0.10	0.01	-0.02	0.16	-0.05	0.10
2	6	0.08	0.09	-0.10	-0.04	-0.04	0.00	0.14	-0.11	-0.07
3	6	0.01	0.05	-0.11	0.02	-0.05	0.03	-0.04	-0.02	-0.05
4	6	-0.03	0.01	0.14	0.02	-0.06	-0.02	0.09	-0.03	0.03
5	6	-0.04	0.01	0.01	0.00	0.00	-0.01	-0.01	0.00	-0.02
6	6	-0.02	-0.07	-0.05	0.02	0.06	-0.06	-0.14	0.15	-0.04
7	6	0.05	-0.15	-0.04	0.00	0.07	0.05	-0.06	0.14	0.10
8	6	-0.09	0.02	0.11	0.05	-0.03	0.05	-0.02	0.12	0.03
9	6	-0.03	0.03	0.01	-0.01	0.05	0.00	0.01	-0.01	-0.03
10	6	-0.08	0.02	-0.07	0.04	-0.03	-0.04	0.01	-0.05	-0.06
11	6	0.05	0.02	0.03	-0.01	0.03	0.02	-0.08	-0.09	-0.03
12	8	0.04	-0.06	0.00	-0.02	0.03	0.00	0.00	-0.01	0.01
13	6	0.04	-0.04	0.01	0.01	-0.05	0.01	-0.01	0.01	0.01
14	7	0.03	0.02	-0.01	-0.01	0.01	0.00	-0.01	-0.01	0.00
15	8	-0.06	0.00	0.02	0.03	0.02	0.00	-0.01	-0.02	-0.01
16	1	0.09	-0.01	0.07	-0.09	0.02	-0.07	0.24	0.23	0.34
17	1	0.06	0.19	-0.11	0.04	-0.18	0.06	0.14	-0.30	-0.12
18	1	0.02	0.02	-0.09	0.06	-0.08	0.06	-0.14	-0.08	-0.02
19	1	0.00	-0.06	0.11	0.08	-0.12	-0.07	-0.04	-0.12	0.02
20	1	-0.13	0.05	0.09	0.06	0.05	-0.08	-0.33	0.16	-0.03
21	1	0.08	-0.11	-0.15	-0.05	0.03	0.10	0.16	0.25	0.32
22	1	-0.20	0.21	0.03	0.09	-0.11	0.08	-0.08	0.02	0.01
23	1	-0.17	0.08	0.00	0.05	-0.15	-0.05	0.00	-0.17	-0.07
24	1	-0.04	0.07	0.03	0.07	0.00	0.01	-0.02	-0.02	-0.04

```
  25   1    -0.04   0.10   0.04     0.04  -0.03  -0.01    -0.09  -0.10  -
0.07
  26   1     0.05  -0.07   0.01    -0.01   0.03  -0.01     0.01  -0.01
0.01
  27   8    -0.02  -0.05   0.00    -0.03  -0.05   0.00     0.00   0.00
0.00
  28   1     0.00   0.72  -0.11    -0.01   0.86  -0.12     0.00  -0.07
0.02
                     28                    29                    30
                     ?A                    ?A                    ?A
 Frequencies --   905.1521              926.9921              947.7770
 Red. masses --     2.3530                2.6503                2.0358
 Frc consts  --     1.1359                1.3418                1.0774
 IR Inten    --     3.1988               11.4685                0.7731
 Raman Activ --     1.9536                1.5046                4.5178
 Depolar     --     0.2933                0.4613                0.5308
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.04   0.05  -0.06    -0.06  -0.02   0.04    -0.07   0.02
0.02
   2   6     0.01  -0.07   0.12     0.07  -0.02   0.01     0.12   0.05
0.04
   3   6     0.04   0.13   0.05     0.03  -0.02  -0.04    -0.05  -0.01  -
0.05
   4   6     0.02   0.05  -0.04    -0.03   0.21  -0.07     0.11   0.03
0.00
   5   6    -0.01   0.00  -0.06    -0.02   0.02   0.07     0.00   0.00
0.05
   6   6     0.06   0.01  -0.11    -0.03   0.03  -0.02    -0.02  -0.09  -
0.05
   7   6    -0.05   0.00   0.04    -0.03  -0.09   0.05    -0.04   0.11  -
0.02
   8   6    -0.11  -0.02   0.08     0.19   0.01  -0.03    -0.04  -0.11
0.01
   9   6     0.00  -0.01   0.05     0.02   0.01   0.07    -0.02   0.01  -
0.03
  10   6    -0.12  -0.04  -0.04    -0.09   0.01  -0.07    -0.03   0.03
0.03
  11   6     0.05  -0.04  -0.01    -0.03  -0.05   0.02     0.04  -0.05  -
0.01
  12   8     0.01  -0.02   0.01     0.02  -0.04  -0.02     0.00   0.01
0.00
  13   6     0.01   0.01  -0.02    -0.01  -0.01  -0.05     0.01   0.00
0.01
  14   7     0.02   0.00   0.00    -0.01   0.00   0.02     0.01   0.00  -
0.01
  15   8    -0.02  -0.01   0.01    -0.03  -0.01  -0.02    -0.03   0.00  -
0.01
  16   1     0.03   0.04  -0.05    -0.17  -0.19   0.24    -0.07   0.07
0.09
  17   1     0.02  -0.37   0.06     0.16  -0.03   0.11     0.28   0.26
0.27
  18   1     0.33   0.37  -0.10     0.14  -0.12   0.05    -0.25  -0.08  -
0.02
```

19	1	0.13	0.02	-0.08	0.00	0.50	0.06	0.32	0.17	0.02
20	1	0.34	0.02	-0.11	0.01	0.14	0.12	-0.09	-0.27	-0.27
21	1	0.03	0.05	0.00	-0.11	-0.17	0.18	-0.03	0.13	-0.05
22	1	-0.15	-0.11	0.08	0.43	-0.01	0.08	-0.10	-0.35	0.02
23	1	-0.28	-0.34	0.05	-0.26	0.01	0.05	-0.04	0.20	0.05
24	1	0.16	-0.18	-0.01	0.05	0.03	0.00	0.09	-0.09	-0.01
25	1	-0.02	0.05	0.03	-0.10	-0.07	-0.09	0.23	-0.21	-0.01
26	1	0.00	-0.01	0.01	0.00	-0.03	-0.02	0.03	-0.01	0.02
27	8	0.01	0.01	0.00	0.00	-0.01	-0.01	0.00	0.00	0.00
28	1	0.01	-0.14	0.01	0.00	0.07	-0.04	0.00	0.03	-0.01

	31			32			33		
	?A			?A			?A		
Frequencies --	978.0466			996.7147			1005.4464		
Red. masses --	2.0690			2.1492			2.7664		
Frc consts --	1.1661			1.2580			1.6477		
IR Inten --	5.9987			2.0180			11.4446		
Raman Activ --	4.1648			7.5494			7.7895		
Depolar --	0.1949			0.4252			0.0332		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.04	-0.03	0.03	0.05	0.01	0.01	-0.11	0.23	0.05
2 6	-0.03	0.13	-0.06	0.00	-0.04	-0.05	-0.04	0.01	0.01
3 6	-0.02	-0.07	0.00	0.16	-0.09	0.03	-0.01	-0.03	-0.01
4 6	0.03	-0.06	-0.02	-0.07	-0.05	-0.02	0.00	0.01	0.01
5 6	0.02	0.00	0.04	0.01	0.00	0.04	0.01	-0.02	-0.03
6 6	0.15	0.02	-0.05	-0.03	0.02	-0.02	0.03	-0.02	0.01
7 6	-0.02	0.03	0.05	0.02	0.07	-0.02	0.22	-0.07	0.05
8 6	-0.04	0.05	-0.04	-0.04	-0.09	-0.02	0.01	0.00	-0.04
9 6	0.00	0.00	0.05	-0.01	0.00	0.05	0.00	-0.01	-0.02
10 6	-0.08	-0.05	0.01	-0.11	0.13	0.03	-0.02	-0.02	0.02
11 6	-0.06	-0.05	0.08	0.00	0.01	-0.03	-0.07	-0.13	-0.07
12 8	-0.01	0.02	0.00	-0.01	0.02	-0.01	-0.01	0.01	0.00

13	6	0.00	0.00	-0.02	0.01	0.00	-0.02	0.00	0.00	0.00
14	7	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	-0.01	0.01	0.00	0.01	-0.02	0.00	0.00
16	1	0.09	0.06	-0.05	0.06	0.08	0.11	0.04	0.65	0.18
17	1	-0.09	0.37	-0.08	-0.10	-0.07	-0.18	0.03	-0.07	0.07
18	1	-0.09	-0.24	0.12	0.50	-0.27	0.21	0.02	0.04	-0.06
19	1	-0.04	-0.03	0.00	-0.21	-0.07	0.00	0.02	-0.01	-0.01
20	1	0.45	0.01	-0.08	-0.04	-0.04	-0.09	-0.05	0.04	0.08
21	1	0.03	0.07	0.02	0.06	0.09	0.06	0.48	0.06	0.18
22	1	0.00	0.05	-0.02	0.00	-0.23	0.02	-0.05	0.07	-0.08
23	1	-0.23	-0.20	0.11	-0.27	0.45	0.17	0.00	0.02	0.01
24	1	0.26	0.28	0.01	-0.09	-0.04	-0.01	-0.03	-0.17	-0.08
25	1	-0.22	-0.17	-0.32	0.08	0.02	0.07	-0.07	-0.15	-0.09
26	1	0.01	0.00	0.00	0.01	0.00	-0.02	0.02	-0.01	0.00
27	8	0.01	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00
28	1	0.00	-0.05	0.00	0.01	-0.04	-0.02	-0.01	-0.02	-0.01

	34			35			36		
	?A			?A			?A		
Frequencies --	1020.7721			1030.4579			1037.8419		
Red. masses --	3.4648			2.5511			2.0100		
Frc consts --	2.1271			1.5960			1.2756		
IR Inten --	8.7357			4.9059			1.8078		
Raman Activ --	0.7098			3.5728			4.8859		
Depolar --	0.7437			0.7361			0.5557		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.08	0.08	0.10	-0.01	-0.05	-0.01	-0.08	-0.03	0.04
2 6	-0.07	0.08	0.07	0.06	0.04	-0.07	-0.01	-0.01	-0.09
3 6	-0.11	-0.12	0.10	-0.03	0.12	0.05	0.03	0.09	0.08
4 6	-0.04	0.09	-0.16	-0.11	-0.02	0.00	0.09	-0.02	-0.10
5 6	-0.01	0.06	-0.05	0.00	0.06	0.03	-0.01	0.03	0.01
6 6	-0.04	0.05	-0.06	0.06	-0.04	0.10	-0.02	-0.09	0.03

```
   7   6    -0.06  -0.06  -0.10     0.07   0.12   0.02     0.05   0.01  -
0.02
   8   6    -0.05  -0.03   0.16     0.08  -0.07   0.07    -0.01   0.07
0.05
   9   6     0.01  -0.02   0.05    -0.01  -0.02  -0.05    -0.01  -0.03  -
0.04
  10   6     0.12   0.07  -0.10    -0.08  -0.09  -0.06    -0.03   0.03  -
0.04
  11   6     0.08  -0.09  -0.04    -0.06   0.04  -0.11    -0.04   0.00
0.10
  12   8     0.04  -0.05   0.00     0.03  -0.05   0.00     0.01  -0.02
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.01
0.01
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.00
0.00
  15   8     0.00  -0.01  -0.01    -0.01   0.01   0.01    -0.02  -0.01
0.00
  16   1     0.03   0.02   0.20    -0.05  -0.03   0.26    -0.13  -0.09
0.13
  17   1    -0.22   0.17  -0.09    -0.10   0.25  -0.21    -0.10  -0.27  -
0.24
  18   1    -0.17  -0.35   0.27    -0.13   0.00   0.12     0.23   0.08
0.13
  19   1    -0.04  -0.16  -0.27    -0.13  -0.09  -0.03     0.35  -0.03  -
0.16
  20   1     0.13   0.15   0.06     0.30  -0.02   0.12    -0.23  -0.03
0.11
  21   1     0.04   0.00  -0.11     0.12   0.16  -0.03     0.11   0.09  -
0.27
  22   1     0.09  -0.11   0.25     0.06  -0.34   0.11    -0.01   0.00
0.06
  23   1     0.20  -0.04  -0.16    -0.01  -0.29  -0.12     0.09   0.18  -
0.12
  24   1    -0.12  -0.03  -0.02    -0.36  -0.13  -0.06     0.05   0.39
0.05
  25   1     0.23  -0.16   0.04     0.14   0.07   0.20     0.00  -0.26  -
0.24
  26   1    -0.14   0.08  -0.01    -0.10   0.06   0.01    -0.03   0.02
0.01
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00  -0.02   0.01    -0.01  -0.01  -0.01     0.00  -0.06
0.01
                     37                     38                     39
                     ?A                     ?A                     ?A
 Frequencies --  1055.3767              1058.3612              1072.0474
 Red. masses --     2.1839                 2.0489                 1.7230
 Frc consts  --     1.4332                 1.3522                 1.1667
 IR Inten    --     4.5048                14.3273                 1.1786
 Raman Activ --    10.3961                 3.3308                 6.3672
 Depolar     --     0.6295                 0.4775                 0.6649
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
```

1	6	-0.05	0.01	-0.10	-0.01	-0.07	0.04	0.06	-0.06	-0.03
2	6	0.15	0.03	0.09	-0.02	-0.01	0.02	-0.02	0.03	0.06
3	6	-0.03	-0.05	0.08	0.01	-0.07	-0.05	-0.03	0.00	0.01
4	6	-0.01	-0.11	-0.06	0.10	0.05	-0.03	-0.03	0.04	-0.02
5	6	0.00	0.03	0.00	0.01	-0.06	0.01	-0.01	0.02	0.01
6	6	-0.03	0.02	0.03	0.01	0.13	0.06	-0.03	-0.05	-0.11
7	6	0.04	-0.04	0.01	0.09	-0.03	-0.08	0.10	-0.01	0.07
8	6	-0.02	0.09	0.00	-0.11	-0.06	0.01	-0.01	-0.01	0.04
9	6	-0.02	-0.03	-0.01	-0.02	0.01	0.01	0.02	-0.01	-0.01
10	6	-0.11	0.02	-0.05	-0.02	-0.05	0.03	0.05	0.04	-0.01
11	6	0.01	0.06	-0.01	-0.02	0.05	-0.03	-0.09	0.03	0.01
12	8	0.01	-0.01	0.00	-0.04	0.04	0.00	0.01	-0.01	0.00
13	6	0.01	0.01	0.00	0.00	0.00	0.00	-0.01	0.00	0.01
14	7	0.02	0.00	0.00	0.01	0.00	0.00	-0.01	0.00	0.00
15	8	0.03	0.00	-0.01	0.00	0.01	-0.01	0.01	0.00	0.00
16	1	-0.04	-0.02	-0.21	-0.11	-0.29	0.04	-0.01	-0.29	-0.21
17	1	0.40	0.03	0.37	0.04	0.01	0.09	0.02	0.04	0.12
18	1	-0.09	-0.33	0.28	0.00	-0.03	-0.10	-0.02	0.02	0.01
19	1	0.07	-0.29	-0.17	0.34	0.22	-0.01	-0.04	0.05	-0.02
20	1	-0.11	0.16	0.19	0.08	0.31	0.26	-0.08	-0.25	-0.34
21	1	0.05	-0.03	-0.02	0.27	0.08	-0.05	0.40	0.14	0.27
22	1	-0.03	0.27	-0.03	-0.17	-0.13	0.00	-0.01	-0.16	0.06
23	1	-0.14	0.03	-0.04	-0.11	-0.20	0.08	0.07	0.13	-0.02
24	1	0.00	-0.07	0.00	-0.42	0.22	-0.01	-0.18	0.21	0.00
25	1	-0.07	0.17	0.07	0.05	0.07	0.08	-0.39	0.24	-0.06
26	1	-0.06	0.05	0.01	0.13	-0.08	-0.01	-0.03	0.02	0.00
27	8	0.01	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00

```
  28   1     0.01  -0.09   0.01     0.00   0.00   0.00    -0.01  -0.01  -
0.01
                     40                    41                    42
                     ?A                    ?A                    ?A
 Frequencies --  1109.6049             1162.0918             1205.5228
 Red. masses --     2.9845                1.3279                2.7339
 Frc consts  --     2.1650                1.0566                2.3409
 IR Inten    --   171.0569                1.2535               50.2483
 Raman Activ --    10.1295                1.7464                2.4437
 Depolar     --     0.6730                0.7465                0.7381
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.02  -0.02   0.01    -0.03  -0.01   0.04     0.00  -0.02
0.04
   2   6    -0.06  -0.05   0.00     0.00  -0.01  -0.02    -0.02   0.03  -
0.03
   3   6     0.04  -0.01  -0.07     0.04  -0.02   0.04     0.07  -0.10
0.07
   4   6     0.07   0.03   0.05     0.03   0.01  -0.01     0.01   0.02
0.02
   5   6     0.06   0.24  -0.05     0.01  -0.01  -0.04     0.19  -0.09  -
0.07
   6   6     0.03   0.06   0.03    -0.02  -0.01  -0.03     0.00  -0.07  -
0.06
   7   6     0.01   0.01  -0.02    -0.01  -0.03   0.06    -0.03   0.00
0.05
   8   6    -0.02  -0.05  -0.07     0.01   0.03  -0.01     0.05   0.09
0.05
   9   6    -0.04   0.00   0.01     0.00  -0.01  -0.04     0.03   0.00  -
0.09
  10   6     0.02  -0.05   0.08    -0.02   0.05   0.04    -0.09   0.13
0.02
  11   6    -0.01   0.01   0.00     0.02   0.03  -0.05     0.00  -0.01  -
0.03
  12   8     0.12  -0.09   0.00     0.00   0.01   0.00    -0.01   0.06  -
0.01
  13   6     0.01  -0.01   0.00     0.00   0.00   0.01     0.00   0.00
0.02
  14   7     0.02   0.01   0.00     0.00   0.00   0.00    -0.02  -0.01
0.00
  15   8    -0.17  -0.04   0.02    -0.01  -0.01   0.01    -0.11  -0.02
0.02
  16   1     0.00  -0.06  -0.18    -0.17  -0.19   0.38     0.02  -0.08  -
0.20
  17   1     0.06  -0.10   0.13    -0.16   0.23  -0.16     0.14  -0.03
0.14
  18   1     0.07  -0.21   0.10    -0.07   0.00   0.02    -0.27   0.22  -
0.23
  19   1     0.03  -0.20  -0.05     0.35  -0.12  -0.13    -0.24   0.07
0.10
  20   1    -0.02  -0.01  -0.05     0.23  -0.15  -0.20    -0.02   0.22
0.28
  21   1    -0.02  -0.03   0.08    -0.10  -0.14   0.34     0.01   0.09  -
0.27
```

```
  22   1    -0.04   0.01  -0.09    -0.17   0.35  -0.15    -0.02  -0.33
0.08
  23   1     0.01  -0.01   0.09     0.01  -0.07   0.01     0.08  -0.26  -
0.13
  24   1    -0.03   0.04   0.00    -0.07  -0.14  -0.02    -0.07  -0.05  -
0.01
  25   1    -0.02   0.00  -0.01     0.03   0.13   0.12     0.01   0.03
0.05
  26   1    -0.63   0.49   0.00     0.01   0.00  -0.01    -0.21   0.21  -
0.02
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.01
0.00
  28   1     0.00   0.03   0.00     0.00   0.00   0.00     0.01  -0.02
0.01
                     43                     44                     45
                     ?A                     ?A                     ?A
 Frequencies --  1212.5039              1218.9030              1234.2356
 Red. masses --     4.3912                 2.2509                 2.1923
 Frc consts  --     3.8036                 1.9704                 1.9677
 IR Inten    --    22.8254                 3.9186                17.7272
 Raman Activ --     3.4172                 1.8826                 4.2053
 Depolar     --     0.2080                 0.2410                 0.2183
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.08  -0.04   0.06    -0.01   0.03  -0.08     0.01   0.01  -
0.07
   2   6    -0.04  -0.01  -0.03     0.06  -0.11   0.03     0.04  -0.06
0.04
   3   6    -0.06   0.12  -0.03     0.03   0.01  -0.02     0.04  -0.01
0.01
   4   6     0.10  -0.15  -0.09    -0.06  -0.06   0.00    -0.04   0.03
0.03
   5   6     0.08   0.00   0.11     0.12  -0.05   0.04    -0.08   0.04  -
0.04
   6   6    -0.05  -0.11  -0.05    -0.13   0.02   0.04    -0.10  -0.02
0.01
   7   6     0.00  -0.06   0.11     0.04   0.01  -0.07     0.04   0.02  -
0.03
   8   6    -0.14   0.10  -0.14    -0.04  -0.05   0.01     0.04  -0.04  -
0.02
   9   6     0.15   0.07   0.20    -0.08  -0.01   0.08     0.19   0.06  -
0.02
  10   6     0.15   0.02  -0.11     0.01   0.05  -0.07     0.03   0.08
0.01
  11   6     0.06   0.09  -0.08     0.00   0.00   0.09    -0.03  -0.01
0.07
  12   8     0.01   0.01   0.00     0.00   0.03  -0.01     0.02  -0.02
0.00
  13   6    -0.03  -0.02  -0.04     0.02   0.00  -0.01    -0.03  -0.01
0.00
  14   7    -0.05  -0.01   0.02     0.04   0.01   0.00    -0.07  -0.02
0.01
  15   8    -0.06  -0.02  -0.02    -0.05   0.00   0.01     0.02   0.00
0.01
```

16	1	-0.04	0.11	0.20	-0.01	0.09	0.11	0.04	0.10	-0.03
17	1	-0.02	0.08	0.02	-0.13	0.29	-0.11	-0.12	0.22	-0.08
18	1	0.09	-0.07	0.15	-0.21	0.11	-0.13	-0.16	-0.05	0.02
19	1	-0.22	0.24	0.15	0.11	0.21	0.09	0.08	-0.06	-0.04
20	1	0.06	0.07	0.17	0.35	-0.08	-0.10	0.13	0.09	0.14
21	1	0.07	-0.01	0.05	0.18	0.07	0.10	-0.03	0.01	-0.22
22	1	0.02	-0.29	-0.01	0.31	0.24	0.12	-0.45	-0.14	-0.24
23	1	-0.25	-0.04	0.18	0.20	-0.18	-0.22	-0.30	-0.40	0.23
24	1	-0.16	-0.20	-0.02	0.17	0.16	0.05	0.09	0.16	0.04
25	1	0.20	0.18	0.25	-0.10	-0.03	-0.12	0.01	-0.18	-0.13
26	1	-0.14	0.13	0.03	-0.18	0.18	0.00	-0.04	0.01	-0.01
27	8	0.00	-0.01	0.00	0.00	0.00	0.00	-0.01	-0.01	0.00
28	1	0.00	0.04	-0.01	0.00	-0.03	0.00	-0.01	0.06	-0.01

	46			47			48		
	?A			?A			?A		
Frequencies --	1244.9220			1257.8979			1268.4315		
Red. masses --	2.0428			1.1161			2.9430		
Frc consts --	1.8653			1.0405			2.7898		
IR Inten --	11.3268			1.1462			10.2629		
Raman Activ --	5.7960			13.1493			6.2319		
Depolar --	0.5809			0.7437			0.6810		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.03	0.00	0.05	-0.01	-0.01	0.02	0.04	-0.03	-0.01
2 6	-0.06	-0.09	-0.06	-0.03	-0.01	0.00	-0.07	-0.05	0.04
3 6	0.13	0.05	-0.03	0.01	0.00	0.01	0.01	0.01	-0.08
4 6	0.06	0.03	-0.04	0.03	0.00	0.03	-0.06	-0.03	-0.13
5 6	-0.11	0.08	0.05	-0.02	0.01	-0.04	0.06	0.01	0.25
6 6	-0.03	-0.02	-0.02	0.00	0.01	-0.01	0.00	0.08	-0.04
7 6	-0.01	-0.04	0.02	0.01	0.02	-0.03	0.05	-0.05	-0.02
8 6	-0.02	0.04	-0.01	0.01	-0.02	-0.03	0.00	0.06	0.10
9 6	-0.08	-0.05	-0.01	-0.01	0.00	0.03	0.04	0.00	-0.17

10	6	-0.01	0.07	0.04	0.00	0.01	0.00	0.01	-0.04	0.07
11	6	0.02	0.02	0.00	0.00	0.00	0.00	-0.02	0.03	0.01
12	8	-0.02	-0.03	0.00	0.00	-0.01	0.01	0.01	0.01	-0.03
13	6	0.01	0.01	0.00	0.00	0.00	-0.01	0.00	0.00	0.04
14	7	0.03	0.01	-0.01	0.01	0.00	0.00	-0.02	-0.01	-0.01
15	8	0.04	-0.01	0.00	0.01	0.00	0.00	-0.02	0.00	-0.02
16	1	0.10	0.18	-0.24	-0.12	-0.14	0.30	0.07	0.20	0.34
17	1	0.16	0.21	0.26	-0.04	0.13	0.02	-0.02	0.18	0.16
18	1	-0.33	-0.09	0.02	0.01	-0.08	0.07	-0.02	0.20	-0.23
19	1	-0.26	-0.16	-0.06	0.03	-0.06	0.01	0.05	-0.21	-0.23
20	1	0.23	0.02	0.02	-0.14	0.07	0.06	-0.09	0.01	-0.13
21	1	0.08	0.01	0.06	0.15	0.17	-0.36	-0.17	-0.14	-0.25
22	1	0.19	-0.15	0.12	0.08	-0.14	0.02	0.03	-0.06	0.14
23	1	0.16	-0.30	-0.11	0.07	-0.07	-0.06	-0.21	0.11	0.24
24	1	-0.08	0.04	0.01	0.41	-0.35	0.00	0.25	-0.19	0.01
25	1	0.09	-0.01	0.05	-0.41	0.34	0.00	-0.07	0.07	0.00
26	1	0.31	-0.28	0.00	0.07	-0.06	0.00	-0.12	0.11	0.01
27	8	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	-0.04	0.01	0.00	-0.01	0.00	0.00	0.00	0.01

	49	50	51
	?A	?A	?A
Frequencies --	1292.2642	1327.2472	1332.4677
Red. masses --	1.7810	1.8317	2.1155
Frc consts --	1.7523	1.9012	2.2130
IR Inten --	5.2868	7.5217	67.0160
Raman Activ --	0.8449	2.6638	3.0826
Depolar --	0.6849	0.7426	0.4148

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	-0.13	-0.04	0.04	0.02	0.01	0.04	0.00	0.04
2	6	-0.02	0.02	0.03	-0.01	0.03	-0.01	-0.07	-0.05	-0.06
3	6	-0.02	-0.03	0.01	-0.02	-0.07	-0.02	0.05	0.10	0.03

```
   4   6     0.01   0.03   0.00    -0.01   0.04  -0.01     0.00   0.07  -
0.05
   5   6    -0.03   0.00  -0.06     0.00   0.03   0.14     0.12  -0.06  -
0.02
   6   6     0.02   0.01  -0.04     0.03  -0.07   0.00     0.01   0.03
0.07
   7   6     0.13   0.01   0.06     0.01   0.08   0.03     0.05   0.04  -
0.02
   8   6    -0.04  -0.01   0.01    -0.01  -0.07  -0.06    -0.01  -0.06
0.04
   9   6    -0.06  -0.03   0.04    -0.02   0.00   0.11     0.09   0.06
0.06
  10   6    -0.01   0.05   0.00    -0.01   0.07  -0.05    -0.04  -0.04  -
0.07
  11   6    -0.08   0.07  -0.01    -0.03  -0.02  -0.02    -0.03  -0.02
0.00
  12   8     0.01   0.00   0.01     0.00  -0.01  -0.02    -0.04   0.01
0.00
  13   6     0.01   0.00  -0.01     0.00   0.00  -0.02    -0.01  -0.01  -
0.01
  14   7     0.02   0.01   0.00     0.01   0.00   0.00    -0.03  -0.01
0.01
  15   8     0.02   0.00   0.00     0.01   0.00  -0.02    -0.05  -0.01
0.01
  16   1     0.19   0.37   0.17    -0.06  -0.20  -0.01     0.06  -0.03  -
0.14
  17   1    -0.03   0.15   0.05     0.06  -0.08   0.05     0.23   0.03
0.31
  18   1     0.18  -0.04   0.05     0.08   0.37  -0.34    -0.28  -0.25
0.25
  19   1     0.00   0.29   0.11     0.07  -0.45  -0.25    -0.10  -0.12  -
0.12
  20   1    -0.24  -0.01  -0.06    -0.25   0.08   0.18    -0.09  -0.20  -
0.20
  21   1    -0.40  -0.28  -0.17    -0.08   0.02   0.04    -0.24  -0.14  -
0.03
  22   1    -0.05   0.04   0.01    -0.09   0.26  -0.15    -0.28   0.25  -
0.13
  23   1     0.19  -0.20  -0.17     0.11  -0.28  -0.16     0.08   0.16  -
0.15
  24   1     0.12  -0.13  -0.01    -0.02  -0.02  -0.02     0.09  -0.07  -
0.01
  25   1     0.24  -0.18   0.02     0.02  -0.05  -0.01    -0.11   0.03  -
0.03
  26   1    -0.04   0.03  -0.01     0.01  -0.01   0.01     0.20  -0.17
0.00
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.01
0.00
  28   1     0.00  -0.03   0.01     0.00   0.00   0.00     0.00   0.03  -
0.01
                     52                    53                    54
                     ?A                    ?A                    ?A
 Frequencies --  1344.8548             1354.7721             1364.9088
 Red. masses --     1.4474                1.4636                1.5805
```

Frc consts --		1.5423			1.5828			1.7348		
IR Inten --		4.1225			0.8038			24.4493		
Raman Activ --		0.5436			2.8828			1.5338		
Depolar --		0.7265			0.7412			0.7500		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	0.03	0.01	-0.04	-0.02	-0.03	-0.01	-0.01	-0.02
2	6	0.02	-0.09	-0.03	0.04	-0.05	-0.04	0.02	0.08	-0.03
3	6	-0.08	0.02	0.00	-0.07	-0.02	0.07	-0.09	0.00	-0.05
4	6	0.01	0.00	-0.01	0.05	0.07	0.03	0.03	0.03	0.00
5	6	0.03	-0.03	-0.01	0.01	-0.01	-0.01	0.07	0.00	0.01
6	6	0.09	0.01	0.03	-0.04	0.03	-0.04	-0.10	-0.02	0.04
7	6	-0.05	-0.01	-0.02	0.00	-0.03	-0.02	0.03	0.00	0.01
8	6	-0.01	0.00	0.02	0.02	0.03	0.00	0.00	-0.02	0.02
9	6	0.02	0.00	-0.05	0.00	0.01	0.04	-0.02	0.00	-0.06
10	6	0.00	0.06	0.01	-0.01	-0.07	0.01	0.05	0.05	0.05
11	6	0.03	-0.02	0.00	-0.01	0.02	0.03	-0.01	0.00	0.01
12	8	0.00	0.01	0.00	0.00	0.00	0.00	-0.02	0.00	0.00
13	6	0.00	0.00	0.01	0.00	0.00	-0.01	0.00	0.00	0.01
14	7	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	-0.01	0.00	0.00	-0.01	0.00	-0.01	-0.02	-0.01	0.00
16	1	-0.01	-0.02	-0.13	-0.01	0.06	0.02	-0.04	-0.04	0.08
17	1	-0.02	0.47	0.05	0.05	0.42	0.07	0.19	-0.35	0.05
18	1	0.45	-0.05	0.13	0.32	0.28	-0.10	0.45	-0.15	0.13
19	1	-0.09	0.02	0.02	-0.26	-0.31	-0.08	-0.23	-0.15	-0.02
20	1	-0.46	-0.12	-0.11	0.24	0.13	0.06	0.47	-0.13	-0.09
21	1	0.10	0.05	0.14	0.04	-0.03	0.07	-0.03	-0.01	-0.15
22	1	0.11	0.08	0.06	-0.22	-0.24	-0.07	0.04	0.12	0.01
23	1	-0.08	-0.41	0.04	0.20	0.39	-0.11	-0.02	-0.31	0.09
24	1	-0.10	0.10	0.01	0.04	0.02	0.02	0.05	-0.03	0.00

```
  25   1    -0.02   0.02   0.00     0.04  -0.05  -0.02    -0.03   0.00  -
0.02
  26   1     0.00   0.00   0.00     0.01  -0.01   0.01     0.17  -0.14
0.01
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.01   0.00     0.00   0.00   0.00     0.00   0.00
0.01
                     55                     56                     57
                     ?A                     ?A                     ?A
 Frequencies --  1376.1874              1383.6413              1389.1497
 Red. masses --     1.4781                 1.6819                 1.7220
 Frc consts  --     1.6493                 1.8972                 1.9578
 IR Inten    --     8.1107                37.1948                 1.9179
 Raman Activ --     1.8478                 3.7609                 2.5341
 Depolar     --     0.7174                 0.7499                 0.7493
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.03   0.04   0.00     0.01   0.06  -0.02     0.06  -0.01
0.02
   2   6    -0.04   0.00  -0.03     0.04  -0.04   0.09    -0.05  -0.04  -
0.01
   3   6    -0.02   0.01  -0.05    -0.01   0.04  -0.06    -0.02   0.08  -
0.02
   4   6    -0.07  -0.07  -0.02    -0.04   0.01   0.05    -0.07   0.00  -
0.02
   5   6    -0.03   0.00   0.03     0.11   0.03   0.00     0.03  -0.04  -
0.01
   6   6     0.00   0.01   0.01     0.00   0.01  -0.05    -0.02  -0.08  -
0.11
   7   6    -0.02  -0.01   0.00     0.05   0.00   0.03    -0.04   0.05
0.04
   8   6     0.06   0.06  -0.01     0.00   0.08  -0.04     0.05  -0.06
0.00
   9   6     0.01   0.00   0.05    -0.05   0.00   0.02    -0.06  -0.02  -
0.03
  10   6    -0.04   0.01   0.05     0.01  -0.01   0.02     0.05  -0.02
0.06
  11   6     0.06  -0.06   0.00    -0.03  -0.02  -0.01    -0.03   0.01
0.00
  12   8     0.01   0.00   0.00    -0.04   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00  -0.01     0.00   0.00   0.00     0.01   0.00
0.01
  14   7     0.00   0.00   0.00     0.01   0.00   0.00     0.02   0.01
0.00
  15   8     0.02   0.00   0.00    -0.03  -0.02   0.00     0.00   0.01
0.01
  16   1     0.01   0.05   0.15    -0.11  -0.26  -0.11     0.09   0.01  -
0.05
  17   1     0.19  -0.06   0.21    -0.30   0.06  -0.27     0.09   0.18
0.20
  18   1     0.22  -0.09   0.06    -0.04  -0.23   0.14     0.14  -0.19
0.21
```

19	1	0.31	0.17	0.01	0.19	-0.27	-0.11	0.27	0.10	-0.05
20	1	0.11	-0.06	-0.08	-0.11	0.09	0.05	0.10	0.42	0.48
21	1	-0.11	-0.05	-0.06	-0.26	-0.17	-0.07	0.15	0.18	0.01
22	1	-0.34	-0.30	-0.13	0.07	-0.39	0.06	-0.07	0.32	-0.11
23	1	0.41	-0.12	-0.29	0.05	0.00	-0.01	-0.02	0.14	0.13
24	1	-0.20	0.18	0.00	-0.09	0.04	-0.02	0.08	-0.01	0.00
25	1	-0.17	0.14	0.00	0.07	-0.15	-0.05	0.11	-0.07	0.04
26	1	-0.09	0.08	0.00	0.30	-0.26	0.01	0.00	0.00	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00

	58			59			60		
	?A			?A			?A		
Frequencies --	1404.3320			1409.2644			1429.3443		
Red. masses --	1.5867			1.5909			1.4842		
Frc consts --	1.8436			1.8615			1.7865		
IR Inten --	18.5101			16.4400			0.2669		
Raman Activ --	2.8721			6.6587			0.7380		
Depolar --	0.5802			0.7029			0.7464		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	-0.04	-0.05	-0.02	-0.11	-0.05	-0.05	-0.05	0.14
2	6	0.01	0.03	0.07	-0.03	0.04	-0.01	0.07	0.01	-0.01
3	6	0.02	0.01	-0.07	0.00	0.00	0.02	-0.02	0.00	-0.02
4	6	0.02	-0.01	-0.03	-0.07	0.08	0.06	-0.03	0.03	-0.03
5	6	0.04	0.02	0.04	0.06	-0.01	-0.03	-0.01	-0.03	0.03
6	6	0.05	0.00	-0.02	0.02	-0.02	0.02	-0.02	-0.02	0.01
7	6	-0.07	-0.06	-0.05	-0.05	-0.03	-0.03	0.03	0.02	-0.07
8	6	0.05	-0.01	0.04	-0.01	0.01	-0.05	0.00	0.01	0.01
9	6	0.03	0.02	0.02	0.00	0.01	0.01	0.00	0.00	0.00
10	6	-0.06	0.01	0.04	0.02	0.01	-0.03	-0.01	0.01	0.01
11	6	-0.02	0.07	0.02	0.05	0.02	0.03	-0.01	0.02	-0.02
12	8	-0.01	0.00	0.00	-0.02	0.00	0.00	0.01	0.00	0.00

13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	-0.02	-0.01	0.00	-0.02	-0.01	0.01	0.01	0.00	0.00
16	1	-0.01	0.08	0.15	0.21	0.53	0.20	0.19	0.18	-0.61
17	1	-0.19	-0.18	-0.19	0.08	-0.11	0.08	-0.15	-0.05	-0.28
18	1	-0.06	-0.19	0.06	-0.04	-0.01	0.02	0.11	-0.02	0.00
19	1	-0.27	0.03	0.04	0.41	-0.32	-0.21	0.23	0.03	-0.09
20	1	-0.15	0.02	0.02	-0.09	-0.06	-0.02	0.10	0.03	0.06
21	1	0.42	0.19	0.23	0.19	0.09	0.15	-0.07	-0.10	0.25
22	1	-0.33	0.06	-0.15	0.21	-0.18	0.07	-0.08	-0.11	-0.01
23	1	0.29	-0.09	-0.22	-0.13	-0.04	0.07	0.07	-0.07	-0.05
24	1	0.18	-0.11	0.02	-0.07	0.14	0.03	0.25	-0.28	-0.01
25	1	0.22	-0.14	0.00	-0.04	0.10	0.03	-0.18	0.18	0.03
26	1	0.11	-0.10	0.00	0.11	-0.09	0.00	-0.08	0.07	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.01	0.00	0.00	0.01	-0.01	0.00	0.00	0.00

	61			62			63		
	?A			?A			?A		
Frequencies --	1443.5937			1446.8587			1473.8383		
Red. masses --	1.5362			1.5263			2.0129		
Frc consts --	1.8862			1.8826			2.5762		
IR Inten --	6.3887			3.6630			42.2579		
Raman Activ --	1.0448			1.1517			6.5066		
Depolar --	0.7461			0.7500			0.7177		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.05	0.03	-0.03	-0.06	-0.04	-0.04	-0.01	-0.02	0.02
2 6	-0.04	0.01	-0.03	0.01	0.01	0.05	0.03	-0.01	0.01
3 6	0.00	-0.01	0.01	0.01	0.00	-0.01	-0.02	-0.03	-0.01
4 6	0.00	-0.03	0.02	0.05	0.00	-0.03	-0.02	-0.02	0.00
5 6	-0.01	0.03	-0.03	0.02	0.04	0.00	0.01	0.09	-0.01
6 6	0.01	-0.06	0.01	0.01	-0.05	-0.04	-0.02	0.01	-0.04

```
   7   6     0.03   0.04  -0.12     0.03   0.08  -0.03    -0.01   0.01
0.07
   8   6    -0.06   0.03   0.01     0.00  -0.03   0.05    -0.09  -0.06  -
0.03
   9   6     0.07   0.01  -0.03    -0.02   0.00  -0.02     0.19   0.05  -
0.04
  10   6    -0.02   0.01   0.02     0.00   0.00   0.01    -0.09  -0.04
0.07
  11   6    -0.05   0.02   0.03     0.09  -0.08   0.01     0.02  -0.01  -
0.02
  12   8     0.00   0.00   0.00    -0.01   0.00   0.00    -0.01  -0.02
0.00
  13   6     0.00   0.00   0.01     0.00   0.00   0.00    -0.01   0.00
0.00
  14   7    -0.02  -0.01   0.00     0.00   0.00   0.00    -0.05  -0.02
0.01
  15   8     0.00   0.00   0.01    -0.01  -0.01   0.00    -0.01  -0.02
0.00
  16   1    -0.09  -0.20   0.21     0.01   0.24   0.18     0.06   0.08  -
0.11
  17   1     0.18  -0.06   0.21    -0.14  -0.01  -0.13    -0.05   0.06  -
0.07
  18   1     0.04   0.02   0.00    -0.06  -0.02   0.00     0.12   0.06  -
0.05
  19   1     0.04   0.06   0.06    -0.31   0.08   0.07     0.15   0.08
0.00
  20   1     0.02   0.12   0.23    -0.07   0.21   0.25     0.10   0.09
0.04
  21   1    -0.13  -0.21   0.65    -0.29  -0.15   0.20     0.03   0.10  -
0.25
  22   1     0.22  -0.20   0.18    -0.11   0.14  -0.02     0.49   0.31
0.17
  23   1     0.07  -0.04  -0.04    -0.02   0.03   0.03     0.43   0.15  -
0.29
  24   1     0.27  -0.10   0.00    -0.25   0.25   0.01    -0.09   0.07  -
0.01
  25   1     0.04  -0.09  -0.04    -0.42   0.33  -0.02     0.02   0.05
0.06
  26   1     0.04  -0.04   0.00     0.09  -0.08   0.00     0.16  -0.14
0.00
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.01
0.00
  28   1     0.00   0.01   0.00     0.00   0.00   0.00     0.00   0.04
0.00
                     64                    65                    66
                     ?A                    ?A                    ?A
 Frequencies --  1494.8268             1635.3684             2532.6597
 Red. masses --     2.1086                1.1039               12.6691
 Frc consts  --     2.7761                1.7394               47.8794
 IR Inten    --    30.3854                2.6106               75.3146
 Raman Activ --     5.4133                9.3215              155.1242
 Depolar     --     0.5734                0.6723                0.1431
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
```

1	6	0.01	-0.01	0.04	-0.01	0.00	0.00	0.00	0.00	0.00
2	6	0.00	-0.01	-0.03	0.00	0.00	0.00	0.00	0.00	0.00
3	6	-0.03	-0.08	0.07	0.00	0.00	0.00	0.00	0.00	0.00
4	6	-0.05	-0.09	-0.04	0.01	0.00	0.00	0.00	0.00	0.00
5	6	0.09	0.21	-0.04	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.02	0.03	0.00	0.00	0.00	0.00	0.00	0.00
7	6	-0.01	-0.01	-0.01	0.00	-0.01	0.00	0.00	0.00	0.00
8	6	0.05	0.01	0.03	0.00	0.00	0.00	0.00	0.00	0.00
9	6	-0.04	0.00	0.01	0.00	0.00	0.00	-0.13	-0.04	0.02
10	6	0.04	0.00	-0.04	0.00	0.00	0.00	0.00	0.00	0.00
11	6	-0.01	0.01	-0.01	-0.05	-0.06	-0.04	0.00	0.00	0.00
12	8	-0.04	-0.03	0.01	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.76	0.24	-0.12
14	7	0.01	0.00	0.00	0.00	0.00	0.00	-0.55	-0.17	0.08
15	8	-0.03	-0.03	0.01	0.00	0.00	0.00	0.00	0.00	0.00
16	1	0.05	0.03	-0.10	-0.02	-0.01	-0.01	0.00	0.00	0.00
17	1	0.07	0.08	0.07	-0.01	-0.01	-0.02	0.00	0.00	0.00
18	1	0.05	0.33	-0.21	0.00	0.00	0.00	0.00	0.00	0.00
19	1	0.16	0.40	0.12	-0.02	-0.02	-0.01	0.00	0.00	0.00
20	1	-0.01	-0.07	-0.07	-0.01	-0.01	-0.02	0.00	0.00	0.00
21	1	0.06	0.04	-0.01	0.00	-0.02	-0.01	0.00	0.00	0.00
22	1	-0.25	-0.01	-0.11	-0.02	-0.02	-0.01	0.00	0.00	0.01
23	1	-0.20	0.04	0.13	0.00	0.00	0.00	0.00	0.00	-0.01
24	1	0.09	-0.06	0.00	0.44	0.54	-0.13	0.00	0.00	0.00
25	1	0.00	0.03	0.03	0.18	0.22	0.64	0.00	0.00	0.00
26	1	0.44	-0.39	0.01	0.00	0.00	0.00	-0.01	0.00	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  28   1     0.00  -0.01   0.00     0.00   0.00   0.00     0.00  -0.01
0.00
                      67                     68                     69
                      ?A                     ?A                     ?A
 Frequencies --  3175.0526              3210.9780              3239.6709
 Red. masses --     1.0576                 1.1051                 1.0872
 Frc consts  --     6.2816                 6.7134                 6.7233
 IR Inten    --    86.6155                52.5204                17.0742
 Raman Activ --   154.3225               108.5152                77.9383
 Depolar     --     0.1922                 0.7493                 0.7500
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01   0.00   0.00     0.00   0.00   0.00    -0.05   0.02  -
0.01
   2   6     0.00   0.00   0.00     0.00   0.00   0.00     0.05   0.01  -
0.04
   3   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.01
0.01
   4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.01
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -0.01
0.01
   7   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   8   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  11   6    -0.04  -0.05  -0.02    -0.02  -0.03   0.09     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1    -0.11   0.04  -0.02     0.02  -0.01   0.00     0.55  -0.23
0.10
  17   1    -0.01   0.00   0.01    -0.01   0.00   0.01    -0.56  -0.11
0.49
  18   1     0.00   0.00   0.00     0.00   0.00   0.00     0.02  -0.07  -
0.09
  19   1     0.00   0.00  -0.01     0.00   0.00   0.01    -0.03   0.05  -
0.12
  20   1     0.00  -0.01   0.01     0.00   0.00   0.00     0.00   0.09  -
0.08
  21   1     0.01  -0.03  -0.01     0.00   0.00   0.00     0.01  -0.01
0.00
```

```
  22   1     0.00   0.00  -0.01     0.00   0.00   0.01     0.00   0.00
0.01
  23   1     0.00   0.00   0.00     0.00   0.00   0.00     0.01   0.00
0.01
  24   1     0.04   0.05   0.64    -0.07  -0.08  -0.75     0.00   0.01
0.06
  25   1     0.42   0.51  -0.36     0.38   0.45  -0.28     0.02   0.02  -
0.01
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     70                    71                    72
                     ?A                    ?A                    ?A
 Frequencies --  3255.3998             3274.1285             3287.8873
 Red. masses --     1.0879                1.0886                1.0888
 Frc consts  --     6.7926                6.8758                6.9351
 IR Inten    --    81.6271               58.8281               52.2106
 Raman Activ --   155.5264              110.8933              121.7604
 Depolar     --     0.4050                0.2945                0.4841
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.05   0.02  -0.01    -0.03   0.01  -0.01     0.00   0.00
0.00
   2   6    -0.04  -0.01   0.03    -0.01   0.00   0.01    -0.01   0.00
0.01
   3   6     0.00  -0.01  -0.01     0.00  -0.01  -0.01     0.00  -0.02  -
0.02
   4   6     0.01  -0.01   0.03    -0.01   0.03  -0.07     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.01  -0.01     0.00   0.01  -0.01     0.00  -0.06
0.05
   7   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   8   6     0.00   0.00   0.00    -0.01   0.00   0.02     0.00   0.00
0.00
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00  -
0.01
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

```
  16   1     0.63  -0.27   0.12     0.31  -0.13   0.06     0.05  -0.02
0.01
  17   1     0.42   0.08  -0.38     0.06   0.01  -0.06     0.11   0.02  -
0.10
  18   1    -0.02   0.08   0.11    -0.02   0.08   0.10    -0.04   0.19
0.25
  19   1    -0.07   0.14  -0.32     0.16  -0.35   0.79     0.00  -0.01
0.01
  20   1     0.00  -0.13   0.11     0.00  -0.08   0.07    -0.01   0.70  -
0.60
  21   1     0.00  -0.01   0.00     0.00   0.00   0.00     0.04  -0.06  -
0.01
  22   1    -0.02   0.01   0.04     0.11  -0.04  -0.25     0.02  -0.01  -
0.05
  23   1    -0.01   0.00  -0.02    -0.01   0.00  -0.02     0.06  -0.01
0.08
  24   1     0.00   0.01   0.06     0.00   0.01   0.04     0.00   0.00
0.01
  25   1     0.03   0.04  -0.03     0.01   0.02  -0.01     0.01   0.01  -
0.01
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  27   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  28   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     73                     74                     75
                     ?A                     ?A                     ?A
 Frequencies --  3295.1634              3304.1202              3340.3342
 Red. masses --     1.0900                 1.0888                 1.0909
 Frc consts  --     6.9732                 7.0031                 7.1716
 IR Inten    --    65.0295                24.8665                31.6971
 Raman Activ --   133.7912               158.2380               149.4293
 Depolar     --     0.1326                 0.1737                 0.1515
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01   0.00   0.00    -0.01   0.00   0.00     0.00   0.00
0.00
   2   6     0.02   0.00  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
   3   6     0.01  -0.05  -0.06     0.00   0.01   0.01     0.00  -0.01  -
0.01
   4   6     0.00   0.00   0.00    -0.01   0.01  -0.02     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00   0.02  -0.01     0.00   0.00   0.00     0.00   0.01  -
0.01
   7   6     0.00   0.00   0.00     0.00   0.01   0.00     0.00   0.00
0.00
   8   6     0.01   0.00  -0.01     0.03  -0.01  -0.07     0.00   0.00
0.00
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

10	6	0.01	0.00	0.01	0.00	0.00	-0.01	-0.05	0.00	-0.07
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	-0.07	0.03	-0.02	0.07	-0.03	0.01	-0.01	0.00	0.00
17	1	-0.17	-0.04	0.15	0.04	0.01	-0.04	-0.04	-0.01	0.03
18	1	-0.10	0.54	0.71	0.01	-0.07	-0.10	-0.02	0.11	0.13
19	1	-0.01	0.02	-0.05	0.06	-0.12	0.26	0.00	0.01	-0.02
20	1	0.00	-0.17	0.15	0.00	0.04	-0.04	0.00	-0.12	0.10
21	1	-0.01	0.01	0.00	0.05	-0.07	-0.01	-0.03	0.04	0.01
22	1	-0.08	0.03	0.17	-0.39	0.13	0.84	0.01	-0.01	-0.03
23	1	-0.12	0.01	-0.17	0.05	0.00	0.07	0.57	-0.04	0.78
24	1	0.00	0.00	-0.01	0.00	0.00	0.03	0.00	0.00	0.00
25	1	-0.01	-0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.00
26	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	76			77			78		
	?A			?A			?A		
Frequencies --	3381.2677			3830.1199			3880.4511		
Red. masses --	1.0898			1.0677			1.0654		
Frc consts --	7.3409			9.2285			9.4516		
IR Inten --	12.8366			5.3966			67.5949		
Raman Activ --	107.1631			230.1695			99.9700		
Depolar --	0.1565			0.2927			0.2170		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
   4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
   6   6     0.00  -0.01   0.01     0.00   0.00   0.00     0.00   0.00
0.00
   7   6     0.04  -0.07  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
   8   6     0.00   0.00  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
   9   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  10   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  11   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.04   0.05  -
0.01
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.02  -0.01   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  17   1     0.01   0.00  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
  18   1     0.00  -0.01  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
  19   1     0.00  -0.01   0.01     0.00   0.00   0.00     0.00   0.00
0.00
  20   1     0.00   0.06  -0.05     0.00   0.00   0.00     0.00   0.00
0.00
  21   1    -0.51   0.83   0.16     0.00  -0.01   0.00     0.00   0.00
0.00
  22   1    -0.03   0.01   0.07     0.00   0.00   0.00     0.00   0.00
0.00
  23   1    -0.02   0.00  -0.03     0.00   0.00   0.00     0.00   0.00
0.00
  24   1     0.01   0.00   0.03     0.00   0.00   0.00     0.00   0.00
0.00
  25   1     0.02   0.02  -0.01     0.00   0.00   0.00     0.00   0.00
0.00
  26   1     0.00   0.00   0.00     0.00   0.00   0.00    -0.60  -0.78
0.17
  27   8     0.00   0.00   0.00     0.06   0.00   0.01     0.00   0.00
0.00
  28   1    -0.01   0.00   0.00    -0.99   0.02  -0.09     0.00   0.00
0.00

 --------------------
 - Thermochemistry -
 --------------------
```

```
Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
Atom  1 has atomic number  6 and mass  12.00000
Atom  2 has atomic number  6 and mass  12.00000
Atom  3 has atomic number  6 and mass  12.00000
Atom  4 has atomic number  6 and mass  12.00000
Atom  5 has atomic number  6 and mass  12.00000
Atom  6 has atomic number  6 and mass  12.00000
Atom  7 has atomic number  6 and mass  12.00000
Atom  8 has atomic number  6 and mass  12.00000
Atom  9 has atomic number  6 and mass  12.00000
Atom 10 has atomic number  6 and mass  12.00000
Atom 11 has atomic number  6 and mass  12.00000
Atom 12 has atomic number  8 and mass  15.99491
Atom 13 has atomic number  6 and mass  12.00000
Atom 14 has atomic number  7 and mass  14.00307
Atom 15 has atomic number  8 and mass  15.99491
Atom 16 has atomic number  1 and mass   1.00783
Atom 17 has atomic number  1 and mass   1.00783
Atom 18 has atomic number  1 and mass   1.00783
Atom 19 has atomic number  1 and mass   1.00783
Atom 20 has atomic number  1 and mass   1.00783
Atom 21 has atomic number  1 and mass   1.00783
Atom 22 has atomic number  1 and mass   1.00783
Atom 23 has atomic number  1 and mass   1.00783
Atom 24 has atomic number  1 and mass   1.00783
Atom 25 has atomic number  1 and mass   1.00783
Atom 26 has atomic number  1 and mass   1.00783
Atom 27 has atomic number  8 and mass  15.99491
Atom 28 has atomic number  1 and mass   1.00783
Molecular mass:   218.08172 amu.
Principal axes and moments of inertia in atomic units:
                          1         2         3
    EIGENVALUES --  2014.78036 2639.58356 3632.75052
          X            0.99995   0.00419   0.00936
          Y           -0.00426   0.99996   0.00773
          Z           -0.00932  -0.00777   0.99993
THIS MOLECULE IS AN ASYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER  1.
WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
          MAY CAUSE SIGNIFICANT ERROR
ROTATIONAL TEMPERATURES (KELVIN)      0.04299     0.03281     0.02384
ROTATIONAL CONSTANTS (GHZ)            0.89575     0.68372     0.49680
   1 IMAGINARY FREQUENCIES IGNORED.
Zero-point vibrational energy     618270.4 (Joules/Mol)
                                  147.77017 (Kcal/Mol)
WARNING-- EXPLICIT CONSIDERATION OF  16 DEGREES OF FREEDOM AS
          VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
VIBRATIONAL TEMPERATURES:    177.96   283.61   304.36   350.68   376.90
         (KELVIN)            401.26   448.56   476.14   530.85   572.25
                             666.24   677.54   779.46   813.59   850.73
                             881.13   909.58   937.09   971.59   982.77
                            1006.11  1172.38  1187.77  1193.05  1214.75
                            1267.75  1302.30  1333.73  1363.63  1407.18
                            1434.04  1446.60  1468.65  1482.59  1493.21
```

1518.44	1522.74	1542.43	1596.46	1671.98
1734.47	1744.51	1753.72	1775.78	1791.15
1809.82	1824.98	1859.27	1909.60	1917.11
1934.93	1949.20	1963.79	1980.02	1990.74
1998.67	2020.51	2027.61	2056.50	2077.00
2081.70	2120.51	2150.71	2352.92	3643.91
4568.17	4619.85	4661.14	4683.77	4710.71
4730.51	4740.98	4753.86	4805.97	4864.86
5510.66	5583.07			

Zero-point correction=	0.235487
(Hartree/Particle)	
Thermal correction to Energy=	0.245857
Thermal correction to Enthalpy=	0.246801
Thermal correction to Gibbs Free Energy=	0.200174
Sum of electronic and zero-point Energies=	-736.125451
Sum of electronic and thermal Energies=	-736.115081
Sum of electronic and thermal Enthalpies=	-736.114137
Sum of electronic and thermal Free Energies=	-736.160764

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	154.278	45.570	98.135
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	42.042
ROTATIONAL	0.889	2.981	31.336
VIBRATIONAL	152.500	39.609	24.756
VIBRATION 1	0.610	1.929	3.042
VIBRATION 2	0.637	1.844	2.160
VIBRATION 3	0.643	1.823	2.030
VIBRATION 4	0.659	1.773	1.775
VIBRATION 5	0.669	1.742	1.649
VIBRATION 6	0.679	1.713	1.540
VIBRATION 7	0.700	1.651	1.353
VIBRATION 8	0.713	1.614	1.256
VIBRATION 9	0.741	1.536	1.084
VIBRATION 10	0.764	1.475	0.971
VIBRATION 11	0.821	1.332	0.757
VIBRATION 12	0.828	1.315	0.735
VIBRATION 13	0.897	1.158	0.562
VIBRATION 14	0.921	1.106	0.513
VIBRATION 15	0.949	1.050	0.465
VIBRATION 16	0.972	1.006	0.429

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.844900D-92	-92.073195	-212.006366
TOTAL V=0	0.174765D+17	16.242455	37.399635
VIB (BOT)	0.424197-106	-106.372433	-244.931578
VIB (BOT) 1	0.165076D+01	0.217683	0.501233
VIB (BOT) 2	0.101265D+01	0.005461	0.012575
VIB (BOT) 3	0.938315D+00	-0.027652	-0.063670
VIB (BOT) 4	0.803099D+00	-0.095231	-0.219277
VIB (BOT) 5	0.740734D+00	-0.130338	-0.300113
VIB (BOT) 6	0.689779D+00	-0.161290	-0.371383
VIB (BOT) 7	0.605895D+00	-0.217602	-0.501048

VIB (BOT)	8	0.564282D+00	-0.248504	-0.572201
VIB (BOT)	9	0.493784D+00	-0.306463	-0.705657
VIB (BOT)	10	0.448873D+00	-0.347877	-0.801015
VIB (BOT)	11	0.366378D+00	-0.436071	-1.004090
VIB (BOT)	12	0.357910D+00	-0.446226	-1.027474
VIB (BOT)	13	0.291965D+00	-0.534669	-1.231121
VIB (BOT)	14	0.273384D+00	-0.563227	-1.296878
VIB (BOT)	15	0.254794D+00	-0.593811	-1.367300
VIB (BOT)	16	0.240702D+00	-0.618521	-1.424196
VIB (V=0)		0.877440D+02	1.943217	4.474423
VIB (V=0)	1	0.222482D+01	0.347294	0.799675
VIB (V=0)	2	0.162937D+01	0.212019	0.488192
VIB (V=0)	3	0.156322D+01	0.194020	0.446747
VIB (V=0)	4	0.144603D+01	0.160177	0.368820
VIB (V=0)	5	0.139369D+01	0.144167	0.331957
VIB (V=0)	6	0.135194D+01	0.130956	0.301538
VIB (V=0)	7	0.128556D+01	0.109093	0.251197
VIB (V=0)	8	0.125393D+01	0.098274	0.226285
VIB (V=0)	9	0.120273D+01	0.080166	0.184590
VIB (V=0)	10	0.117193D+01	0.068901	0.158650
VIB (V=0)	11	0.111987D+01	0.049166	0.113208
VIB (V=0)	12	0.111490D+01	0.047235	0.108763
VIB (V=0)	13	0.107900D+01	0.033022	0.076037
VIB (V=0)	14	0.106986D+01	0.029326	0.067526
VIB (V=0)	15	0.106118D+01	0.025788	0.059379
VIB (V=0)	16	0.105492D+01	0.023220	0.053466
ELECTRONIC		0.100000D+01	0.000000	0.000000
TRANSLATIONAL		0.126587D+09	8.102389	18.656441
ROTATIONAL		0.157343D+07	6.196849	14.268771

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000383	0.000000496	-0.000000380
2	6	-0.000000249	-0.000000046	-0.000000253
3	6	0.000000903	0.000000508	0.000000790
4	6	0.000000337	-0.000000804	0.000000519
5	6	-0.000000282	0.000001436	-0.000003615
6	6	0.000001719	0.000000512	-0.000000447
7	6	0.000000638	-0.000000191	-0.000000318
8	6	-0.000000056	0.000001064	0.000000848
9	6	0.000001974	0.000002529	-0.000006581
10	6	-0.000002151	-0.000004281	0.000000081
11	6	0.000000298	-0.000000239	0.000000008
12	8	-0.000001523	-0.000003015	0.000000992
13	6	-0.000001106	-0.000000645	-0.000001033
14	7	0.000008892	-0.000003862	0.000011426
15	8	-0.000012199	0.000002738	0.000004392
16	1	0.000000207	-0.000000151	0.000000120
17	1	0.000000206	-0.000000104	0.000000100
18	1	-0.000000225	-0.000000029	0.000000403
19	1	-0.000000244	0.000000232	0.000000173
20	1	-0.000000034	0.000000090	0.000000364

21	1	-0.000000094	-0.000000311	-0.000000185
22	1	-0.000000347	0.000000080	0.000000130
23	1	-0.000001027	-0.000000179	0.000000098
24	1	-0.000000101	-0.000000101	-0.000000017
25	1	-0.000000076	0.000000194	-0.000000077
26	1	0.000001580	0.000002026	-0.000000349
27	8	0.000002426	0.000002638	-0.000005816
28	1	0.000000918	-0.000000586	-0.000001371

Cartesian Forces: Max 0.000012199 RMS 0.000002616

Internal Coordinate Forces (Hartree/Bohr or radian)

Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	C		0.000000(1)		0.000000(29)		0.000000(57)	
2	C		0.000000(2)		0.000000(30)		0.000000(58)	
3	C		0.000001(3)		0.000001(31)		0.000001(59)	
4	C		0.000000(4)		-0.000001(32)		0.000001(60)	
5	C		0.000000(5)		0.000001(33)		-0.000004(61)	
6	C		0.000002(6)		0.000001(34)		0.000000(62)	
7	C		0.000001(7)		0.000000(35)		0.000000(63)	
8	C		0.000000(8)		0.000001(36)		0.000001(64)	
9	C		0.000002(9)		0.000003(37)		-0.000007(65)	
10	C		-0.000002(10)		-0.000004(38)		0.000000(66)	
11	C		0.000000(11)		0.000000(39)		0.000000(67)	
12	O		-0.000002(12)		-0.000003(40)		0.000001(68)	
13	C		-0.000001(13)		-0.000001(41)		-0.000001(69)	
14	N		0.000009(14)		-0.000004(42)		0.000011(70)	
15	O		-0.000012(15)		0.000003(43)		0.000004(71)	
16	H		0.000000(16)		0.000000(44)		0.000000(72)	
17	H		0.000000(17)		0.000000(45)		0.000000(73)	
18	H		0.000000(18)		0.000000(46)		0.000000(74)	
19	H		0.000000(19)		0.000000(47)		0.000000(75)	
20	H		0.000000(20)		0.000000(48)		0.000000(76)	
21	H		0.000000(21)		0.000000(49)		0.000000(77)	
22	H		0.000000(22)		0.000000(50)		0.000000(78)	
23	H		-0.000001(23)		0.000000(51)		0.000000(79)	
24	H		0.000000(24)		0.000000(52)		0.000000(80)	
25	H		0.000000(25)		0.000000(53)		0.000000(81)	
26	H		0.000002(26)		0.000002(54)		0.000000(82)	
27	O		0.000002(27)		0.000003(55)		-0.000006(83)	
28	H		0.000001(28)		-0.000001(56)		-0.000001(84)	

Internal Forces: Max 0.000012199 RMS 0.000002616

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number 1 out of a maximum of 94
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
Eigenvalues --- -0.18630 0.00284 0.00312 0.00631 0.01072
Eigenvalues --- 0.01248 0.01491 0.01789 0.01938 0.02750
Eigenvalues --- 0.03106 0.03901 0.04141 0.04271 0.04490

```
    Eigenvalues ---    0.04582   0.04708   0.04766   0.05038   0.05067
    Eigenvalues ---    0.05133   0.05212   0.05298   0.05502   0.05774
    Eigenvalues ---    0.05938   0.06291   0.06967   0.07539   0.09549
    Eigenvalues ---    0.10184   0.10577   0.11057   0.12172   0.14314
    Eigenvalues ---    0.15076   0.15544   0.17849   0.18848   0.19420
    Eigenvalues ---    0.20204   0.21234   0.24740   0.27380   0.28281
    Eigenvalues ---    0.31305   0.34998   0.35976   0.36781   0.39118
    Eigenvalues ---    0.40106   0.48617   0.48936   0.49964   0.51560
    Eigenvalues ---    0.52005   0.58060   0.58692   0.61423   0.63957
    Eigenvalues ---    0.67248   0.72023   0.75217   0.83694   0.85050
    Eigenvalues ---    0.86890   0.93684   0.94992   0.95556   0.98122
    Eigenvalues ---    0.99643   1.02294   1.05500   1.06782   1.09000
    Eigenvalues ---    1.10760   1.12093   3.09469
Eigenvalue   1 out of range, new value =    0.186300 Eigenvector:
                          1
          X1          -0.00818
          Y1           0.00057
          Z1          -0.01746
          X2          -0.00956
          Y2           0.00172
          Z2          -0.00616
          X3           0.00030
          Y3           0.03370
          Z3          -0.04798
          X4          -0.00966
          Y4          -0.02104
          Z4          -0.05278
          X5          -0.05150
          Y5           0.02299
          Z5          -0.11439
          X6           0.01948
          Y6          -0.01835
          Z6           0.03162
          X7           0.03210
          Y7           0.00759
          Z7           0.03703
          X8           0.05088
          Y8          -0.00620
          Z8          -0.01865
          X9           0.75602
          Y9          -0.13404
          Z9          -0.29506
          X10          0.03703
          Y10         -0.01789
          Z10         -0.01204
          X11          0.00458
          Y11          0.00201
          Z11          0.01331
          X12          0.00809
          Y12         -0.00814
          Z12          0.07677
          X13         -0.09197
          Y13          0.00997
          Z13          0.04640
```

```
          X14         -0.03350
          Y14          0.00407
          Z14          0.02292
          X15         -0.38071
          Y15          0.06284
          Z15          0.07190
          X16         -0.00683
          Y16          0.00243
          Z16         -0.01407
          X17         -0.00800
          Y17          0.00141
          Z17         -0.00237
          X18          0.01566
          Y18          0.01213
          Z18         -0.02857
          X19          0.01331
          Y19         -0.00939
          Z19         -0.02888
          X20          0.01904
          Y20         -0.00999
          Z20          0.02073
          X21          0.02677
          Y21          0.00310
          Z21          0.02937
          X22          0.02054
          Y22          0.00916
          Z22          0.00376
          X23          0.01140
          Y23         -0.03306
          Z23          0.01122
          X24          0.00114
          Y24          0.00188
          Z24          0.00503
          X25          0.00154
          Y25          0.00013
          Z25          0.01217
          X26          0.03698
          Y26         -0.00890
          Z26          0.01473
          X27         -0.23641
          Y27          0.04538
          Z27          0.15685
          X28         -0.10728
          Y28          0.02873
          Z28          0.12047
Angle between quadratic step and forces=  70.57 degrees.
Linear search not attempted -- first point.
TrRot=  0.000000 -0.000019 -0.000002 -0.000005  0.000002 -0.000005
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   X1       -0.85806   0.00000   0.00000  -0.00001  -0.00003  -0.85809
   Y1       -0.79992   0.00000   0.00000  -0.00003  -0.00004  -0.79996
   Z1       -4.05130   0.00000   0.00000   0.00000   0.00000  -4.05130
   X2       -0.78783   0.00000   0.00000   0.00000   0.00001  -0.78782
```

Y2	2.03190	0.00000	0.00000	-0.00002	-0.00003	2.03187
Z2	-3.26103	0.00000	0.00000	-0.00002	-0.00002	-3.26105
X3	1.53598	0.00000	0.00000	-0.00001	0.00001	1.53599
Y3	2.38902	0.00000	0.00000	-0.00001	-0.00005	2.38897
Z3	-1.48555	0.00000	0.00000	-0.00001	-0.00002	-1.48557
X4	0.71444	0.00000	0.00000	-0.00003	-0.00005	0.71439
Y4	-2.03633	0.00000	0.00000	-0.00002	-0.00005	-2.03638
Z4	-1.92482	0.00000	0.00000	0.00001	0.00001	-1.92481
X5	2.82725	0.00000	0.00000	-0.00004	-0.00005	2.82720
Y5	-0.18805	0.00000	0.00000	-0.00003	-0.00008	-0.18813
Z5	-1.25184	0.00000	0.00000	0.00001	0.00000	-1.25184
X6	-2.58748	0.00000	0.00000	0.00000	0.00001	-2.58747
Y6	2.10290	0.00000	0.00000	0.00000	0.00001	2.10290
Z6	-0.88843	0.00000	0.00000	-0.00002	-0.00002	-0.88845
X7	-3.49465	0.00000	0.00000	-0.00002	-0.00003	-3.49467
Y7	-0.67246	0.00000	0.00000	0.00001	0.00003	-0.67243
Z7	-0.64136	0.00000	0.00000	-0.00001	0.00000	-0.64136
X8	-1.10004	0.00000	0.00000	-0.00003	-0.00005	-1.10009
Y8	-1.96456	0.00000	0.00000	0.00002	0.00001	-1.96455
Z8	0.44777	0.00000	0.00000	0.00001	0.00001	0.44779
X9	0.02296	0.00000	0.00000	0.00004	0.00004	0.02300
Y9	-0.00684	0.00000	0.00000	0.00001	-0.00001	-0.00684
Z9	2.29907	-0.00001	0.00000	0.00000	-0.00001	2.29907
X10	-0.24665	0.00000	0.00000	-0.00001	0.00001	-0.24664
Y10	2.49995	0.00000	0.00000	0.00000	-0.00001	2.49993
Z10	0.87724	0.00000	0.00000	-0.00002	-0.00002	0.87722
X11	-3.58016	0.00000	0.00000	-0.00002	-0.00004	-3.58020
Y11	-1.58636	0.00000	0.00000	-0.00001	0.00001	-1.58636
Z11	-3.40579	0.00000	0.00000	-0.00001	0.00000	-3.40579
X12	5.00795	0.00000	0.00000	-0.00001	-0.00002	5.00793
Y12	-0.44491	0.00000	0.00000	-0.00016	-0.00023	-0.44514
Z12	-2.88336	0.00000	0.00000	0.00009	0.00008	-2.88328
X13	0.96191	0.00000	0.00000	0.00005	0.00006	0.96197
Y13	-0.44815	0.00000	0.00000	-0.00008	-0.00010	-0.44825
Z13	4.80849	0.00000	0.00000	0.00002	0.00001	4.80850
X14	1.68935	0.00001	0.00000	0.00016	0.00017	1.68952
Y14	-0.78500	0.00000	0.00000	-0.00022	-0.00025	-0.78525
Z14	6.81668	0.00001	0.00000	-0.00004	-0.00004	6.81664
X15	3.42191	-0.00001	0.00000	-0.00015	-0.00015	3.42176
Y15	-0.55139	0.00000	0.00000	0.00004	-0.00001	-0.55140
Z15	1.27497	0.00000	0.00000	0.00005	0.00005	1.27502
X16	-0.17759	0.00000	0.00000	0.00000	-0.00002	-0.17762
Y16	-1.19248	0.00000	0.00000	-0.00005	-0.00006	-1.19254
Z16	-5.93887	0.00000	0.00000	0.00001	0.00001	-5.93886
X17	-1.10001	0.00000	0.00000	0.00001	0.00003	-1.09998
Y17	3.37140	0.00000	0.00000	-0.00003	-0.00004	3.37136
Z17	-4.77214	0.00000	0.00000	-0.00003	-0.00003	-4.77217
X18	2.82678	0.00000	0.00000	0.00000	0.00003	2.82682
Y18	3.93828	0.00000	0.00000	-0.00002	-0.00007	3.93821
Z18	-1.77889	0.00000	0.00000	-0.00002	-0.00002	-1.77891
X19	1.42178	0.00000	0.00000	-0.00003	-0.00007	1.42171
Y19	-3.90647	0.00000	0.00000	-0.00002	-0.00006	-3.90653
Z19	-2.33802	0.00000	0.00000	0.00004	0.00003	-2.33799
X20	-4.06863	0.00000	0.00000	0.00000	0.00003	-4.06860

Y20	3.50017	0.00000	0.00000	0.00001	0.00003	3.50020
Z20	-0.79922	0.00000	0.00000	-0.00003	-0.00002	-0.79924
X21	-5.14998	0.00000	0.00000	-0.00004	-0.00004	-5.15002
Y21	-0.91338	0.00000	0.00000	0.00002	0.00005	-0.91333
Z21	0.50059	0.00000	0.00000	-0.00003	-0.00002	0.50057
X22	-1.42352	0.00000	0.00000	-0.00005	-0.00008	-1.42360
Y22	-3.77812	0.00000	0.00000	0.00002	0.00002	-3.77811
Z22	1.31876	0.00000	0.00000	0.00003	0.00003	1.31879
X23	-0.19570	0.00000	0.00000	-0.00004	0.00000	-0.19571
Y23	4.13917	0.00000	0.00000	0.00002	0.00000	4.13917
Z23	2.07544	0.00000	0.00000	-0.00004	-0.00004	2.07540
X24	-3.89070	0.00000	0.00000	-0.00003	-0.00007	-3.89077
Y24	-3.60992	0.00000	0.00000	-0.00001	0.00001	-3.60992
Z24	-3.57274	0.00000	0.00000	0.00000	0.00001	-3.57273
X25	-4.99352	0.00000	0.00000	-0.00001	-0.00002	-4.99354
Y25	-0.59246	0.00000	0.00000	-0.00001	0.00002	-0.59244
Z25	-4.51762	0.00000	0.00000	-0.00002	-0.00001	-4.51763
X26	6.44458	0.00000	0.00000	0.00016	0.00015	6.44473
Y26	-0.82672	0.00000	0.00000	0.00085	0.00076	-0.82595
Z26	-1.81977	0.00000	0.00000	0.00021	0.00020	-1.81957
X27	-3.27419	0.00000	0.00000	0.00008	0.00009	-3.27410
Y27	0.58259	0.00000	0.00000	0.00020	0.00021	0.58279
Z27	3.98169	-0.00001	0.00000	-0.00009	-0.00009	3.98161
X28	-3.21035	0.00000	0.00000	0.00006	0.00008	-3.21027
Y28	0.74872	0.00000	0.00000	-0.00009	-0.00008	0.74865
Z28	5.80457	0.00000	0.00000	-0.00007	-0.00006	5.80450

Item		Value	Threshold	Converged?
Maximum	Force	0.000012	0.000450	YES
RMS	Force	0.000003	0.000300	YES
Maximum	Displacement	0.000765	0.001800	YES
RMS	Displacement	0.000108	0.001200	YES

Predicted change in Energy=-3.781442D-09
Optimization completed.
   -- Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1|1|UNPC-UNK|Freq|RHF|3-21+G*|C12H12N1O3(1-)|PCUSER|08-May-2002|0||#N
RHF/3-21+G* FREQ||Freq calc of output str of mech1st8ts2||-1,1|C,-0.45
4065087,-0.4232990522,-2.1438560261|C,-0.416901087,1.0752339478,-1.725
6630261|C,0.812803913,1.2642149478,-0.7861190261|C,0.378067913,-1.0775
820522,-1.0185720261|C,1.496115913,-0.0995130522,-0.6624460261|C,-1.36
9238087,1.1128049478,-0.4701390261|C,-1.849288087,-0.3558500522,-0.339
3930261|C,-0.582116087,-1.0395980522,0.2369519739|C,0.012150913,-0.003
6180522,1.2166179739|C,-0.130524087,1.3229149478,0.4642179739|C,-1.894
539087,-0.8394670522,-1.8022670261|O,2.650094913,-0.2354370522,-1.5258
080261|C,0.509020913,-0.2371500522,2.5445419739|N,0.893966913,-0.41540
20522,3.6072319739|O,1.810796913,-0.2917850522,0.6746849739|H,-0.09397
8087,-0.6310310522,-3.1427140261|H,-0.582099087,1.7840689478,-2.525308
0261|H,1.495868913,2.0840459478,-0.9413490261|H,0.752375913,-2.0672150
522,-1.2372270261|H,-2.153026087,1.8522089478,-0.4229280261|H,-2.72525
0087,-0.4833420522,0.2649019739|H,-0.753292087,-1.9992970522,0.6978569
739|H,-0.103562087,2.1903559478,1.0982759739|H,-2.058872087,-1.9102900
522,-1.8906150261|H,-2.642458087,-0.3135150522,-2.3906230261|H,3.41032
3913,-0.4374800522,-0.9629800261|O,-1.732627087,0.3082909478,2.1070219

739|H,-1.698845087,0.3962059478,3.0716459739||Version=x86-Win32-G98Rev
A.7|HF=-736.3609381|RMSD=9.837e-009|RMSF=2.616e-006|Dipole=-0.8263189,
0.2961867,-2.8533515|DipoleDeriv=0.057927,0.0189129,-0.0948577,0.00857
53,0.0015759,0.0447671,-0.0675692,0.0562149,0.1376055,-0.0262835,-0.03
35633,0.061186,0.0041739,0.0828675,-0.0865766,0.0339485,-0.0993964,0.0
317537,-0.0297867,0.138599,-0.0000504,0.1452085,-0.0628889,0.0200851,0
.063471,-0.0120793,-0.0245224,-0.118557,-0.1173267,-0.0382795,-0.18332
67,0.0417222,0.0040084,0.0207972,0.0112582,-0.0284001,1.1368363,-0.078
5984,-0.1284493,-0.0578724,0.5749813,0.0020783,-0.5648517,0.0745706,1.
0063883,0.1110889,-0.1117378,-0.0148744,-0.0730819,0.0713803,0.0368646
,-0.0300711,0.0065073,0.1058448,0.0692895,0.0318742,0.0391776,0.019597
5,0.026435,0.016736,-0.0256428,0.0318699,0.1230066,-0.0698143,0.081775
5,0.0623664,0.0864954,0.1186361,-0.0017866,0.0296407,-0.0380106,0.0515
891,2.3693894,-0.3320226,-1.2113187,-0.3353321,0.3864004,0.1715136,-0.
8532568,0.1082065,1.2058012,-0.0824459,0.0061896,0.0179056,-0.0144563,
0.1284126,-0.0647372,0.0191144,0.025137,0.0321132,0.0640205,-0.046055,
0.0697092,-0.0550173,0.1953106,-0.0729989,0.081856,-0.0694556,-0.07100
92,-1.2046064,0.0438714,0.427639,0.0485182,-0.6458105,-0.0737764,0.529
8833,-0.0891397,-0.7318944,0.1158119,-0.0267804,0.2189278,-0.0396062,0
.0788345,-0.0964162,0.2577194,-0.1067575,0.5657962,-0.4087719,0.020417
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62442,-0.0208174,-1.3369223,0.0189354,0.0139761,0.0895864,0.004844,0.0
332468,-0.0557444,0.0658061,-0.0597703,-0.2156185,0.0361731,0.0298486,
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246,-0.0678721,-0.1365771,0.0267189,-0.1244516,-0.086337,0.0300302,0.0
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,-0.0095608,-0.0204236,-0.0728864,-0.0826519,-0.0092473,-0.1010824,-0.
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,-0.0239286,-0.0168378,0.0494686,-0.1202053,0.0451786,-0.143462,0.1245
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090494,-0.0873684,0.012795,0.3524121,0.0291391,-0.1288811,0.0368932,0.
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.2572376,-0.3736871,0.4194825,-0.0871006,1.1288889,1.0367045,2.2122674
,-0.4712844,0.4431561,-4.0998993,1.6154264,13.6793773|HyperPolar=11.65
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,-0.00395260,-0.09173123,0.00482314,0.12827894,0.64430895,-0.01363153,
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-0.00018303,-0.00008578,0.00012035,-0.00001904,-0.00001977,-0.00000143
,-0.00015752,0.00005784,-0.00004550,0.00007031,-0.00085984,-0.00016977
,0.00115134,0.00057716,0.00032312,-0.00004285,0.00021073,-0.00004579,0
.00005998,-0.00009797,0.00005951,0.00269163,-0.00114406,0.00164410,0.1
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-0.00006451,-0.00000873,-0.00001652,-0.00030009,-0.00007116,0.00006820
,-0.00001014,0.00002386,0.00000519,0.00000458,-0.00005249,-0.00013478,
0.00009099,0.00016382,-0.00007836,-0.00011337,0.00007816,0.00000536,0.
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78,-0.00032079,-0.00015768,0.00020091,-0.00106245,0.00015893,0.0000304
9,-0.00003782,-0.00001115,0.08919689,-0.02200547,0.05829741,-0.0002034
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3,0.00027027,-0.00494644,0.02345209,-0.00018470,-0.00035603,-0.0007496
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0.00311927,-0.00151968,-0.00256069,-0.00128148,-0.00349936,-0.01083542
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,0.00005987,-0.00004232,-0.00007021,0.00001430,0.00005092,-0.00007890,
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00000439,-0.00000021,0.00000015,-0.00000012,-0.00000021,0.00000010,-0.
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00019,0.00000035,-0.00000008,-0.00000013,0.00000103,0.00000018,-0.0000
0010,0.00000010,0.00000010,0.00000002,0.00000008,-0.00000019,0.0000000
8,-0.00000158,-0.00000203,0.00000035,-0.00000243,-0.00000264,0.0000058
2,-0.00000092,0.00000059,0.00000137|||@

CONFIDENCE IS WHAT YOU FEEL BEFORE YOU FULLY
COMPREHEND THE SITUATION.
Job cpu time: 0 days 18 hours 54 minutes 56.0 seconds.
File lengths (MBytes): RWF= 307 Int=   0 D2E=   0 Chk=   5 Scr=
1
Normal termination of Gaussian 98.

```
%nproc=2
%chk=mech1st8ts2
%nosave
# opt=(calcfc,gdiis,ts,noeigentest) rhf/3-21+g(d) geom=connectivity
optcyc=100

TS search for mech1str5 using input@1.65A from mech1str8S2 & calcfc

-1  1
 C
 C                  1             B1
 C                  2             B2    1             A1
 C                  1             B3    2             A2    3
D1
 C                  3             B4    2             A3    1
D2
 C                  2             B5    1             A4    4
D3
 C                  6             B6    2             A5    1
D4
 C                  7             B7    6             A6    2
D5
 C                  8             B8    7             A7    6
D6
 C                  9             B9    8             A8    7
D7
 C                  1            B10    2             A9    3
D8
 O                  5            B11    3            A10    2
D9
 C                  9            B12    8            A11    7
D10
 N                 13            B13    9            A12    8
D11
 O                  5            B14    3            A13    2
D12
 H                  1            B15    2            A14    3
D13
 H                  2            B16    1            A15   11
D14
 H                  3            B17    2            A16    1
D15
 H                  4            B18    1            A17    2
D16
 H                  6            B19    2            A18    1
D17
 H                  7            B20    6            A19    2
D18
 H                  8            B21    7            A20    6
D19
 H                 10            B22    9            A21    8
D20
 H                 11            B23    1            A22    2
D21
```

```
 H                 11             B24    1             A23    2
D22
 H                 12             B25    5             A24    3
D23
 O                 13             B26    9             A25    8
D24
 H                 27             B27   13             A26    9
D25
```

B1	1.553242
B2	1.559140
B3	1.545805
B4	1.526458
B5	1.579019
B6	1.553574
B7	1.545600
B8	1.561373
B9	1.549880
B10	1.539191
B11	1.434202
B12	1.446896
B13	1.186554
B14	1.405605
B15	1.082720
B16	1.081329
B17	1.077720
B18	1.084805
B19	1.081073
B20	1.075122
B21	1.079645
B22	1.076574
B23	1.087424
B24	1.087555
B25	0.964662
B26	1.554897
B27	0.975274
A1	107.997203
A2	101.207418
A3	107.313641
A4	103.138694
A5	102.854220
A6	101.277852
A7	106.640611
A8	101.961910
A9	103.097210
A10	112.139797
A11	124.506462
A12	161.029231
A13	105.480403
A14	115.177475
A15	115.343498
A16	120.130276
A17	114.862631
A18	118.124527

```
  A19          115.479459
  A20          115.388940
  A21          113.401652
  A22          113.130547
  A23          112.866238
  A24          112.369839
  A25           66.576131
  A26          124.316813
  D1            21.327784
  D2            -1.338564
  D3           -72.520398
  D4            -0.461272
  D5            74.420755
  D6            36.616797
  D7           -39.475326
  D8           127.885143
  D9           105.655748
  D10          108.852931
  D11          108.139287
  D12         -129.119537
  D13         -103.519677
  D14          -96.473230
  D15          130.688353
  D16         -162.345499
  D17         -128.660631
  D18         -161.142798
  D19          161.944276
  D20          158.573570
  D21         -171.133896
  D22           64.181496
  D23         -155.813099
  D24          -72.132864
  D25         -174.747903

1  2 1.0  4 1.0  11 1.0  16 1.0
2  3 1.0  6 1.0  17 1.0
3  5 1.0  10 1.0  18 1.0
4  5 1.0  8 1.0  19 1.0
5  12 1.0  15 1.0
6  7 1.0  10 1.0  20 1.0
7  8 1.0  11 1.0  21 1.0
8  9 1.0  22 1.0
9  10 1.0  13 1.5
10  23 1.0
11  24 1.0  25 1.0
12  26 1.0
13  14 3.0
14
15
16
17
18
19
20
```

```
21
22
23
24
25
26
27  28 1.0
28
```

```
 Entering Gaussian System, Link 0=g98
 Input=mech1str5F.gjf
 Output=mech1str5F.out
 Initial command:
 /usr/g98/l1.exe /usr/scratch/Singh/Gau-15958.inp -
scrdir=/usr/scratch/Singh/
 Default is to use a total of   2 processors:
                                2 via shared-memory
                                1 via Linda
 Entering Link 1 = /usr/g98/l1.exe PID=     18492.
```

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

Cite this work as:
Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

```
**********************************************
Gaussian 98:  DEC-AXP-OSF/1-G98RevA.7 11-Apr-1999
                  22-Apr-2002
**********************************************
%nproc=2
Will use up to    2 processors via shared memory.
%chk=mech1str5tsF
%nosave
-------------------
#N RHF/3-21+G* FREQ
-------------------
1/10=4,30=1,38=1/1,3;
2/17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
```

```
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;
-------------------------------------
Freq calc of output str of mech1str5ts
-------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                    -2.09041  -0.14148  -0.40646
C                    -1.65988  -0.14313   1.08501
C                    -0.53992   0.92996   1.25835
C                    -0.86999   0.51235  -1.0893
C                    -0.32766   1.57633  -0.12298
C                    -0.58186  -1.28914   1.14931
C                    -0.51896  -1.79965  -0.31172
C                     0.21692  -0.64328  -1.02278
C                     1.27059  -0.09811  -0.01517
C                     0.53477  -0.21041   1.34214
C                    -1.97489  -1.62843  -0.79789
O                    -0.24927   2.91292  -0.30612
C                     2.60545  -0.64019  -0.1071
N                     3.64955  -1.09441  -0.1704
O                     1.2092    1.33148  -0.31752
H                    -3.03314   0.34416  -0.61026
H                    -2.46568  -0.1618    1.80108
H                    -0.58898   1.63972   2.06582
H                    -1.03095   0.88823  -2.08696
H                    -0.68441  -2.05064   1.90576
H                    -0.07438  -2.77556  -0.44446
H                     0.64176  -0.88136  -1.98598
H                     1.17596  -0.24734   2.20733
H                    -2.08882  -1.79783  -1.86261
H                    -2.67001  -2.26132  -0.25776
H                     1.20717   2.46056  -0.31856

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  88 maximum allowed number of steps= 156.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

--------------------------------------------------------------------------
                          Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
--------------------------------------------------------------------------
  1   1  C     0  -2.090408         -0.141479         -0.406460
  2   2  C     0  -1.659875         -0.143131          1.085012
  3   3  C     0  -0.539923          0.929959          1.258348
  4   4  C     0  -0.869986          0.512346         -1.089299
  5   5  C     0  -0.327661          1.576328         -0.122975
  6   6  C     0  -0.581855         -1.289137          1.149305
```

7	7	C	0	-0.518956	-1.799647	-0.311715
8	8	C	0	0.216921	-0.643284	-1.022779
9	9	C	0	1.270594	-0.098112	-0.015174
10	10	C	0	0.534774	-0.210405	1.342136
11	11	C	0	-1.974888	-1.628431	-0.797885
12	12	O	0	-0.249269	2.912917	-0.306116
13	13	C	0	2.605453	-0.640189	-0.107102
14	14	N	0	3.649552	-1.094414	-0.170400
15	15	O	0	1.209203	1.331479	-0.317519
16	16	H	0	-3.033144	0.344156	-0.610258
17	17	H	0	-2.465678	-0.161801	1.801080
18	18	H	0	-0.588976	1.639719	2.065820
19	19	H	0	-1.030947	0.888229	-2.086960
20	20	H	0	-0.684409	-2.050635	1.905763
21	21	H	0	-0.074375	-2.775564	-0.444455
22	22	H	0	0.641760	-0.881364	-1.985985
23	23	H	0	1.175958	-0.247340	2.207329
24	24	H	0	-2.088823	-1.797829	-1.862608
25	25	H	0	-2.670010	-2.261317	-0.257757
26	26	H	0	1.207171	2.460559	-0.318561

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.090408	-0.141479	-0.406460
2	6	0	-1.659875	-0.143131	1.085012
3	6	0	-0.539923	0.929959	1.258348
4	6	0	-0.869986	0.512346	-1.089299
5	6	0	-0.327661	1.576328	-0.122975
6	6	0	-0.581855	-1.289137	1.149305
7	6	0	-0.518956	-1.799647	-0.311715
8	6	0	0.216921	-0.643284	-1.022779
9	6	0	1.270594	-0.098112	-0.015174
10	6	0	0.534774	-0.210405	1.342136
11	6	0	-1.974888	-1.628431	-0.797885
12	8	0	-0.249269	2.912917	-0.306116
13	6	0	2.605453	-0.640189	-0.107102
14	7	0	3.649552	-1.094414	-0.170400
15	8	0	1.209203	1.331479	-0.317519
16	1	0	-3.033144	0.344156	-0.610258
17	1	0	-2.465678	-0.161801	1.801080
18	1	0	-0.588976	1.639719	2.065820
19	1	0	-1.030947	0.888229	-2.086960
20	1	0	-0.684409	-2.050635	1.905763
21	1	0	-0.074375	-2.775564	-0.444455
22	1	0	0.641760	-0.881364	-1.985985
23	1	0	1.175958	-0.247340	2.207329
24	1	0	-2.088823	-1.797829	-1.862608
25	1	0	-2.670010	-2.261317	-0.257757
26	1	0	1.207171	2.460559	-0.318561

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.552369	0.000000			
3	C	2.514671	1.560724	0.000000		
4	C	1.543757	2.404413	2.407237	0.000000	
5	C	2.477600	2.488085	1.539773	1.536215	0.000000
6	C	2.452194	1.574672	2.222169	2.887855	3.145505
7	C	2.286473	2.448793	3.149014	2.464380	3.386654
8	C	2.440374	2.866234	2.872533	1.587852	2.456195
9	C	3.383980	3.130509	2.440647	2.471535	2.317281
10	C	3.154983	2.210684	1.569211	2.899585	2.466325
11	C	1.541942	2.418812	3.582259	2.426655	3.665971
12	O	3.567800	3.642043	2.542469	2.600270	1.351353
13	C	4.731748	4.456593	3.771367	3.791006	3.676460
14	N	5.823311	5.538142	4.867351	4.883879	4.790964
15	O	3.614547	3.517553	2.388308	2.364244	1.568359
16	H	1.079873	2.235454	3.170332	2.221941	3.012529
17	H	2.239302	1.078156	2.279261	3.369718	3.360684
18	H	3.396930	2.299427	1.076186	3.362248	2.205250
19	H	2.237596	3.394210	3.381410	1.078204	2.196663
20	H	3.311810	2.294284	3.053516	3.946354	4.171080
21	H	3.317263	3.432606	4.104531	3.443715	4.371095
22	H	3.241461	3.908137	3.899098	2.243178	3.232775
23	H	4.184764	3.051623	2.287104	3.953576	3.319179
24	H	2.205417	3.407416	4.424962	2.724056	4.184848
25	H	2.202672	2.703722	4.125541	3.409509	4.498031
26	H	4.201471	4.119365	2.807439	2.950280	1.782085

		6	7	8	9	10
6	C	0.000000				
7	C	1.548921	0.000000			
8	C	2.402731	1.544119	0.000000		
9	C	2.491208	2.487096	1.556505	0.000000	
10	C	1.564515	2.524136	2.425126	1.548009	0.000000
11	C	2.418101	1.544479	2.413528	3.672556	3.590110
12	O	4.459386	4.720278	3.657527	3.385399	3.617540
13	C	3.486922	3.338883	2.558038	1.443657	2.563731
14	N	4.436704	4.230104	3.565533	2.583825	3.573665
15	O	3.496726	3.576383	2.319850	1.462502	2.363623
16	H	3.431111	3.317553	3.421715	4.367137	4.104804
17	H	2.290084	3.306988	3.924582	4.154824	3.035738
18	H	3.068916	4.181724	3.924413	3.287642	2.282431
19	H	3.926324	3.261642	2.243922	3.249963	3.926471
20	H	1.078251	2.237762	3.371853	3.365172	2.278273
21	H	2.237649	1.080595	2.228437	3.026875	3.184809
22	H	3.390215	2.234656	1.079322	2.212015	3.396766
23	H	2.301013	3.409981	3.392657	2.229517	1.077516
24	H	3.406074	2.206752	2.711963	4.193773	4.435489
25	H	2.699139	2.200701	3.396713	4.501851	4.127534
26	H	4.406298	4.596620	3.333221	2.577375	3.216222

		11	12	13	14	15
11	C	0.000000				
12	O	4.882974	0.000000			
13	C	4.736383	4.562193	0.000000		
14	N	5.684473	5.592667	1.140381	0.000000	

15	O	4.373815	2.151329	2.425132	3.444112	0.000000
16	H	2.246377	3.800131	5.745944	6.849919	4.365548
17	H	3.024318	4.336662	5.439337	6.492499	4.497010
18	H	4.560961	2.713395	4.485972	5.517362	3.001460
19	H	2.980993	2.807452	4.413536	5.432416	2.888886
20	H	3.025443	5.451477	4.106601	4.899799	4.468495
21	H	2.247838	5.692850	3.443125	4.094997	4.304821
22	H	2.969265	4.244109	2.728453	3.519737	2.828859
23	H	4.567992	4.282044	2.748523	3.534091	2.978025
24	H	1.084118	5.291290	5.143749	6.023895	4.801754
25	H	1.084194	5.712707	5.520984	6.426987	5.287726
26	H	5.203373	1.525123	3.408012	4.315670	1.129082

		16	17	18	19	20
16	H	0.000000				
17	H	2.528351	0.000000			
18	H	3.848874	2.614875	0.000000		
19	H	2.546656	4.275263	4.243307	0.000000	
20	H	4.193083	2.598379	3.695056	4.969793	0.000000
21	H	4.302843	4.194343	5.104999	4.127497	2.534006
22	H	4.110893	4.951344	4.928255	2.437130	4.274532
23	H	5.099530	3.665224	2.587665	4.959926	2.608406
24	H	2.654849	4.030039	5.431282	2.895573	4.029505
25	H	2.654169	2.947631	4.994777	3.994014	2.944116
26	H	4.748107	4.985927	3.095997	3.257089	5.373692

		21	22	23	24	25
21	H	0.000000				
22	H	2.545026	0.000000			
23	H	3.871332	4.274487	0.000000		
24	H	2.650495	2.882918	5.443087	0.000000	
25	H	2.652664	3.982319	4.992416	1.768657	0.000000
26	H	5.392142	3.777359	3.703216	5.601922	6.110020

		26
26	H	0.000000

Interatomic angles:

C1-C2-C3=107.7574	C2-C1-C4=101.898	C1-C4-C3= 75.5519
C3-C2-C4= 71.1711	C2-C1-C5= 72.1508	C1-C5-C3= 73.3525
C2-C3-C5=106.7331	C1-C4-C5=107.1089	C2-C4-C5= 74.6899
C3-C5-C4=102.9966	C1-C2-C6=103.2893	C1-C6-C3= 64.8731
C3-C2-C6= 90.2633	C4-C1-C6= 89.5707	C4-C2-C6= 90.5971
C4-C3-C6= 77.0744	C5-C1-C6= 79.2928	C5-C2-C6= 98.987
C5-C3-C6=112.1963	C5-C4-C6= 84.7915	C2-C1-C7= 76.6326
C3-C1-C7= 81.8247	C3-C2-C7=101.1935	C4-C1-C7= 77.4167
C4-C2-C7= 61.0245	C3-C4-C7= 80.5321	C5-C1-C7= 90.5207
C5-C2-C7= 86.6233	C5-C4-C7=113.6413	C1-C7-C6= 76.8297
C2-C6-C7=103.2474	C3-C6-C7=112.003	C4-C7-C6= 89.0046
C2-C1-C8= 88.8658	C3-C1-C8= 70.8434	C3-C2-C8= 74.4416
C1-C4-C8=102.3787	C2-C4-C8= 89.3458	C3-C4-C8= 89.5157
C1-C8-C5= 60.7928	C2-C5-C8= 70.8565	C3-C5-C8= 88.8459
C5-C4-C8=103.6545	C1-C8-C6= 60.833	C2-C6-C8= 89.7167
C3-C6-C8= 76.6829	C4-C8-C6= 90.3403	C5-C8-C6= 80.6785
C1-C7-C8= 76.4296	C2-C7-C8= 88.7453	C3-C8-C7= 85.3481
C4-C8-C7=103.7748	C5-C8-C7=113.7275	C6-C7-C8=101.9403
C1-C3-C9= 86.1275	C2-C3-C9=100.6464	C1-C4-C9=112.8208
C2-C4-C9= 79.8739	C4-C3-C9= 61.2987	C1-C5-C9= 89.7157

C2-C5-C9= 81.2193 C3-C5-C9= 75.5234 C4-C5-C9= 76.8374
C1-C6-C9= 86.3958 C2-C6-C9= 98.1657 C6-C3-C9= 64.3894
C4-C9-C6= 71.1683 C5-C9-C6= 81.6247 C1-C7-C9= 90.19
C2-C7-C9= 78.7222 C3-C9-C7= 79.4341 C7-C4-C9= 60.5135
C5-C9-C7= 89.5724 C6-C7-C9= 72.017 C1-C8-C9=113.8618
C2-C8-C9= 84.6114 C3-C9-C8= 89.0345 C4-C8-C9=103.6262
C5-C9-C8= 75.8817 C6-C8-C9= 74.5728 C7-C8-C9=106.6669
C1-C2-C10=112.7746 C1-C3-C10= 98.5103 C2-C3-C10= 89.8694
C1-C4-C10= 84.6363 C4-C2-C10= 77.7218 C4-C3-C10= 91.1406
C1-C5-C10= 79.3082 C2-C10-C5= 64.0053 C5-C3-C10=104.9841
C4-C5-C10= 89.7345 C1-C6-C10=101.2198 C2-C6-C10= 89.5328
C3-C10-C6= 90.3256 C4-C6-C10= 74.7301 C5-C10-C6=100.1784
C1-C7-C10= 81.8052 C7-C2-C10= 65.3687 C3-C10-C7= 97.8547
C4-C7-C10= 71.0658 C5-C10-C7= 85.4643 C7-C6-C10=108.3323
C1-C8-C10= 80.8475 C2-C10-C8= 76.2252 C3-C10-C8= 89.3058
C4-C8-C10= 90.0378 C5-C8-C10= 60.693 C8-C6-C10= 71.8691
C7-C8-C10= 75.3491 C2-C10-C9=111.5736 C3-C10-C9=103.062
C4-C9-C10= 89.272 C5-C9-C10= 76.4298 C6-C10-C9=106.332
C7-C9-C10= 73.3154 C8-C9-C10=102.7337 C2-C1-C11=102.8318
C3-C1-C11=122.1912 C3-C2-C11=127.0213 C4-C1-C11=103.7044
C4-C2-C11= 60.4122 C3-C4-C11= 95.6447 C5-C1-C11=130.1171
C5-C2-C11= 96.6704 C5-C4-C11=134.1234 C1-C11-C6= 72.7485
C2-C6-C11= 71.0254 C3-C6-C11=100.9823 C4-C11-C6= 73.1789
C1-C11-C7= 95.6021 C2-C11-C7= 72.5585 C4-C11-C7= 72.9254
C6-C7-C11=102.8323 C1-C11-C8= 72.4264 C2-C11-C8= 72.7596
C3-C8-C11= 84.8527 C4-C8-C11= 71.2973 C5-C8-C11= 97.6647
C6-C8-C11= 60.2736 C8-C7-C11=102.7837 C9-C4-C11= 97.1381
C9-C6-C11= 96.8374 C9-C7-C11=129.7897 C9-C8-C11=134.2192
C10-C2-C11=101.6038 C10-C4-C11= 84.2604 C10-C6-C11=127.3846
C10-C7-C11=122.004 C10-C8-C11= 95.7978 C1-C3-O12= 89.7378
C2-C3-O12=123.3632 C1-C4-O12=116.5188 C2-C4-O12= 93.3095
C4-C3-O12= 63.3127 C1-C5-O12=135.3592 C2-C5-O12=141.2959
C3-C5-O12=123.009 C4-C5-O12=128.3353 C6-C3-O12=138.6613
C6-C4-O12=108.5788 C7-C4-O12=137.4829 C8-C3-O12= 84.7439
C8-C4-O12=119.7278 C8-C5-O12=146.2321 C9-C3-O12= 85.5636
C9-C4-O12= 83.7067 C9-C5-O12=132.9209 C10-C3-O12=121.4228
C10-C4-O12= 82.0623 C10-C5-O12=140.9648 C11-C4-O12=152.4938
C1-C8-C13=142.3895 C2-C8-C13=110.3623 C3-C8-C13= 87.7702
C4-C8-C13=130.7887 C5-C8-C13= 94.2896 C6-C8-C13= 89.2633
C7-C8-C13=106.3231 C3-C9-C13=151.3191 C4-C9-C13=149.9847
C5-C9-C13=154.9711 C6-C9-C13=122.5341 C7-C9-C13=113.6299
C8-C9-C13=116.9488 C2-C10-C13=137.8318 C3-C10-C13=130.1503
C4-C10-C13= 87.654 C5-C10-C13= 93.9035 C6-C10-C13=113.0292
C7-C10-C13= 82.0241 C10-C8-C13= 61.8572 C10-C9-C13=117.9114
C11-C8-C13=144.5969 C3-C9-N14=151.2552 C4-C9-N14=150.0605
C5-C9-N14=155.6237 C6-C9-N14=121.8954 C7-C9-N14=113.0491
C8-C9-N14=116.7006 C10-C9-N14=117.5388 C8-C13-N14=146.569
C9-C13-N14=178.5171 C10-C13-N14=146.8916 C1-C3-O15= 94.9544
C2-C3-O15=124.6003 C1-C4-O15=134.2335 C2-C4-O15= 95.0578
C3-O15-C4= 60.8614 C1-C5-O15=125.0822 C2-C5-O15=118.4909
C3-C5-O15=100.418 C4-C5-O15= 99.1943 C6-C3-O15= 98.588
C6-C4-O15= 82.8388 C7-C4-O15= 95.5535 C1-C8-O15= 98.7776
C2-C8-O15= 84.7197 C3-O15-C8= 75.1804 C4-C8-O15= 71.6992
C5-O15-C8= 75.6088 C6-C8-O15= 95.5195 C7-C8-O15=134.5339

C3-O15-C9= 74.3357 C4-O15-C9= 76.4514 C5-O15-C9= 99.6771
C6-C9-O15=122.1916 C7-C9-O15=127.8718 C8-C9-O15=100.3772
C2-C10-O15=100.4715 C3-C10-O15= 71.5705 C4-O15-C10= 75.6565
C5-O15-C10= 74.6411 C6-C10-O15=124.534 C7-C10-O15= 94.0009
C8-O15-C10= 62.362 C10-C9-O15=103.4278 C11-C4-O15=131.826
C11-C8-O15=135.0378 C3-O15-O12= 67.8881 C4-O15-O12= 70.1363
O12-C5-O15= 94.632 C8-O15-O12=109.7174 C9-O15-O12=138.238
C10-O15-O12=106.4017 C3-O15-C13=103.1631 C4-O15-C13=104.6531
C5-O15-C13=132.8705 C8-O15-C13= 65.2012 C13-C9-O15=113.1219
C10-O15-C13= 64.7224 O12-O15-C13=170.9328 N14-C9-O15=113.7749
N14-C13-O15=147.7951 C2-C1-H16=115.0822 C3-C1-H16=118.1385
C3-C2-H16=112.0349 C4-C1-H16=114.5958 C2-H16-C4= 65.2877
C3-C4-H16= 86.3511 C5-C1-H16=109.3241 C5-C2-H16= 79.0528
C3-C5-H16= 81.3503 C5-C4-H16=105.0996 C6-C1-H16=150.1425
C6-C2-H16=127.6013 C6-C4-H16= 83.2688 C7-C1-H16=159.0605
C7-C2-H16= 90.0645 C7-C4-H16= 89.9789 C8-C1-H16=150.4845
C8-C2-H16= 83.258 C8-C4-H16=127.0336 C8-C5-H16= 76.7173
C9-C4-H16=136.9524 C9-C5-H16=109.3531 C10-C2-H16=134.8049
C10-C4-H16=105.7832 C10-C5-H16= 96.5355 C11-C1-H16=116.819
C2-H16-C11= 65.3249 C4-H16-C11= 65.7845 C5-H16-C11= 87.1108
C6-C11-H16= 94.6414 C7-C11-H16=121.0068 C8-C11-H16= 94.426
O12-C4-H16=103.7298 O12-C5-H16=115.7677 O15-C4-H16=144.293
O15-C5-H16=142.7615 C1-C2-H17=115.5211 C1-H17-C3= 67.6243
C3-C2-H17=118.3242 C4-C1-H17=124.9161 C4-C2-H17=148.3043
C4-C3-H17= 91.9071 C5-C1-H17= 90.7292 C5-C2-H17=137.2737
C5-C3-H17=122.0839 C1-H17-C6= 65.5463 C6-C2-H17=118.1605
C6-C3-H17= 61.1451 C4-C6-H17= 80.2973 C7-C1-H17= 93.8846
C7-C2-H17=135.6696 C7-C6-H17=117.6525 C8-C1-H17=113.9256
C8-C2-H17=167.1048 C8-C3-H17= 98.5902 C8-C6-H17=113.4804
C9-C3-H17=123.3153 C9-C6-H17=120.6217 C10-C2-H17=131.6205
C10-C3-H17=102.582 C10-C6-H17=102.2754 C11-C1-H17=104.7176
C11-C2-H17=114.1444 C11-C6-H17= 79.8845 O12-C3-H17=128.0753
O15-C3-H17=148.9177 H16-C1-H17= 92.5119 H16-C2-H17= 92.7692
C3-H17-H16= 82.3385 C4-H16-H17= 90.1296 C5-H16-H17= 74.0986
C6-H17-H16= 90.6703 C11-H16-H17= 78.3579 C1-C2-H18=122.5578
C1-C3-H18=138.5585 C2-C3-H18=120.2701 C4-C2-H18= 91.2237
C4-C3-H18=147.1295 C1-C5-H18= 92.8194 C2-H18-C5= 67.0167
C5-C3-H18=113.7364 C4-C5-H18=127.0428 C6-C2-H18=103.1809
C6-C3-H18=133.9922 C7-C2-H18=123.4216 C8-C2-H18= 98.2804
C8-C3-H18=165.7075 C8-C5-H18=114.5733 C9-C3-H18=134.6785
C9-C5-H18= 93.229 C2-C10-H18= 61.5386 C10-C3-H18=118.0622
C4-C10-H18= 79.9388 C5-H18-C10= 66.6502 C6-C10-H18=104.2754
C7-C10-H18=120.8355 C8-C10-H18=112.9143 C9-C10-H18=116.9515
C11-C2-H18=150.3198 C2-H18-O12= 92.8231 O12-C3-H18= 87.2787
C4-O12-H18= 78.4755 O12-C5-H18= 96.4857 C10-H18-O12= 92.3811
C13-C10-H18=135.4617 C2-H18-O15= 81.992 O15-C3-H18=114.6818
C4-O15-H18= 76.5807 O15-C5-H18=104.1063 C8-O15-H18= 94.1614
C9-O15-H18= 87.7865 O15-C10-H18= 80.4642 O15-O12-H18= 75.2016
C13-O15-H18=111.071 H16-C2-H18=116.1398 H16-C5-H18= 93.7776
C1-H17-H18= 88.4689 H17-C2-H18= 94.4857 H17-C3-H18= 95.6662
C5-H18-H17= 87.9801 C6-H17-H18= 77.1489 C10-H18-H17= 76.2786
O12-H18-H17=108.9428 O15-H18-H17=106.1904 H16-H17-H18= 96.8789
C2-C1-H19=126.2097 C3-C1-H19= 90.5271 C1-C4-H19=116.0345
C2-C4-H19=151.9751 C3-C4-H19=149.5853 C1-H19-C5= 67.9302

C2-C5-H19= 92.6467 C3-C5-H19=128.788 C5-C4-H19=113.1593
C6-C1-H19=113.6141 C6-C4-H19=161.7393 C7-C1-H19= 92.26
C7-C4-H19=129.8131 C1-H19-C8= 65.9865 C2-C8-H19= 82.2715
C3-C8-H19= 81.7371 C8-C4-H19=113.2457 C5-H19-C8= 67.1534
C6-C8-H19=115.2969 C7-C8-H19=117.6773 C9-C4-H19=128.1365
C9-C5-H19= 92.0667 C9-C8-H19=116.3856 C10-C4-H19=159.2487
C10-C5-H19=114.5915 C10-C8-H19=114.4271 C11-C1-H19=102.5711
C2-C11-H19= 77.1129 C11-C4-H19=110.5298 C5-H19-C11= 88.8086
C6-C11-H19= 92.7134 C7-C11-H19= 86.0555 C11-C8-H19= 79.4995
C1-H19-O12= 89.2729 C3-O12-H19= 78.23 O12-C4-H19= 89.5694
O12-C5-H19=101.96 C8-H19-O12= 92.0947 C11-H19-O12=115.0059
C13-C8-H19=133.4876 C1-H19-O15= 88.7255 C3-O15-H19= 79.0729
O15-C4-H19=108.2133 O15-C5-H19= 98.8544 O15-C8-H19= 78.5248
C9-O15-H19= 90.5267 C10-O15-H19= 96.2418 C11-H19-O15= 96.3277
O15-O12-H19= 69.8338 C13-O15-H19=112.0152 H16-C1-H19= 93.7075
C2-H16-H19= 90.191 H16-C4-H19= 94.6198 C5-H19-H16= 78.4746
C8-H19-H16= 90.94 C11-H16-H19= 76.6319 O12-H19-H16= 90.2955
O15-H19-H16=106.6946 H17-C1-H19=145.4772 H17-H16-H19=114.7916
H18-C5-H19=149.1454 H18-O12-H19=100.4423 H18-O15-H19= 92.1521
C1-C2-H20=117.5489 C3-C2-H20=103.1099 C4-C2-H20=114.2351
C5-C2-H20=121.3728 C1-C6-H20=135.8166 C2-C6-H20=118.5229
C3-C6-H20=132.2701 C4-C6-H20=167.1366 C1-C7-H20= 94.1051
C2-H20-C7= 65.3981 C4-C7-H20=114.0392 C7-C6-H20=115.648
C8-C2-H20= 80.7695 C8-C6-H20=148.8338 C8-C7-H20=125.1385
C9-C6-H20=137.4174 C9-C7-H20= 90.6751 C2-C10-H20= 61.4517
C3-C10-H20=103.5151 C4-C10-H20= 98.5996 C5-C10-H20=123.0244
C10-C6-H20=117.928 C7-H20-C10= 67.9565 C8-C10-H20= 91.5434
C9-C10-H20=121.9971 C11-C2-H20= 79.8229 C11-C6-H20=114.2707
C11-C7-H20=104.7536 C13-C10-H20=115.8908 O15-C10-H20=148.5744
H16-C2-H20=135.5379 C1-H17-H20= 86.0681 H17-C2-H20= 93.7715
C3-H17-H20= 77.2077 H17-C6-H20= 93.9996 C7-H20-H17= 85.9418
C10-H20-H17= 76.6866 H16-H17-H20=109.74 H18-C2-H20=107.0994
H18-C10-H20=108.2298 H18-H17-H20= 90.2711 C1-C6-H21= 89.916
C2-C6-H21=127.5626 C3-C6-H21=133.9502 C4-C6-H21= 83.3904
C1-C7-H21=158.8484 C2-C7-H21=150.772 C4-C7-H21=150.1265
C6-C7-H21=115.4827 C1-C8-H21= 90.4366 C2-C8-H21= 83.7151
C3-C8-H21=106.4705 C4-C8-H21=128.1545 C5-C8-H21=137.7851
C6-H21-C8= 65.0941 C8-C7-H21=115.0684 C9-C6-H21= 79.3981
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C10-C7-H21=118.5131 C10-C8-H21= 86.2646 C1-C11-H21=121.0347
C2-C11-H21= 94.6384 C4-C11-H21= 94.8256 C6-H21-C11= 65.2436
C11-C7-H21=116.6979 C8-H21-C11= 65.2543 C13-C8-H21= 91.7372
O15-C8-H21=142.3288 H16-C11-H21=146.4391 H17-C6-H21=135.7477
H19-C8-H21=134.7044 H19-C11-H21=103.362 C2-H20-H21= 90.4822
H20-C6-H21= 92.9874 H20-C7-H21= 92.9148 C8-H21-H20= 89.9101
C10-H20-H21= 82.6921 C11-H21-H20= 78.2461 H17-H20-H21=109.6107
C1-C4-H22=116.5161 C2-C4-H22=114.4251 C3-C4-H22=113.9053
C5-C4-H22=116.3499 C6-C4-H22= 81.6655 C1-C7-H22= 91.6005
C2-C7-H22=113.0395 C4-H22-C7= 66.7819 C6-C7-H22=126.325
C1-C8-H22=130.0081 C2-C8-H22=162.2699 C3-C8-H22=158.9396
C4-C8-H22=113.1157 C5-C8-H22=127.8457 C6-C8-H22=151.4397
C7-C8-H22=115.6804 C3-C9-H22=113.7763 C4-H22-C9= 67.3833
C5-C9-H22= 91.0509 C6-C9-H22= 92.0509 C7-H22-C9= 68.0149
C9-C8-H22=112.8618 C10-C4-H22= 81.5951 C10-C7-H22= 90.8791

C10-C8-H22=149.0977 C10-C9-H22=128.3444 C1-C11-H22= 85.697
C2-C11-H22= 92.4193 C11-C4-H22= 78.857 C6-C11-H22= 77.246
C11-C7-H22=102.0193 C11-C8-H22=110.5225 C9-H22-C11= 89.0322
O12-C4-H22=122.2163 C4-H22-C13= 98.9078 C7-H22-C13= 83.9275
C13-C8-H22= 87.2593 C13-C9-H22= 94.1959 C10-C13-H22= 79.7928
C11-H22-C13=112.3918 N14-C9-H22= 94.1106 N14-C13-H22=125.8393
C3-O15-H22= 96.3586 O15-C4-H22= 75.7046 C5-O15-H22= 89.9266
C7-H22-O15= 89.0682 O15-C8-H22=106.9006 O15-C9-H22= 98.6269
C10-O15-H22= 81.177 C11-H22-O15= 97.9079 O12-O15-H22=116.2418
O15-C13-H22= 66.281 H16-C4-H22=134.0474 H16-C11-H22=103.1579
H18-O15-H22=115.3722 C1-H19-H22= 87.6912 H19-C4-H22= 86.9809
C5-H19-H22= 88.319 C7-H22-H19= 88.4481 H19-C8-H22= 86.9169
C9-H22-H19= 88.5631 C11-H22-H19= 66.0731 O12-H19-H22=107.8346
C13-H22-H19=117.2785 O15-H22-H19= 66.0543 H16-H19-H22=111.1283
H20-C7-H22=145.7849 C4-H22-H21= 91.7574 C6-H21-H22= 90.0469
H21-C7-H22= 93.7491 H21-C8-H22= 94.1282 C9-H22-H21= 78.6897
C11-H21-H22= 76.2815 C13-H22-H21= 81.4427 O15-H22-H21=106.3438
H19-H22-H21=111.8627 H20-H21-H22=114.6195 C1-C3-H23=121.1951
C2-C3-H23=103.3277 C4-C3-H23=114.7224 C5-C3-H23=119.0053
C1-C6-H23=123.3521 C2-C6-H23=102.2546 C6-C3-H23= 61.3456
C4-C6-H23= 98.6396 C7-C6-H23=123.4986 C8-C3-H23= 81.3676
C8-C6-H23= 92.2927 C3-H23-C9= 65.4032 C4-C9-H23=114.3934
C5-C9-H23= 93.7534 C6-H23-C9= 66.6947 C7-C9-H23= 92.4371
C8-C9-H23=126.3799 C2-C10-H23=133.2494 C3-C10-H23=118.38
C4-C10-H23=165.9639 C5-C10-H23=135.2272 C6-C10-H23=120.0025
C7-C10-H23=138.8455 C8-C10-H23=148.7475 C9-C10-H23=115.0666
C11-C6-H23=150.9127 O12-C3-H23=124.8218 C3-H23-C13= 96.5677
C6-H23-C13= 86.871 C8-C13-H23= 79.3952 C13-C9-H23= 94.4502
C13-C10-H23= 88.1394 N14-C9-H23= 94.1955 N14-C13-H23=125.4403
O15-C3-H23= 79.0977 C4-O15-H23= 94.7762 C5-O15-H23= 88.0894
C6-H23-O15= 81.8782 C8-O15-H23= 78.5613 O15-C9-H23=105.648
O15-C10-H23=114.6059 O12-O15-H23=112.1885 O15-C13-H23= 69.9656
H17-C3-H23=106.769 H17-C6-H23=105.9421 C2-H18-H23= 77.0297
H18-C3-H23= 93.5754 C5-H18-H23= 87.2771 C6-H23-H18= 77.5249
C9-H23-H18= 85.7348 H18-C10-H23= 93.7941 O12-H18-H23=107.734
C13-H23-H18=114.3883 O15-H23-H18= 64.8261 H17-H18-H23= 89.5778
H19-O15-H23=115.4227 C2-H20-H23= 76.6917 C3-H23-H20= 76.8685
H20-C6-H23= 94.0041 C7-H20-H23= 89.0999 C9-H23-H20= 87.782
H20-C10-H23= 95.2847 C13-H23-H20=100.0656 O15-H23-H20=106.0491
H17-H20-H23= 89.4865 H18-H23-H20= 90.6522 H21-C6-H23=117.065
H21-H20-H23= 97.6607 H22-C9-H23=148.4723 H22-C13-H23=102.6023
H22-O15-H23= 94.7669 C2-C1-H24=129.2985 C3-C1-H24=139.1717
C4-C1-H24= 91.4594 C2-C4-H24= 83.0231 C3-C4-H24=119.0339
C5-C1-H24=126.5665 C5-C4-H24=157.5024 C6-C1-H24= 93.8392
C6-C4-H24= 74.6727 C1-H24-C7= 62.4258 C2-C7-H24= 93.9481
C4-C7-H24= 71.1037 C6-C7-H24=129.3274 C8-C1-H24= 71.2244
C2-C8-H24= 75.2445 C3-C8-H24=104.7777 C4-C8-H24= 73.4342
C5-C8-H24=108.0385 C6-C8-H24= 83.2733 C8-C7-H24= 90.8465
C9-C4-H24=107.5433 C9-C7-H24=126.52 C9-C8-H24=157.6879
C10-C4-H24=104.0889 C10-C7-H24=139.1953 C10-C8-H24=119.3019
C1-C11-H24=113.0864 C2-C11-H24=150.9444 C4-C11-H24= 93.8852
C6-C11-H24=150.8465 C7-C11-H24=113.0102 C8-C11-H24= 93.8822
O12-C4-H24=167.2248 C13-C8-H24=154.8557 O15-C4-H24=141.2591
O15-C8-H24=145.1054 H16-C1-H24=102.3436 C2-H16-H24= 87.8998

C4-H16-H24= 67.2373 C5-H16-H24= 94.9831 C7-H24-H16= 85.5368
C8-H24-H16= 79.2138 H16-C11-H24= 99.7721 H17-C1-H24=130.1057
H17-H16-H24=102.0404 H19-C1-H24= 81.3384 H19-C4-H24= 88.0619
C5-H19-H24=109.7719 C7-H24-H19= 78.189 H19-C8-H24= 70.7851
C11-H24-H19= 83.8433 O12-H19-H24=136.1846 O15-H19-H24=112.2206
H19-H16-H24= 67.616 H20-C7-H24=130.0846 C1-H24-H21= 85.6598
C4-H24-H21= 79.6819 C6-H21-H24= 87.9184 H21-C7-H24=101.9522
C8-H21-H24= 66.8912 H21-C11-H24= 99.412 H16-H24-H21=108.3952
H19-H24-H21= 96.0838 H20-H21-H24=101.9903 C1-H24-H22= 77.8886
H22-C4-H24= 70.1932 H22-C7-H24= 80.9449 H22-C8-H24= 87.9593
C9-H22-H24=110.1021 C11-H24-H22= 83.847 C13-H22-H24=132.8678
O15-H22-H24=114.4199 H16-H24-H22= 95.774 H19-H22-H24= 65.3244
H22-H21-H24= 67.3702 C2-C1-H25= 90.4063 C3-C1-H25=121.8435
C3-C2-H25=149.5317 C4-C1-H25=130.2021 C4-C2-H25= 83.5234
C5-C1-H25=147.86 C5-C2-H25=120.0222 C6-C1-H25= 70.6483
C2-C6-H25= 73.2147 C3-C6-H25=113.5696 C4-C6-H25= 75.1314
C1-H25-C7= 62.5646 C2-C7-H25= 70.8844 C4-C7-H25= 93.7452
C6-C7-H25= 90.3623 C8-C1-H25= 93.896 C8-C2-H25= 75.0906
C8-C6-H25= 83.2666 C8-C7-H25=129.3614 C9-C6-H25=120.2516
C9-C7-H25=147.5543 C10-C2-H25=113.88 C10-C6-H25=149.8552
C10-C7-H25=121.6051 C1-C11-H25=112.8564 C2-C11-H25= 93.1038
C4-C11-H25=150.0797 C6-C11-H25= 92.8714 C7-C11-H25=112.5106
C8-C11-H25=150.1041 H16-C1-H25=102.4639 C2-H16-H25= 66.5001
C4-H16-H25= 88.2661 C5-H16-H25=104.9015 C6-H25-H16= 79.718
C7-H25-H16= 85.6723 H16-C11-H25= 99.7264 H17-C1-H25= 83.1435
H17-C2-H25= 92.1232 C3-H17-H25=103.4989 H17-C6-H25= 71.8972
C7-H25-H17= 78.4599 C11-H25-H17= 83.5545 H17-H16-H25= 69.2793
H18-C2-H25=173.3481 H18-H17-H25=127.6755 H19-C1-H25=128.1827
H19-C11-H25=155.6804 H19-H16-H25=100.3213 C1-H25-H20= 78.6545
H20-C2-H25= 71.6485 H20-C6-H25= 92.1645 H20-C7-H25= 83.1024
C10-H20-H25=103.7044 C11-H25-H20= 83.7953 H16-H25-H20= 96.8703
H17-H20-H25= 63.9006 C1-H25-H21= 85.6609 C2-H25-H21= 79.7033
C6-H21-H25= 66.3704 H21-C7-H25=102.4561 C8-H21-H25= 87.7464
H21-C11-H25= 99.5465 H16-H25-H21=108.3506 H17-H25-H21= 96.8581
H20-H21-H25= 69.1269 H22-C7-H25=127.7541 H22-C11-H25=155.6731
H22-H21-H25=100.0019 H23-C6-H25=173.6048 H23-H20-H25=127.9846
C1-H25-H24= 66.4264 C2-H25-H24= 97.0403 C4-H24-H25= 96.4122
C6-H25-H24= 97.1468 C7-H25-H24= 66.521 C8-H24-H25= 96.3125
H24-C11-H25=109.31 H16-H25-H24= 70.5612 H17-H25-H24=115.1094
H19-H24-H25=115.6869 H20-H25-H24=115.2412 H21-H24-H25= 70.5843
H22-H24-H25=115.6822 C1-C3-H26=104.1307 C2-C3-H26=139.3788
C1-C4-H26=136.1136 C2-C4-H26=100.0829 C4-C3-H26= 68.4153
C1-C5-H26=160.7729 C2-C5-H26=149.0182 C3-C5-H26=115.1804
C4-C5-H26=125.3565 C6-C3-H26=121.9123 C6-C4-H26= 98.0003
C7-C4-H26=115.8998 C8-C3-H26= 71.8554 C8-C4-H26= 89.2963
C8-C5-H26=102.546 C3-C9-H26= 67.9754 C4-C9-H26= 71.4778
C9-C5-H26= 76.6805 C6-C9-H26=120.7535 C7-C9-H26=130.3488
C8-C9-H26=104.7649 C10-C3-H26= 89.9996 C10-C4-H26= 66.6992
C10-C5-H26= 97.0933 C10-C9-H26= 99.4117 C11-C4-H26=150.6628
C3-O12-H26= 83.273 C4-O12-H26= 87.2303 C5-O12-H26= 76.2987
C9-H26-O12=108.481 C13-C9-H26=112.8314 N14-C9-H26=113.4768
C3-O15-H26= 99.6372 C4-O15-H26=110.1563 C5-O15-H26= 80.9227
C8-O15-H26=148.2328 C9-O15-H26=167.894 C10-O15-H26=130.7283
O12-H26-O15=107.3564 C13-O15-H26=144.5014 H16-C4-H26=132.7726

```
    H16-C5-H26=163.4691     H17-C3-H26=157.0265     H18-C3-H26= 95.1775
    H18-C5-H26=101.3455    H18-O12-H26= 89.2847    H18-O15-H26= 84.0856
    H19-C4-H26= 96.6972     H19-C5-H26=109.4535    H19-O12-H26= 92.6829
   H19-O15-H26= 98.7122     H22-C4-H26= 92.3054     H22-C9-H26=103.8658
   H22-O15-H26=141.3827     H23-C3-H26= 92.6836     H23-C9-H26=100.5296
   H23-O15-H26=122.0675     H24-C4-H26=161.6586
 Stoichiometry    C12H11NO2
 Framework group  C1[X(C12H11NO2)]
 Deg. of freedom   72
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -2.092005   -0.095578   -0.411596
    2          6             0       -1.665516   -0.101788    1.081026
    3          6             0       -0.522029    0.946295    1.253711
    4          6             0       -0.855324    0.528105   -1.093376
    5          6             0       -0.291591    1.582899   -0.129233
    6          6             0       -0.613872   -1.271651    1.152127
    7          6             0       -0.558723   -1.788522   -0.306968
    8          6             0        0.204982   -0.651572   -1.019991
    9          6             0        1.268084   -0.126874   -0.011422
   10          6             0        0.526370   -0.217785    1.344279
   11          6             0       -2.009134   -1.586112   -0.797633
   12          8             0       -0.182502    2.916729   -0.316721
   13          6             0        2.590573   -0.699316   -0.097910
   14          7             0        3.624290   -1.177255   -0.156849
   15          8             0        1.239843    1.302682   -0.318806
   16          1             0       -3.022977    0.410543   -0.619584
   17          1             0       -2.473403   -0.099744    1.794984
   18          1             0       -0.557121    1.659781    2.058622
   19          1             0       -1.005134    0.904067   -2.092743
   20          1             0       -0.735603   -2.028004    1.910900
   21          1             0       -0.135991   -2.774698   -0.435182
   22          1             0        0.626840   -0.902541   -1.981233
   23          1             0        1.164292   -0.266207    2.211315
   24          1             0       -2.124092   -1.756585   -1.862075
   25          1             0       -2.719805   -2.201237   -0.257221
   26          1             0        1.263359    2.431508   -0.323706
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.0167878      0.7871262      0.5892410
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,O-16,C-
12,N-14,
 O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1
 Standard basis: 3-21+G* (6D, 7F)
 There are   217 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    131072 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
```

```
  217 basis functions      318 primitive gaussians
   53 alpha electrons       53 beta electrons
      nuclear repulsion energy      1060.0790644747 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   217 RedAO= T  NBF=   217
 NBsUse=   217 1.00D-04 NBFU=   217
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -661.256897752     A.U. after   18 cycles
            Convg  =    0.7268D-08             -V/T =  2.0018
            S**2   =   0.0000
 Range of M.O.s used for correlation:     1   217
 NBasis=   217 NAE=    53 NBE=    53 NFC=     0 NFV=     0
 NROrb=    217 NOA=    53 NOB=    53 NVA=   164 NVB=   164

 **** Warning!!: The largest alpha MO coefficient is  0.10281511D+03

          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   2 vectors were produced by pass 12.
   1 vectors were produced by pass 13.
 Inv2:  IOpt= 1 Iter= 1 AM= 7.79D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  39 with in-core refinement.
 G2DrvN: will do   13 atoms at a time, making    2 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  41 IRICut=      41 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
          There are  81 degrees of freedom in the 1st order CPHF.
```

```
 78 vectors were produced by pass  0.
 AX will form  39 AO Fock derivatives at one time.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  1.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  3.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  4.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  5.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  6.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 46 vectors were produced by pass  7.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  3 vectors were produced by pass  8.
 Inv2:  IOpt= 1 Iter= 1 AM= 5.31D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 595 with in-core refinement.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.

 ********************************************************************

           Population analysis using the SCF density.

 ********************************************************************

 Alpha  occ. eigenvalues --  -20.55086 -20.41754 -15.55182 -11.33540 -
11.31239
 Alpha  occ. eigenvalues --  -11.26167 -11.22743 -11.22606 -11.21088 -
11.21022
 Alpha  occ. eigenvalues --  -11.20642 -11.20482 -11.20388 -11.20222 -
11.19542
 Alpha  occ. eigenvalues --   -1.48023  -1.30309  -1.28691  -1.26004  -
1.12490
 Alpha  occ. eigenvalues --   -1.10396  -1.06913  -0.99074  -0.94356  -
0.90875
 Alpha  occ. eigenvalues --   -0.85680  -0.82071  -0.81021  -0.77953  -
0.74530
 Alpha  occ. eigenvalues --   -0.74190  -0.69459  -0.67128  -0.65980  -
0.63362
 Alpha  occ. eigenvalues --   -0.63182  -0.60454  -0.58866  -0.55332  -
0.54762
 Alpha  occ. eigenvalues --   -0.53466  -0.53184  -0.52552  -0.51541  -
0.50661
```

```
 Alpha  occ. eigenvalues --   -0.49448  -0.48431  -0.47486  -0.47106  -
0.46552
 Alpha  occ. eigenvalues --   -0.44369  -0.41556  -0.38217
 Alpha virt. eigenvalues --    0.04928   0.06224   0.06629   0.07097
0.08363
 Alpha virt. eigenvalues --    0.08582   0.08803   0.09327   0.09598
0.11414
 Alpha virt. eigenvalues --    0.11918   0.12126   0.13038   0.13362
0.13451
 Alpha virt. eigenvalues --    0.14166   0.14761   0.15351   0.16544
0.17159
 Alpha virt. eigenvalues --    0.17608   0.18145   0.18429   0.19064
0.19309
 Alpha virt. eigenvalues --    0.19651   0.19846   0.20234   0.21962
0.23376
 Alpha virt. eigenvalues --    0.23714   0.24161   0.24303   0.24622
0.25029
 Alpha virt. eigenvalues --    0.25056   0.25425   0.25649   0.26474
0.26561
 Alpha virt. eigenvalues --    0.27351   0.27677   0.28391   0.28966
0.29184
 Alpha virt. eigenvalues --    0.29480   0.30109   0.30626   0.31626
0.32729
 Alpha virt. eigenvalues --    0.32912   0.34172   0.35430   0.35648
0.36218
 Alpha virt. eigenvalues --    0.36595   0.37344   0.38659   0.39561
0.39868
 Alpha virt. eigenvalues --    0.41830   0.42518   0.43212   0.43986
0.45271
 Alpha virt. eigenvalues --    0.45289   0.45788   0.46962   0.48148
0.48681
 Alpha virt. eigenvalues --    0.49431   0.50190   0.51720   0.51993
0.53187
 Alpha virt. eigenvalues --    0.53679   0.54179   0.55101   0.55520
0.55795
 Alpha virt. eigenvalues --    0.57018   0.57982   0.59069   0.59422
0.60561
 Alpha virt. eigenvalues --    0.61080   0.62484   0.62835   0.65445
0.67853
 Alpha virt. eigenvalues --    0.71627   0.73089   0.99872   1.07926
1.09902
 Alpha virt. eigenvalues --    1.10709   1.11149   1.12100   1.13784
1.14379
 Alpha virt. eigenvalues --    1.15158   1.15714   1.16652   1.17490
1.17832
 Alpha virt. eigenvalues --    1.19439   1.19525   1.20225   1.21045
1.21280
 Alpha virt. eigenvalues --    1.23509   1.24139   1.25933   1.28181
1.29886
 Alpha virt. eigenvalues --    1.30938   1.31589   1.34554   1.36402
1.37881
 Alpha virt. eigenvalues --    1.39032   1.43898   1.45028   1.47208
1.48560
```

```
 Alpha virt. eigenvalues --    1.49568   1.50187   1.50980   1.52599
1.55557
 Alpha virt. eigenvalues --    1.56770   1.56918   1.59115   1.60408
1.66829
 Alpha virt. eigenvalues --    1.69023   1.72810   1.74523   1.76412
1.80687
 Alpha virt. eigenvalues --    1.85947   1.92970   1.98588   2.05377
2.10411
 Alpha virt. eigenvalues --    2.15207   2.23343   2.25798   2.31442
2.36254
 Alpha virt. eigenvalues --    2.39258   2.39738   2.49076   2.53276
2.62534
 Alpha virt. eigenvalues --    2.78897   2.93915   3.15053   3.18680
3.48847
 Alpha virt. eigenvalues --    3.63124   3.79584   3.93564   4.08521
          Condensed to atoms (all electrons):
               1         2         3         4         5         6
  1  C   13.822302  -6.213738   2.205413  -7.093227   0.470716   3.685909
  2  C   -6.213738  19.027183 -11.921231   1.354348   5.561698  -9.734794
  3  C    2.205413 -11.921231  35.309100  12.928828 -30.342271   7.968111
  4  C   -7.093227   1.354348  12.928828  33.004382 -28.952468  -1.859996
  5  C    0.470716   5.561698 -30.342271 -28.952468  63.535009  -1.885365
  6  C    3.685909  -9.734794   7.968111  -1.859996  -1.885365  18.275825
  7  C   -1.333115   2.572037  -0.500294   3.032853  -1.471736  -5.495044
  8  C    4.347578  -1.509713  -9.030028 -19.874223  23.697986   3.938205
  9  C   -1.245440  -2.825574  18.903533  19.290957 -31.988269   1.248690
 10  C   -2.509627   9.247593 -20.314880  -7.608364  22.660347  -9.066289
 11  C   -3.138652   0.652398   0.446546   2.458422  -0.705341  -0.395989
 12  O   -0.006399  -0.192772   1.121218   1.167542  -2.432681   0.047002
 13  C    2.249444  -0.296694  -0.253672  -1.432727 -12.922604  -0.531130
 14  N   -0.073798   0.014178   0.084513   0.178677   0.184976  -0.085350
 15  O   -0.001046   0.000107  -0.737483  -0.728346   1.647546   0.146272
 16  H    0.465750  -0.085844   0.023834  -0.082093   0.014504   0.032396
 17  H   -0.071574   0.535994  -0.143101  -0.005998   0.054993  -0.111087
 18  H    0.017510  -0.082413   0.539721   0.021474  -0.081723   0.032634
 19  H   -0.034155  -0.005238   0.051889   0.580138  -0.167734   0.006039
 20  H    0.006651  -0.121455   0.074493  -0.000372   0.001414   0.580968
 21  H   -0.044733   0.042688  -0.005352   0.076547   0.012110  -0.108915
 22  H    0.024708   0.001722  -0.017084  -0.136373   0.057048   0.009657
 23  H   -0.002066   0.041276  -0.066301  -0.007508   0.039498  -0.064841
 24  H   -0.076743   0.026837   0.004779   0.019383  -0.017965   0.034420
 25  H   -0.029171  -0.004022  -0.010578  -0.023930   0.015836   0.029508
 26  H    0.019446  -0.013823   0.167543   0.148693  -0.467827  -0.002084
               7         8         9        10        11        12
  1  C   -1.333115   4.347578  -1.245440  -2.509627  -3.138652  -0.006399
  2  C    2.572037  -1.509713  -2.825574   9.247593   0.652398  -0.192772
  3  C   -0.500294  -9.030028  18.903533 -20.314880   0.446546   1.121218
  4  C    3.032853 -19.874223  19.290957  -7.608364   2.458422   1.167542
  5  C   -1.471736  23.697986 -31.988269  22.660347  -0.705341  -2.432681
  6  C   -5.495044   3.938205   1.248690  -9.066289  -0.395989   0.047002
  7  C   12.552052  -5.523389   0.178170   2.129955  -1.540201   0.072527
  8  C   -5.523389  34.913180 -23.489166  12.606313  -1.653919  -0.793367
  9  C    0.178170 -23.489166  90.352744 -22.689570   1.473815   1.146936
 10  C    2.129955  12.606313 -22.689570  36.335217   0.465425  -0.678932
```

11	C	-1.540201	-1.653919	1.473815	0.465425	10.824364	0.013392
12	O	0.072527	-0.793367	1.146936	-0.678932	0.013392	9.113750
13	C	0.364406	-11.841246	-47.479430	-14.755925	-1.947834	0.359469
14	N	0.173086	0.155505	2.958816	0.539831	0.056041	-0.001526
15	O	0.082297	1.324158	-2.189465	1.290402	-0.062413	-0.346350
16	H	-0.023903	0.035598	-0.006253	-0.013128	-0.005217	0.000852
17	H	0.004526	0.015336	-0.033055	0.099789	0.022237	0.000070
18	H	0.000777	0.013565	-0.027341	-0.055629	0.001143	-0.001822
19	H	0.016778	-0.137875	0.031664	-0.009107	0.021121	0.004814
20	H	-0.111767	0.030820	0.031671	-0.119756	0.018469	-0.000051
21	H	0.473870	-0.123517	0.087543	0.039443	0.027560	-0.000050
22	H	-0.062435	0.602049	-0.128019	0.075457	0.009896	0.000126
23	H	0.008982	0.083958	-0.063696	0.593019	-0.002315	0.000169
24	H	-0.084659	0.058917	-0.029550	0.005749	0.379073	0.000103
25	H	-0.097388	0.086593	-0.028874	0.007925	0.368211	-0.000034
26	H	-0.002402	-0.160631	0.316629	-0.166819	0.003245	0.231722

		13	14	15	16	17	18
1	C	2.249444	-0.073798	-0.001046	0.465750	-0.071574	0.017510
2	C	-0.296694	0.014178	0.000107	-0.085844	0.535994	-0.082413
3	C	-0.253672	0.084513	-0.737483	0.023834	-0.143101	0.539721
4	C	-1.432727	0.178677	-0.728346	-0.082093	-0.005998	0.021474
5	C	-12.922604	0.184976	1.647546	0.014504	0.054993	-0.081723
6	C	-0.531130	-0.085350	0.146272	0.032396	-0.111087	0.032634
7	C	0.364406	0.173086	0.082297	-0.023903	0.004526	0.000777
8	C	-11.841246	0.155505	1.324158	0.035598	0.015336	0.013565
9	C	-47.479430	2.958816	-2.189465	-0.006253	-0.033055	-0.027341
10	C	-14.755925	0.539831	1.290402	-0.013128	0.099789	-0.055629
11	C	-1.947834	0.056041	-0.062413	-0.005217	0.022237	0.001143
12	O	0.359469	-0.001526	-0.346350	0.000852	0.000070	-0.001822
13	C	98.260186	-4.675115	-1.771844	-0.006428	-0.003807	-0.025048
14	N	-4.675115	8.150748	0.006464	0.000021	0.000005	0.000120
15	O	-1.771844	0.006464	9.724960	-0.000751	0.000066	0.005297
16	H	-0.006428	0.000021	-0.000751	0.372684	-0.000621	-0.000013
17	H	-0.003807	0.000005	0.000066	-0.000621	0.366714	-0.000570
18	H	-0.025048	0.000120	0.005297	-0.000013	-0.000570	0.337955
19	H	-0.009536	-0.000034	0.004357	-0.000595	-0.000015	-0.000009
20	H	-0.029987	-0.000232	-0.000135	-0.000009	-0.000456	-0.000067
21	H	-0.128683	0.002481	-0.000596	-0.000012	-0.000012	0.000000
22	H	-0.087838	-0.000324	0.008018	-0.000016	0.000000	0.000000
23	H	-0.209683	0.001665	0.012330	0.000000	-0.000069	-0.000665
24	H	-0.003310	0.000067	0.000072	-0.000213	-0.000028	0.000000
25	H	0.003709	-0.000018	0.000244	-0.000407	0.000123	0.000000
26	H	0.210930	-0.004324	-0.109153	-0.000002	0.000001	0.000290

		19	20	21	22	23	24
1	C	-0.034155	0.006651	-0.044733	0.024708	-0.002066	-0.076743
2	C	-0.005238	-0.121455	0.042688	0.001722	0.041276	0.026837
3	C	0.051889	0.074493	-0.005352	-0.017084	-0.066301	0.004779
4	C	0.580138	-0.000372	0.076547	-0.136373	-0.007508	0.019383
5	C	-0.167734	0.001414	0.012110	0.057048	0.039498	-0.017965
6	C	0.006039	0.580968	-0.108915	0.009657	-0.064841	0.034420
7	C	0.016778	-0.111767	0.473870	-0.062435	0.008982	-0.084659
8	C	-0.137875	0.030820	-0.123517	0.602049	0.083958	0.058917
9	C	0.031664	0.031671	0.087543	-0.128019	-0.063696	-0.029550
10	C	-0.009107	-0.119756	0.039443	0.075457	0.593019	0.005749

11	C	0.021121	0.018469	0.027560	0.009896	-0.002315	0.379073
12	O	0.004814	-0.000051	-0.000050	0.000126	0.000169	0.000103
13	C	-0.009536	-0.029987	-0.128683	-0.087838	-0.209683	-0.003310
14	N	-0.000034	-0.000232	0.002481	-0.000324	0.001665	0.000067
15	O	0.004357	-0.000135	-0.000596	0.008018	0.012330	0.000072
16	H	-0.000595	-0.000009	-0.000012	-0.000016	0.000000	-0.000213
17	H	-0.000015	-0.000456	-0.000012	0.000000	-0.000069	-0.000028
18	H	-0.000009	-0.000067	0.000000	0.000000	-0.000665	0.000000
19	H	0.344684	0.000000	-0.000018	-0.000558	0.000000	0.000070
20	H	0.000000	0.366518	-0.000209	-0.000018	-0.000297	-0.000028
21	H	-0.000018	-0.000209	0.372831	-0.000258	-0.000027	-0.000244
22	H	-0.000558	-0.000018	-0.000258	0.353628	-0.000016	0.000027
23	H	0.000000	-0.000297	-0.000027	-0.000016	0.350691	0.000000
24	H	0.000070	-0.000028	-0.000244	0.000027	0.000000	0.429813
25	H	-0.000023	0.000060	-0.000449	-0.000025	0.000001	-0.015537
26	H	0.000205	0.000000	0.000000	-0.000055	-0.000080	0.000000

		25	26
1	C	-0.029171	0.019446
2	C	-0.004022	-0.013823
3	C	-0.010578	0.167543
4	C	-0.023930	0.148693
5	C	0.015836	-0.467827
6	C	0.029508	-0.002084
7	C	-0.097388	-0.002402
8	C	0.086593	-0.160631
9	C	-0.028874	0.316629
10	C	0.007925	-0.166819
11	C	0.368211	0.003245
12	O	-0.000034	0.231722
13	C	0.003709	0.210930
14	N	-0.000018	-0.004324
15	O	0.000244	-0.109153
16	H	-0.000407	-0.000002
17	H	0.000123	0.000001
18	H	0.000000	0.000290
19	H	-0.000023	0.000205
20	H	0.000060	0.000000
21	H	-0.000449	0.000000
22	H	-0.000025	-0.000055
23	H	0.000001	-0.000080
24	H	-0.015537	0.000000
25	H	0.429328	0.000000
26	H	0.000000	0.267316

Total atomic charges:

		1
1	C	0.558055
2	C	-0.070747
3	C	-0.487245
4	C	-0.456619
5	C	-0.517698
6	C	-0.694751
7	C	0.584014
8	C	-1.772685
9	C	2.202533

```
10  C   -2.108440
11  C   -1.789475
12  O   -0.825709
13  C    2.964396
14  N   -0.666474
15  O   -0.305006
16  H    0.279866
17  H    0.270540
18  H    0.304814
19  H    0.303136
20  H    0.273773
21  H    0.278001
22  H    0.290683
23  H    0.285973
24  H    0.268966
25  H    0.268916
26  H    0.561181
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  C    0.837922
 2  C    0.199794
 3  C   -0.182431
 4  C   -0.153483
 5  C   -0.517698
 6  C   -0.420978
 7  C    0.862015
 8  C   -1.482003
 9  C    2.202533
10  C   -1.822467
11  C   -1.251593
12  O   -0.825709
13  C    2.964396
14  N   -0.666474
15  O    0.256175
16  H    0.000000
17  H    0.000000
18  H    0.000000
19  H    0.000000
20  H    0.000000
21  H    0.000000
22  H    0.000000
23  H    0.000000
24  H    0.000000
25  H    0.000000
26  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  2162.6291
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=    -3.3419    Y=    -4.5758    Z=     1.2907  Tot=     5.8114
Quadrupole moment (Debye-Ang):
  XX=  -101.5566   YY=  -107.5372   ZZ=   -83.2855
  XY=    10.7413   XZ=     1.0384   YZ=     2.7728
```

```
 Octapole moment (Debye-Ang**2):
  XXX=   -83.8577  YYY=   -55.9204  ZZZ=     0.0133  XYY=     5.6070
  XXY=    34.5448  XXZ=     4.4098  XZZ=    -1.7007  YZZ=     1.7818
  YYZ=     8.7937  XYZ=    -1.7666
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -1749.1412 YYYY= -1236.3411 ZZZZ=  -471.2319 XXXY=   131.0021
 XXXZ=    12.2396 YYYX=    81.5819 YYYZ=    19.2427 ZZZX=     2.5667
 ZZZY=     1.4407 XXYY=  -437.0466 XXZZ=  -316.5426 YYZZ=  -251.8104
 XXYZ=    -8.4711 YYXZ=    -6.9307 ZZXY=     2.0150
 N-N= 1.060079064475D+03 E-N=-3.663972689242D+03  KE= 6.600482073076D+02
  Exact polarizability: 129.634  -5.439 117.219   0.557   0.672  98.557
 Approx polarizability: 116.889  -7.947 109.553  -0.512  -0.358  95.099
 Full mass-weighted force constant matrix:
 Low frequencies ----1746.1312   -1.1392   -0.0017   -0.0004    0.0006
0.6892
 Low frequencies ---    0.9479  132.2759  163.9862
 ******    1 imaginary frequencies (negative Signs) ******
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                      1                      2                      3
                     ?A                     ?A                     ?A
 Frequencies -- -1746.1312               132.2759               163.9862
 Red. masses --     1.0958                 7.8843                 7.9092
 Frc consts  --     1.9684                 0.0813                 0.1253
 IR Inten    --  1025.3312                 6.0832                 4.3685
 Raman Activ --    13.4087                 2.8525                 2.0870
 Depolar     --     0.7452                 0.7254                 0.7499
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00    -0.03   0.09   0.00    -0.06   0.02
0.09
   2   6     0.00   0.00   0.00    -0.05   0.05   0.00     0.08  -0.02
0.05
   3   6     0.00   0.00   0.00     0.02  -0.04   0.02     0.11  -0.04  -
0.04
   4   6     0.00   0.00   0.00     0.04  -0.03   0.02    -0.12   0.02  -
0.02
   5   6    -0.03   0.05   0.00     0.09  -0.06   0.02    -0.02  -0.01  -
0.05
   6   6     0.00   0.00   0.00    -0.14  -0.03   0.01     0.07  -0.03  -
0.07
   7   6     0.00   0.00   0.00    -0.17  -0.04   0.02    -0.06   0.00  -
0.09
   8   6     0.00   0.00   0.00    -0.05  -0.11   0.02    -0.09   0.00  -
0.11
   9   6     0.01  -0.01   0.01    -0.02  -0.16   0.02    -0.01  -0.01  -
0.16
  10   6     0.00   0.00   0.00    -0.05  -0.13   0.02     0.08  -0.03  -
0.13
  11   6     0.00   0.00   0.00    -0.15   0.08   0.00    -0.11   0.03
0.06
  12   8    -0.05  -0.01   0.00     0.13  -0.06  -0.10     0.04   0.01
0.19
```

13	6	0.00	0.00	0.00	0.08	0.08	-0.01	0.02	0.02	0.05
14	7	0.00	0.00	0.00	0.26	0.48	-0.08	0.08	0.10	0.47
15	8	0.01	0.01	-0.01	0.00	-0.13	0.09	-0.01	-0.05	-0.30
16	1	0.00	0.00	0.00	0.03	0.17	-0.02	-0.07	0.03	0.19
17	1	0.00	0.00	0.00	-0.06	0.11	-0.01	0.15	-0.02	0.13
18	1	0.00	0.00	0.00	0.08	-0.05	0.03	0.18	-0.03	-0.04
19	1	0.00	0.00	0.00	0.08	-0.01	0.02	-0.20	0.02	-0.01
20	1	0.00	0.00	0.00	-0.21	-0.02	0.01	0.13	-0.05	-0.07
21	1	0.00	0.00	0.00	-0.26	-0.08	0.03	-0.10	-0.01	-0.15
22	1	0.01	0.00	0.00	-0.07	-0.16	0.02	-0.16	0.03	-0.15
23	1	0.00	0.00	0.00	-0.07	-0.18	0.02	0.14	-0.06	-0.18
24	1	0.00	0.00	0.00	-0.16	0.09	0.00	-0.22	0.05	0.07
25	1	0.00	0.00	0.00	-0.21	0.14	-0.01	-0.06	0.03	0.12
26	1	0.76	-0.65	0.07	0.15	-0.16	-0.23	-0.04	-0.01	0.26

	4	5	6
	?A	?A	?A
Frequencies --	184.4695	344.1383	398.4251
Red. masses --	4.2193	6.1555	2.6133
Frc consts --	0.0846	0.4295	0.2444
IR Inten --	25.8610	4.0365	12.9379
Raman Activ --	1.4394	1.4763	0.3614
Depolar --	0.7396	0.7465	0.5840

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	-0.03	-0.08	-0.06	-0.14	0.05	0.02	-0.01	-0.08
2	6	-0.05	0.04	-0.06	-0.02	-0.11	0.02	-0.01	0.04	-0.08
3	6	-0.04	0.02	-0.08	-0.10	0.02	0.01	-0.01	0.00	-0.04
4	6	0.00	-0.04	-0.07	-0.13	0.06	0.04	0.04	-0.01	-0.08
5	6	-0.01	-0.02	-0.08	0.01	0.13	0.02	0.03	0.01	0.00
6	6	-0.06	0.04	0.06	0.06	-0.04	-0.01	0.00	0.02	-0.04
7	6	0.01	-0.02	0.09	0.10	0.00	-0.04	0.00	-0.01	-0.01
8	6	0.02	-0.04	0.07	-0.07	0.09	-0.03	0.00	-0.01	-0.08

9	6	-0.01	0.01	0.09	-0.10	0.00	-0.02	0.00	-0.01	-0.06
10	6	-0.04	0.05	0.06	-0.05	0.04	-0.01	-0.01	-0.01	-0.05
11	6	0.03	-0.06	0.01	0.09	-0.16	0.01	-0.07	-0.09	0.20
12	8	0.10	0.03	0.28	0.40	0.13	-0.09	0.00	0.04	0.08
13	6	-0.01	0.01	0.01	-0.13	-0.02	-0.01	0.01	0.01	-0.04
14	7	0.01	0.07	-0.16	-0.08	0.10	0.02	0.00	-0.02	0.02
15	8	0.03	-0.06	-0.19	-0.04	-0.07	0.05	0.00	0.05	0.16
16	1	-0.02	-0.07	-0.13	-0.14	-0.27	0.09	0.02	-0.01	-0.12
17	1	-0.07	0.10	-0.09	0.00	-0.18	0.05	-0.03	0.03	-0.11
18	1	-0.09	0.10	-0.14	-0.16	-0.05	0.08	-0.01	-0.02	-0.03
19	1	0.05	-0.12	-0.11	-0.21	0.04	0.04	0.06	0.03	-0.07
20	1	-0.10	0.09	0.09	0.12	-0.07	-0.03	-0.02	0.03	-0.03
21	1	0.03	-0.02	0.15	0.23	0.06	-0.07	0.02	-0.01	0.01
22	1	0.07	-0.08	0.11	-0.08	0.17	-0.05	0.00	-0.06	-0.07
23	1	-0.10	0.09	0.10	-0.01	0.09	-0.03	0.00	-0.01	-0.07
24	1	0.09	-0.13	0.01	0.08	-0.15	0.01	-0.39	-0.43	0.29
25	1	0.01	-0.03	0.01	0.16	-0.23	0.02	0.07	0.10	0.61
26	1	-0.01	-0.01	0.72	0.31	-0.17	-0.17	0.05	0.03	-0.01

	7			8			9		
	?A			?A			?A		
Frequencies --	448.6085			474.7717			490.8366		
Red. masses --	3.2913			8.7270			7.5639		
Frc consts --	0.3903			1.1590			1.0737		
IR Inten --	52.6424			7.3039			25.0147		
Raman Activ --	0.6364			6.8580			3.0687		
Depolar --	0.5502			0.1650			0.4743		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	-0.03	-0.06	-0.20	-0.07	0.05	0.05	0.03	0.02
2 6	-0.03	0.06	-0.02	-0.17	0.00	0.03	0.04	-0.10	0.00
3 6	0.03	0.01	0.02	-0.16	0.05	-0.03	-0.04	-0.05	0.01
4 6	0.03	0.00	0.02	-0.18	0.04	0.06	0.05	-0.08	0.00

```
   5   6     0.04   0.03   0.08    -0.14   0.06   0.01     0.05   0.05  -
0.05
   6   6    -0.06   0.06   0.09    -0.08   0.08  -0.03     0.02  -0.12  -
0.03
   7   6    -0.02  -0.05   0.16    -0.03   0.08  -0.02    -0.09  -0.12  -
0.03
   8   6    -0.04  -0.09   0.00    -0.02   0.07   0.00     0.08  -0.14
0.07
   9   6    -0.02  -0.05  -0.16     0.21  -0.01  -0.02     0.07   0.09
0.08
  10   6     0.03  -0.01  -0.07    -0.06   0.06  -0.03     0.01  -0.05
0.04
  11   6     0.10  -0.04  -0.09    -0.04  -0.06  -0.02    -0.15   0.07
0.00
  12   8     0.00   0.07   0.10     0.04   0.04   0.00     0.15   0.15  -
0.03
  13   6     0.02   0.03  -0.17     0.43  -0.09  -0.02     0.20   0.41
0.05
  14   7     0.01  -0.03   0.08     0.41  -0.22  -0.03    -0.08  -0.18  -
0.02
  15   8    -0.11   0.02   0.04     0.01  -0.01   0.02    -0.28   0.05  -
0.07
  16   1     0.01  -0.08  -0.13    -0.24  -0.15   0.01     0.11   0.16
0.08
  17   1    -0.07   0.13  -0.06    -0.11  -0.02   0.10     0.02  -0.15  -
0.02
  18   1     0.07  -0.04   0.07    -0.15   0.03  -0.01    -0.09  -0.08
0.04
  19   1     0.09   0.04   0.03    -0.22   0.00   0.05     0.07  -0.20  -
0.05
  20   1    -0.06   0.14   0.17    -0.03   0.04  -0.05     0.04  -0.10
0.00
  21   1     0.02  -0.05   0.26     0.03   0.10   0.04    -0.25  -0.18  -
0.09
  22   1    -0.19  -0.23  -0.03    -0.15   0.12  -0.07     0.15  -0.12
0.10
  23   1     0.12   0.00  -0.14    -0.20   0.11   0.08    -0.06  -0.08
0.09
  24   1     0.39   0.05  -0.14    -0.03  -0.02  -0.02    -0.22   0.07
0.01
  25   1    -0.06  -0.08  -0.35     0.04  -0.18  -0.04    -0.18   0.15
0.04
  26   1     0.07  -0.02  -0.42    -0.06   0.00  -0.02     0.18  -0.04  -
0.04
                     10                     11                     12
                     ?A                     ?A                     ?A
 Frequencies --   535.1356               571.9128               603.0171
 Red. masses --     3.1628                 3.7361                 6.5102
 Frc consts  --     0.5336                 0.7200                 1.3948
 IR Inten    --     1.4433                 8.0841                22.1988
 Raman Activ --     1.3351                 1.6156                 8.3763
 Depolar     --     0.7389                 0.5229                 0.1914
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
```

1	6	0.04	0.03	-0.10	-0.08	-0.02	-0.01	-0.01	0.00
0.13									
2	6	-0.06	0.02	-0.06	-0.02	0.12	0.00	-0.06	0.14
0.11									
3	6	-0.01	0.00	0.16	0.16	-0.06	0.00	-0.04	0.13
0.01									
4	6	0.06	0.06	0.10	-0.09	0.04	-0.01	0.01	-0.13
0.02									
5	6	0.01	0.01	0.17	0.05	-0.06	-0.05	0.02	-0.18
0.03									
6	6	-0.05	0.02	-0.06	-0.14	0.01	-0.01	0.01	0.20 -
0.11									
7	6	0.06	0.03	-0.04	0.04	0.09	0.01	0.10	0.09 -
0.13									
8	6	0.03	0.03	0.02	-0.04	0.11	0.02	0.12	-0.07 -
0.20									
9	6	0.00	-0.01	0.00	0.02	0.03	0.04	-0.02	-0.03 -
0.06									
10	6	-0.03	-0.02	0.05	0.02	-0.19	0.07	-0.07	0.12 -
0.08									
11	6	0.04	-0.04	0.06	0.08	-0.09	0.02	0.08	0.05
0.01									
12	8	-0.01	-0.02	-0.02	0.01	-0.07	-0.07	0.06	-0.22
0.11									
13	6	0.01	-0.02	0.03	0.04	0.20	-0.10	0.02	0.14
0.11									
14	7	0.01	0.00	-0.02	-0.06	-0.04	0.05	-0.08	-0.02 -
0.04									
15	8	-0.06	-0.05	-0.22	0.01	-0.01	0.01	-0.15	-0.14
0.08									
16	1	0.04	-0.01	-0.19	-0.14	-0.16	-0.07	0.03	0.01 -
0.02									
17	1	-0.12	-0.05	-0.13	0.03	0.27	0.06	0.01	0.07
0.18									
18	1	-0.07	-0.09	0.24	0.26	-0.03	-0.03	0.09	0.29 -
0.13									
19	1	0.20	0.22	0.14	-0.09	0.06	0.00	-0.15	-0.06
0.07									
20	1	-0.12	0.00	-0.08	-0.31	-0.05	-0.09	0.09	0.13 -
0.18									
21	1	0.09	0.04	-0.01	0.19	0.14	0.06	0.04	0.04
0.06									
22	1	0.03	0.10	0.00	-0.03	0.13	0.02	0.17	-0.01 -
0.19									
23	1	-0.03	-0.14	0.05	-0.01	-0.34	0.08	-0.06	0.06 -
0.09									
24	1	-0.15	-0.26	0.12	0.07	-0.11	0.02	0.00	0.24 -
0.02									
25	1	0.13	0.07	0.32	0.16	-0.16	0.04	0.20	-0.14 -
0.06									
26	1	-0.04	-0.05	-0.53	0.03	0.00	0.41	0.09	-0.22 -
0.21									

	13	14	15
	?A	?A	?A

Frequencies --		610.5575			619.4439			663.2744		
Red. masses --		9.3468			5.6892			4.9516		
Frc consts --		2.0529			1.2862			1.2835		
IR Inten --		63.9170			6.7031			9.0581		
Raman Activ --		1.8937			7.4185			1.1023		
Depolar --		0.6582			0.2667			0.6718		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.05	-0.05	0.00	-0.06	-0.12	0.08	-0.12	-0.01	-0.16
2	6	-0.16	-0.10	0.03	-0.01	0.11	0.05	0.13	0.00	-0.14
3	6	-0.14	0.00	0.09	0.17	0.06	0.01	0.09	-0.02	-0.02
4	6	0.09	-0.08	0.12	-0.01	-0.08	0.09	-0.13	0.11	-0.06
5	6	-0.03	-0.01	0.13	0.09	0.11	0.03	0.01	-0.06	0.07
6	6	-0.03	0.01	0.00	-0.12	0.02	-0.10	0.14	0.06	0.02
7	6	-0.09	-0.07	0.04	-0.05	-0.13	-0.07	-0.08	0.01	0.06
8	6	0.00	-0.05	0.01	0.03	-0.09	-0.04	-0.16	0.03	0.01
9	6	0.06	0.19	-0.12	0.00	-0.01	0.00	0.01	0.02	0.03
10	6	-0.06	0.11	-0.10	-0.05	-0.07	-0.12	0.17	0.09	0.04
11	6	-0.13	-0.05	-0.04	-0.04	-0.18	-0.06	-0.10	-0.07	-0.08
12	8	0.08	-0.19	-0.01	-0.06	0.18	0.02	0.01	-0.13	0.04
13	6	0.01	0.31	-0.16	-0.02	-0.02	0.31	0.05	0.10	0.23
14	7	-0.14	-0.02	0.05	-0.03	0.02	-0.11	-0.03	-0.02	-0.07
15	8	0.47	0.05	-0.05	0.12	0.13	-0.03	0.00	-0.06	0.05
16	1	0.03	0.05	-0.08	-0.05	-0.15	-0.01	-0.19	-0.08	-0.01
17	1	-0.18	-0.19	0.00	0.09	0.21	0.15	0.17	-0.03	-0.09
18	1	-0.18	-0.07	0.15	0.35	-0.01	0.08	-0.04	-0.01	-0.04
19	1	0.13	0.01	0.15	-0.08	-0.13	0.08	0.04	0.28	-0.03
20	1	0.13	0.07	0.08	-0.13	0.06	-0.06	0.09	0.16	0.12
21	1	-0.13	-0.09	0.09	-0.02	-0.14	0.08	-0.02	0.04	-0.01
22	1	-0.11	-0.07	-0.04	0.03	-0.01	-0.07	-0.20	-0.02	0.01
23	1	-0.06	0.14	-0.10	-0.07	-0.22	-0.12	0.23	0.15	0.00

24	1	-0.08	-0.03	-0.04	-0.04	-0.01	-0.09	0.10	-0.17	-0.09
25	1	-0.18	-0.02	-0.07	-0.01	-0.30	-0.15	-0.19	-0.03	-0.15
26	1	0.03	0.01	-0.01	0.01	0.15	-0.27	0.02	-0.10	-0.44

	16	17	18
	?A	?A	?A
Frequencies --	694.3433	744.3176	800.3281
Red. masses --	5.7168	1.9945	5.3959
Frc consts --	1.6239	0.6510	2.0363
IR Inten --	3.6223	98.2289	102.4796
Raman Activ --	6.4080	1.5266	2.1593
Depolar --	0.4071	0.7453	0.6322

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.08	0.08	0.02	-0.04	-0.01	0.05	0.12	0.02	0.06
2	6	-0.10	-0.07	0.07	-0.02	-0.03	0.00	0.17	0.08	-0.07
3	6	-0.05	-0.17	-0.08	-0.02	-0.05	-0.13	0.00	0.15	-0.03
4	6	-0.01	0.14	-0.08	0.00	-0.01	-0.02	-0.09	0.10	-0.06
5	6	-0.06	0.01	-0.03	0.14	-0.04	-0.04	-0.21	0.13	0.02
6	6	-0.05	-0.11	0.13	-0.03	-0.07	0.04	-0.03	-0.07	-0.02
7	6	0.04	0.08	0.17	0.02	0.05	-0.02	0.04	-0.16	-0.07
8	6	-0.02	0.02	-0.10	0.00	0.05	0.04	-0.03	-0.07	-0.02
9	6	-0.01	-0.01	-0.13	0.01	-0.02	0.03	-0.06	-0.10	0.04
10	6	-0.10	-0.11	-0.20	-0.05	0.02	0.07	-0.08	-0.03	0.09
11	6	0.18	0.13	0.12	0.00	0.01	0.01	0.10	0.03	0.04
12	8	0.01	-0.01	-0.01	-0.02	0.00	0.08	-0.07	0.07	0.04
13	6	0.05	0.09	0.28	-0.01	0.01	-0.04	0.07	0.15	-0.07
14	7	-0.02	-0.03	-0.09	-0.01	0.00	0.01	-0.02	-0.04	0.02
15	8	0.05	-0.02	-0.03	0.04	0.04	-0.03	0.15	-0.22	0.03
16	1	0.02	-0.01	0.04	-0.04	-0.01	0.07	0.02	-0.12	0.20
17	1	-0.19	0.07	-0.04	0.02	0.09	0.06	0.15	0.11	-0.10
18	1	0.12	-0.28	0.02	-0.06	0.04	-0.21	-0.09	0.16	-0.04
19	1	-0.09	0.19	-0.05	-0.06	-0.08	-0.04	-0.17	0.04	-0.07

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  20   1     0.12  -0.15   0.12    -0.04  -0.14  -0.04    -0.27  -0.01
0.01
  21   1     0.03   0.08   0.12     0.04   0.07  -0.09    -0.02  -0.18  -
0.14
  22   1    -0.20  -0.21  -0.12     0.05   0.05   0.06     0.00   0.02  -
0.04
  23   1    -0.04   0.05  -0.24    -0.10   0.16   0.12    -0.14   0.01
0.14
  24   1     0.26   0.04   0.13    -0.04   0.04   0.01     0.02   0.14
0.04
  25   1     0.11   0.20   0.11     0.06  -0.04   0.02     0.04   0.09
0.02
  26   1    -0.03  -0.02  -0.08     0.10   0.00  -0.85    -0.29  -0.10  -
0.41
                     19                    20                    21
                     ?A                    ?A                    ?A
 Frequencies --   803.8146              825.3193              839.1783
 Red. masses --     4.0219                4.7479                3.1342
 Frc consts  --     1.5311                1.9054                1.3004
 IR Inten    --    31.1082               15.0037                9.2860
 Raman Activ --     7.5779               12.7648                1.1002
 Depolar     --     0.0465                0.0359                0.7351
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.11  -0.02   0.04    -0.01   0.06   0.04     0.11  -0.06  -
0.06
   2   6     0.01  -0.04   0.04     0.02   0.02  -0.16    -0.02   0.06
0.14
   3   6    -0.06   0.10   0.07     0.00   0.02  -0.20     0.07   0.04  -
0.08
   4   6     0.04   0.11  -0.01     0.00   0.07   0.30     0.10   0.04
0.04
   5   6     0.25  -0.06  -0.02     0.13  -0.04   0.02    -0.09   0.02
0.02
   6   6    -0.01  -0.03   0.09     0.04  -0.03  -0.12    -0.01  -0.10
0.16
   7   6    -0.03  -0.06  -0.03     0.05  -0.15   0.00    -0.05   0.00  -
0.09
   8   6    -0.14   0.00  -0.22    -0.10   0.01   0.18     0.01   0.13
0.04
   9   6    -0.06  -0.08  -0.03     0.00  -0.04   0.01    -0.01  -0.01
0.01
  10   6    -0.09   0.06   0.15    -0.09   0.06  -0.18    -0.02   0.05  -
0.08
  11   6     0.00  -0.09  -0.02     0.09   0.04   0.05    -0.08  -0.10  -
0.10
  12   8    -0.06  -0.01  -0.03    -0.03  -0.06  -0.02     0.01  -0.03
0.00
  13   6     0.06   0.04   0.02     0.01   0.02  -0.01     0.01   0.02  -
0.01
  14   7     0.04  -0.04  -0.01     0.00  -0.01   0.00     0.00  -0.01
0.00
  15   8     0.00   0.06  -0.04    -0.05   0.00   0.02    -0.05  -0.07
0.01
```

16	1	0.09	-0.03	0.12	-0.04	-0.03	0.00	0.18	0.05	-0.10
17	1	-0.08	-0.08	-0.06	0.11	0.03	-0.06	-0.11	0.38	0.05
18	1	-0.23	0.22	-0.04	0.00	-0.05	-0.15	0.34	0.04	-0.06
19	1	-0.10	0.38	0.11	0.16	0.04	0.27	0.17	0.08	0.04
20	1	-0.01	-0.05	0.08	0.07	0.14	0.05	0.23	-0.16	0.14
21	1	0.06	-0.02	-0.06	0.03	-0.14	-0.12	0.09	0.08	-0.20
22	1	-0.18	-0.05	-0.23	-0.31	0.25	0.04	0.03	0.24	0.02
23	1	-0.01	0.06	0.09	-0.22	0.18	-0.08	-0.03	0.34	-0.06
24	1	0.04	-0.04	-0.03	0.03	0.01	0.06	-0.23	-0.19	-0.07
25	1	-0.09	-0.04	-0.08	0.05	0.11	0.08	-0.05	0.00	0.07
26	1	0.10	0.11	0.52	0.04	0.03	0.42	-0.09	-0.06	0.03

	22			23			24		
	?A			?A			?A		
Frequencies --	876.3470			883.1277			912.5566		
Red. masses --	4.2355			3.5977			2.6968		
Frc consts --	1.9165			1.6532			1.3232		
IR Inten --	10.2978			0.2380			7.2939		
Raman Activ --	4.5091			14.4764			0.4972		
Depolar --	0.2494			0.0157			0.7291		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.20	-0.05	0.10	0.13	-0.04	0.08	-0.04	-0.04	0.05
2	6	0.14	0.06	-0.11	0.13	-0.14	-0.03	-0.01	0.03	-0.11
3	6	-0.02	-0.03	0.00	-0.05	0.02	-0.06	-0.05	-0.12	-0.06
4	6	-0.06	-0.03	-0.01	0.12	-0.04	0.04	0.00	-0.05	0.11
5	6	-0.09	-0.03	0.03	-0.01	0.02	-0.03	0.02	0.02	0.05
6	6	-0.17	-0.02	0.02	-0.07	0.14	-0.08	-0.06	0.04	0.12
7	6	0.00	-0.11	0.02	-0.05	0.22	0.08	0.04	0.05	-0.05
8	6	0.00	0.10	-0.03	-0.07	0.08	0.06	0.09	-0.01	-0.08
9	6	0.04	0.19	-0.05	-0.02	-0.07	-0.01	-0.01	-0.09	-0.05
10	6	-0.01	-0.01	0.00	-0.01	-0.06	-0.06	0.14	0.04	0.04
11	6	-0.04	-0.01	0.01	-0.07	-0.09	-0.04	-0.04	0.04	-0.01

12	8	0.10	-0.16	0.02	-0.03	0.05	0.01	-0.03	0.07	-0.03
13	6	-0.02	-0.09	0.03	0.02	0.04	0.02	0.00	0.03	0.03
14	7	0.04	0.01	-0.01	-0.01	-0.01	-0.01	-0.03	0.00	-0.01
15	8	-0.06	0.14	-0.01	0.01	-0.08	0.00	0.02	-0.06	0.00
16	1	0.21	0.03	0.26	0.24	0.23	0.28	0.00	0.01	0.02
17	1	0.02	0.18	-0.25	0.12	-0.32	-0.04	0.03	0.29	-0.08
18	1	-0.18	-0.07	0.02	-0.13	0.00	-0.05	-0.36	-0.32	0.09
19	1	-0.28	-0.03	0.03	0.07	-0.13	0.02	-0.07	-0.03	0.13
20	1	-0.46	0.14	0.13	-0.15	0.09	-0.16	-0.30	0.03	0.07
21	1	0.08	-0.08	0.06	0.25	0.32	0.28	0.00	0.02	0.00
22	1	0.00	0.17	-0.05	-0.18	-0.06	0.05	0.08	0.11	-0.12
23	1	0.00	-0.02	-0.01	-0.07	-0.19	-0.03	0.35	0.37	-0.09
24	1	-0.09	0.19	-0.02	0.00	-0.09	-0.04	-0.16	0.12	-0.01
25	1	-0.15	0.06	-0.07	-0.05	-0.12	-0.04	0.06	-0.04	0.03
26	1	0.10	0.01	-0.15	-0.07	-0.03	-0.03	-0.05	0.00	0.24

	25	26	27
	?A	?A	?A
Frequencies --	925.6229	957.9829	982.7641
Red. masses --	2.8257	2.1281	2.2284
Frc consts --	1.4264	1.1507	1.2681
IR Inten --	10.0214	4.3779	7.0740
Raman Activ --	1.8475	2.7024	3.9333
Depolar --	0.6045	0.7375	0.0809

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.06	-0.03	0.06	-0.09	0.05	0.01	0.03	-0.02	0.03
2	6	0.05	-0.06	0.02	0.12	0.06	0.05	0.01	0.11	-0.08
3	6	0.01	-0.04	-0.08	-0.06	0.01	-0.02	0.03	-0.12	0.02
4	6	0.01	0.22	-0.05	0.10	0.01	-0.02	0.02	-0.07	-0.04
5	6	0.02	0.00	0.05	-0.04	0.01	0.05	0.00	0.02	0.07
6	6	-0.03	0.07	-0.01	-0.06	-0.13	-0.05	0.12	-0.01	-0.04
7	6	-0.04	-0.04	0.06	-0.03	0.07	-0.01	-0.01	0.06	0.03

8	6	0.21	-0.03	-0.05	-0.03	-0.09	0.02	-0.05	0.02	-0.05
9	6	0.04	0.00	0.07	0.01	0.04	-0.05	-0.01	0.01	0.07
10	6	-0.05	0.00	-0.05	0.00	0.04	0.02	-0.13	0.03	0.00
11	6	-0.06	-0.06	0.00	0.05	-0.05	0.01	-0.05	-0.03	0.08
12	8	-0.01	-0.02	-0.02	0.02	-0.03	-0.01	0.00	0.02	-0.02
13	6	-0.03	-0.02	-0.06	-0.01	-0.02	0.01	0.01	0.00	-0.04
14	7	-0.02	0.02	0.02	0.01	0.00	0.00	0.02	-0.01	0.01
15	8	-0.03	-0.02	-0.02	-0.02	0.03	0.00	0.00	-0.02	-0.01
16	1	-0.14	-0.09	0.27	-0.09	0.05	0.05	0.07	0.04	0.00
17	1	0.15	-0.05	0.13	0.30	0.20	0.25	-0.02	0.33	-0.12
18	1	0.04	-0.12	-0.01	-0.25	-0.03	0.01	0.04	-0.38	0.25
19	1	0.06	0.51	0.05	0.34	0.12	-0.02	-0.04	-0.01	-0.01
20	1	0.01	0.15	0.07	-0.22	-0.29	-0.24	0.33	-0.07	-0.07
21	1	-0.14	-0.12	0.29	-0.04	0.07	-0.08	0.04	0.09	-0.02
22	1	0.43	-0.04	0.04	-0.14	-0.32	0.03	0.03	-0.05	0.00
23	1	-0.21	0.05	0.06	0.05	0.22	0.00	-0.32	0.12	0.14
24	1	-0.01	-0.02	-0.01	0.10	-0.07	0.01	0.26	0.26	-0.01
25	1	-0.08	-0.08	-0.06	0.18	-0.21	-0.01	-0.17	-0.20	-0.28
26	1	-0.01	0.00	0.03	0.01	0.01	0.14	-0.02	0.00	0.04

	28	29	30
	?A	?A	?A
Frequencies --	994.7261	997.5654	1010.9207
Red. masses --	2.7742	2.2117	5.7400
Frc consts --	1.6173	1.2968	3.4562
IR Inten --	2.8023	1.7894	1.7811
Raman Activ --	8.3195	7.2309	0.3323
Depolar --	0.0485	0.5044	0.6311

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.06	0.22	0.03	0.05	-0.02	-0.03	-0.12	-0.14	-0.13
2	6	-0.02	0.01	0.00	0.02	-0.10	-0.01	0.13	-0.07	-0.12
3	6	0.02	-0.03	0.03	0.15	-0.06	0.03	0.12	0.22	-0.06

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   4   6    -0.03   0.00  -0.02    -0.08  -0.02   0.00    -0.04  -0.11
0.14
   5   6    -0.01   0.00  -0.02     0.00   0.00   0.02    -0.03   0.01
0.09
   6   6     0.00  -0.04   0.01    -0.09   0.02  -0.02     0.07  -0.13
0.12
   7   6     0.24  -0.07   0.05    -0.01   0.06  -0.02     0.11   0.14
0.13
   8   6     0.01  -0.03   0.00    -0.02  -0.09   0.00     0.14   0.01  -
0.10
   9   6    -0.01   0.01  -0.04    -0.01   0.00   0.02     0.02   0.02  -
0.13
  10   6    -0.05   0.02   0.01    -0.06   0.16   0.02    -0.21  -0.12
0.07
  11   6    -0.12  -0.09  -0.09     0.05   0.04  -0.05    -0.13   0.15  -
0.01
  12   8    -0.01   0.01   0.00     0.01   0.00  -0.01     0.02  -0.01  -
0.01
  13   6     0.00   0.00   0.01     0.01   0.00  -0.02    -0.01  -0.01
0.02
  14   7     0.00   0.00   0.00     0.01   0.00   0.01    -0.01   0.01  -
0.01
  15   8     0.00  -0.02   0.01     0.00   0.02   0.02    -0.01   0.03  -
0.01
  16   1     0.07   0.55   0.17     0.03  -0.03   0.05    -0.11  -0.11  -
0.08
  17   1     0.00  -0.06   0.02    -0.04  -0.23  -0.07     0.21   0.00  -
0.02
  18   1     0.11  -0.03   0.03     0.45  -0.16   0.13     0.08   0.31  -
0.14
  19   1    -0.02  -0.06  -0.04    -0.19  -0.04   0.01     0.04   0.07
0.20
  20   1    -0.07   0.00   0.04    -0.21  -0.06  -0.12     0.02  -0.24
0.00
  21   1     0.59   0.05   0.19    -0.05   0.04   0.07     0.02   0.11
0.07
  22   1    -0.05  -0.04  -0.03    -0.04  -0.22   0.03    -0.06  -0.09  -
0.17
  23   1    -0.02   0.10   0.00    -0.12   0.52   0.08    -0.26  -0.19
0.10
  24   1    -0.17  -0.12  -0.08    -0.14  -0.15   0.01    -0.05   0.03
0.00
  25   1    -0.10  -0.09  -0.04     0.15   0.14   0.20    -0.17   0.22
0.01
  26   1    -0.02  -0.01   0.00     0.01   0.01   0.08     0.01   0.00
0.13
                      31                     32                     33
                      ?A                     ?A                     ?A
 Frequencies --  1034.1343              1042.4705              1056.3764
 Red. masses --     2.1246                 1.8752                 2.0908
 Frc consts  --     1.3387                 1.2007                 1.3746
 IR Inten    --     1.8405                 1.5321                 2.9809
 Raman Activ --     2.1060                 6.6059                 9.1208
 Depolar     --     0.6682                 0.7339                 0.5274
```

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.09	0.04	-0.05	-0.06	0.03	-0.03	-0.05	0.06	-0.07
2	6	-0.03	0.03	0.07	-0.02	-0.06	0.02	0.14	0.00	0.07
3	6	-0.03	-0.05	-0.10	0.05	-0.01	-0.02	-0.04	-0.08	0.02
4	6	-0.06	0.01	0.12	0.09	-0.05	0.01	-0.02	-0.08	0.00
5	6	-0.05	0.00	-0.01	-0.04	0.00	-0.01	0.01	0.00	0.00
6	6	0.04	0.01	-0.08	-0.05	-0.01	-0.04	0.01	0.09	0.07
7	6	-0.04	0.00	0.06	-0.01	-0.08	0.04	-0.03	-0.03	-0.02
8	6	-0.01	-0.06	-0.09	-0.01	0.11	-0.09	-0.01	0.05	-0.03
9	6	0.07	0.03	0.03	-0.01	0.00	0.00	-0.06	-0.04	0.01
10	6	0.06	-0.02	0.09	0.02	0.04	0.04	-0.10	-0.01	-0.02
11	6	0.01	-0.03	-0.04	0.00	0.00	0.12	0.07	0.02	-0.07
12	8	0.01	0.02	0.00	0.01	0.02	0.00	0.01	0.00	0.00
13	6	-0.03	-0.01	0.00	0.00	0.00	0.01	0.02	0.01	-0.01
14	7	-0.02	0.02	0.00	0.00	0.00	0.00	0.02	-0.01	0.00
15	8	0.01	0.00	0.00	-0.01	-0.03	0.00	0.01	0.03	-0.01
16	1	0.19	0.14	-0.24	0.01	0.07	-0.23	0.00	0.14	-0.07
17	1	0.06	0.21	0.17	0.10	-0.32	0.16	0.37	0.06	0.33
18	1	-0.11	0.04	-0.19	0.22	0.06	-0.07	-0.20	-0.23	0.13
19	1	-0.33	0.05	0.18	0.18	-0.02	0.01	0.00	-0.19	-0.04
20	1	0.13	-0.21	-0.29	-0.35	0.02	-0.06	0.06	0.29	0.27
21	1	-0.08	-0.05	0.33	-0.07	-0.10	0.03	-0.15	-0.09	-0.02
22	1	-0.09	0.02	-0.15	0.02	0.39	-0.15	0.04	0.27	-0.07
23	1	-0.10	-0.03	0.21	0.03	0.25	0.05	-0.17	-0.11	0.02
24	1	0.10	-0.29	-0.01	0.36	0.13	0.05	-0.02	-0.31	0.00
25	1	-0.13	0.22	0.06	-0.21	-0.06	-0.23	0.15	0.12	0.17
26	1	-0.01	-0.01	-0.06	-0.04	-0.03	-0.03	0.02	0.02	-0.03

	34			35			36		
	?A			?A			?A		
Frequencies --	1064.5738			1083.6626			1126.4565		
Red. masses --	1.8026			2.4612			7.1241		
Frc consts --	1.2037			1.7029			5.3261		
IR Inten --	1.8494			3.4969			40.7417		
Raman Activ --	5.6199			0.8605			5.5279		
Depolar --	0.7268			0.6710			0.7252		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.01	-0.11	-0.02	-0.03	0.03	0.06	-0.03	-0.02	0.02
2 6	0.01	0.02	0.09	-0.06	-0.05	-0.05	0.02	0.00	0.00
3 6	-0.02	-0.06	-0.02	0.06	-0.04	-0.09	0.02	-0.04	0.10
4 6	0.06	0.03	-0.04	0.10	0.01	0.03	0.01	-0.03	-0.04
5 6	-0.01	0.00	0.01	-0.11	0.01	0.01	0.21	-0.06	-0.05
6 6	-0.02	0.07	-0.04	0.04	0.11	0.09	-0.06	-0.06	0.00
7 6	0.11	-0.06	0.00	0.00	0.00	-0.10	-0.05	-0.04	0.04
8 6	-0.09	-0.02	0.01	-0.08	-0.08	-0.06	0.00	0.09	0.00
9 6	0.00	0.01	0.00	0.08	0.07	0.00	0.23	0.40	-0.13
10 6	0.00	0.01	0.02	-0.01	-0.07	0.10	-0.06	0.09	-0.02
11 6	-0.05	0.09	-0.02	0.04	-0.02	-0.01	0.04	0.02	-0.06
12 8	0.00	0.01	-0.01	0.03	0.01	0.00	-0.11	0.15	0.00
13 6	0.00	0.00	0.00	-0.02	-0.02	0.01	-0.05	-0.07	0.02
14 7	0.00	0.00	0.00	-0.02	0.02	0.00	-0.01	0.03	-0.01
15 8	0.00	0.00	0.00	-0.01	0.02	0.00	-0.03	-0.34	0.06
16 1	-0.12	-0.43	-0.20	0.01	0.14	0.16	-0.09	-0.12	0.06
17 1	0.16	0.05	0.26	-0.10	-0.07	-0.10	0.07	0.11	0.06
18 1	-0.04	-0.08	-0.01	0.18	0.04	-0.16	-0.29	0.02	0.04
19 1	0.22	0.08	-0.04	0.24	0.12	0.05	-0.12	-0.05	-0.03
20 1	-0.04	0.07	-0.04	0.03	0.30	0.28	0.00	0.12	0.20
21 1	0.41	0.05	0.14	-0.09	-0.02	-0.27	-0.18	-0.08	-0.11
22 1	-0.17	-0.09	0.00	-0.29	-0.18	-0.13	-0.21	-0.02	-0.07

```
  23   1    -0.07  -0.02   0.07    -0.24  -0.15   0.27    -0.16  -0.17
0.05
  24   1    -0.31   0.28  -0.02    -0.09   0.05   0.00    -0.11  -0.17  -
0.01
  25   1    -0.18   0.28   0.03     0.26  -0.22   0.05     0.10   0.12
0.15
  26   1     0.00   0.00   0.01    -0.03  -0.02  -0.04    -0.03  -0.21
0.06
                     37                    38                    39
                     ?A                    ?A                    ?A
 Frequencies --  1160.9361             1181.5624             1216.8079
 Red. masses --     2.0427                2.2095                2.5872
 Frc consts  --     1.6221                1.8174                2.2569
 IR Inten    --     6.2682                6.4947               29.5190
 Raman Activ --     2.7612                2.1387                6.5335
 Depolar     --     0.6898                0.5233                0.0874
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01   0.02  -0.06    -0.07   0.00   0.04     0.01   0.01  -
0.04
   2   6     0.02  -0.02   0.03     0.00  -0.03  -0.03     0.07   0.05
0.04
   3   6    -0.06   0.07  -0.04    -0.02   0.08  -0.01    -0.10   0.04
0.06
   4   6    -0.04  -0.06   0.00     0.05  -0.09  -0.04    -0.06   0.02  -
0.01
   5   6     0.04  -0.01   0.08     0.00   0.00   0.05     0.02  -0.02  -
0.05
   6   6    -0.04  -0.03   0.05    -0.05  -0.04   0.00    -0.01  -0.01
0.01
   7   6     0.04   0.03  -0.03     0.01  -0.03   0.06     0.00   0.01  -
0.01
   8   6    -0.05  -0.03  -0.05    -0.09   0.02  -0.11     0.04   0.01
0.00
   9   6     0.05   0.05   0.16     0.01   0.02   0.16     0.26  -0.15  -
0.01
  10   6     0.06  -0.04  -0.12     0.08  -0.01  -0.08     0.03  -0.02  -
0.03
  11   6    -0.01   0.00   0.05     0.06   0.06  -0.06    -0.02  -0.01
0.02
  12   8    -0.01   0.02  -0.01     0.00   0.00   0.00    -0.01   0.00
0.01
  13   6    -0.01  -0.01  -0.03     0.00   0.00  -0.03    -0.05   0.01
0.01
  14   7     0.00   0.01   0.01     0.00   0.00   0.01    -0.09   0.04
0.00
  15   8     0.00  -0.01  -0.01    -0.01   0.00  -0.01    -0.01   0.03  -
0.01
  16   1     0.13   0.15  -0.30    -0.17  -0.01   0.44    -0.09  -0.11
0.11
  17   1     0.13  -0.16   0.15    -0.17   0.21  -0.22    -0.11  -0.14  -
0.16
  18   1     0.05   0.00   0.02     0.06  -0.04   0.10     0.18  -0.16
0.26
```

19	1	-0.34	0.25	0.15	0.26	0.04	-0.02	0.14	-0.22	-0.13
20	1	-0.19	0.17	0.22	0.20	-0.20	-0.11	-0.08	0.03	0.04
21	1	0.22	0.14	-0.34	0.02	-0.07	0.43	0.02	0.03	-0.10
22	1	0.14	-0.37	0.12	0.01	0.24	-0.12	-0.40	0.13	-0.23
23	1	-0.02	0.05	-0.06	0.00	0.03	-0.01	-0.37	0.27	0.28
24	1	0.11	0.09	0.02	-0.14	-0.13	-0.01	0.06	0.01	0.00
25	1	-0.06	-0.05	-0.08	0.14	0.16	0.17	-0.09	0.00	-0.07
26	1	0.02	-0.01	-0.01	-0.01	0.00	-0.05	0.01	0.05	0.01

	40	41	42
	?A	?A	?A
Frequencies --	1234.1843	1250.1693	1262.5332
Red. masses --	2.2030	3.9469	2.1141
Frc consts --	1.9771	3.6345	1.9855
IR Inten --	7.0833	39.4466	90.5494
Raman Activ --	0.3534	3.0529	5.0586
Depolar --	0.4862	0.6088	0.7495

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	0.03	-0.11	0.04	0.01	0.00	0.00	0.04	-0.01
2	6	0.07	-0.10	0.07	-0.07	-0.03	0.04	-0.02	-0.08	-0.01
3	6	0.03	-0.03	0.00	-0.02	0.06	-0.12	0.03	0.10	-0.04
4	6	-0.10	-0.01	0.02	-0.08	-0.09	-0.19	0.01	0.07	0.00
5	6	0.01	-0.06	0.02	0.06	-0.01	0.32	0.07	0.16	-0.02
6	6	-0.12	0.06	0.04	0.02	0.06	-0.04	-0.01	0.04	0.07
7	6	0.04	0.01	-0.10	-0.01	-0.08	-0.01	0.00	0.01	-0.06
8	6	0.00	-0.08	0.04	-0.03	0.10	0.11	-0.02	-0.06	0.00
9	6	0.01	0.02	-0.01	0.03	-0.05	-0.16	0.00	0.07	0.01
10	6	-0.01	0.06	-0.02	0.04	-0.08	0.06	0.01	-0.06	0.01
11	6	-0.02	-0.01	0.11	0.03	0.02	-0.01	0.00	-0.02	0.04
12	8	0.00	0.04	-0.01	-0.01	0.03	-0.05	-0.02	-0.11	0.02
13	6	0.00	0.00	0.00	0.00	0.01	0.04	0.00	-0.01	0.00
14	7	0.00	0.00	0.00	-0.02	0.01	-0.01	0.01	0.00	0.00

15	8	0.02	0.00	0.01	0.00	0.00	-0.02	-0.03	-0.03	0.01
16	1	0.02	0.12	0.14	0.15	0.24	0.11	0.03	-0.04	-0.31
17	1	-0.18	0.32	-0.22	0.02	0.03	0.14	0.09	0.02	0.11
18	1	-0.20	0.17	-0.20	0.06	0.08	-0.14	-0.11	-0.37	0.37
19	1	0.31	0.09	-0.01	-0.10	-0.01	-0.16	-0.11	-0.43	-0.17
20	1	0.34	-0.16	-0.11	0.04	-0.06	-0.16	0.09	-0.21	-0.16
21	1	0.06	-0.01	0.07	-0.13	-0.14	0.13	-0.01	-0.04	0.27
22	1	-0.01	0.26	-0.06	0.20	0.03	0.23	-0.03	0.16	-0.07
23	1	0.00	-0.26	-0.05	-0.24	0.31	0.29	0.00	0.07	0.02
24	1	0.20	0.22	0.04	-0.09	0.05	0.00	-0.08	0.22	0.00
25	1	-0.09	-0.16	-0.17	0.17	-0.09	0.05	0.02	-0.14	-0.06
26	1	0.04	-0.03	0.02	0.04	0.01	0.30	-0.06	0.07	0.01

	43			44			45		
	?A			?A			?A		
Frequencies --	1267.3852			1269.2438			1300.8679		
Red. masses --	1.6353			1.3781			1.6606		
Frc consts --	1.5476			1.3081			1.6557		
IR Inten --	1.7517			7.7813			1.4101		
Raman Activ --	5.3384			11.2785			0.6981		
Depolar --	0.6119			0.7003			0.5958		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.02	0.01	-0.03	-0.01	0.01	0.01	-0.01	0.13	0.04
2 6	0.06	0.07	0.02	0.01	-0.02	-0.03	0.02	0.00	-0.03
3 6	-0.09	-0.03	0.01	0.05	-0.01	0.03	0.02	-0.01	0.00
4 6	-0.04	-0.01	0.02	0.01	0.00	-0.02	0.00	-0.04	0.02
5 6	0.02	-0.06	-0.03	-0.03	-0.01	0.00	-0.02	-0.02	0.03
6 6	0.07	0.01	0.04	-0.04	-0.07	-0.02	0.00	-0.01	0.03
7 6	0.00	0.02	-0.01	-0.03	-0.01	0.05	-0.13	0.01	-0.06
8 6	-0.02	-0.04	0.02	0.01	0.05	-0.01	0.03	0.00	-0.02
9 6	-0.05	0.08	0.01	0.04	-0.08	0.01	0.01	0.01	-0.03
10 6	-0.03	-0.09	-0.01	0.01	0.07	-0.01	-0.01	-0.03	0.00

11	6	-0.01	-0.01	-0.01	0.02	0.00	0.00	0.07	-0.07	0.01
12	8	0.00	0.04	0.00	0.01	0.01	0.00	0.00	0.02	-0.01
13	6	0.01	-0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00
14	7	0.02	-0.01	0.00	-0.02	0.01	0.00	0.00	0.00	0.00
15	8	0.02	-0.01	0.00	0.00	0.01	0.00	0.00	0.01	0.00
16	1	0.03	-0.03	-0.15	0.12	0.09	-0.40	-0.27	-0.41	-0.11
17	1	-0.07	-0.31	-0.14	0.08	-0.04	0.04	-0.01	-0.15	-0.08
18	1	0.28	0.07	-0.06	-0.19	0.09	-0.07	-0.10	0.14	-0.14
19	1	0.14	0.20	0.07	-0.15	0.08	0.03	0.02	-0.11	0.00
20	1	-0.15	-0.08	-0.09	0.25	0.04	0.14	0.17	0.00	0.07
21	1	-0.17	-0.09	0.35	0.00	-0.03	0.25	0.48	0.24	0.18
22	1	0.01	0.22	-0.03	-0.12	-0.06	-0.04	0.19	-0.06	0.07
23	1	0.05	0.33	-0.05	-0.07	-0.18	0.03	-0.04	0.16	0.04
24	1	-0.27	0.27	-0.03	-0.37	0.37	-0.02	-0.10	0.11	-0.01
25	1	0.24	-0.28	0.01	0.33	-0.32	0.05	-0.25	0.29	-0.01
26	1	0.05	-0.04	-0.05	-0.02	0.00	0.00	0.01	-0.02	0.02

	46			47			48		
	?A			?A			?A		
Frequencies --	1327.6566			1358.4909			1363.0636		
Red. masses --	1.5893			1.6516			1.4935		
Frc consts --	1.6505			1.7958			1.6349		
IR Inten --	5.4758			9.7182			8.4440		
Raman Activ --	2.5157			1.4563			1.8136		
Depolar --	0.7007			0.5329			0.6010		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.05	-0.01	-0.01	-0.03	0.01	-0.05	-0.03	-0.04	-0.04
2	6	0.03	-0.02	0.01	0.07	-0.02	0.03	0.04	0.04	0.02
3	6	-0.01	0.06	0.00	-0.12	-0.04	-0.03	0.01	-0.02	0.02
4	6	0.02	-0.05	0.03	0.03	0.02	0.05	0.03	0.03	0.03
5	6	-0.01	-0.01	-0.13	0.04	0.06	0.03	0.01	0.04	0.00
6	6	-0.03	0.04	-0.01	-0.01	-0.04	-0.03	-0.10	0.02	-0.06

7	6	-0.03	-0.06	-0.02	-0.02	0.00	0.02	0.02	-0.03	0.00
8	6	-0.01	0.05	0.03	0.01	0.01	-0.04	0.03	0.04	-0.02
9	6	-0.01	-0.01	-0.08	-0.06	0.02	-0.04	-0.04	0.02	0.02
10	6	0.03	-0.02	0.04	0.07	0.07	0.04	0.01	-0.09	0.03
11	6	0.03	0.02	0.02	0.00	0.01	0.01	-0.02	0.03	0.02
12	8	0.00	0.00	0.02	-0.01	-0.02	0.00	0.00	-0.02	0.00
13	6	0.00	0.00	0.02	0.01	0.00	0.01	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.01	-0.01	0.00	0.01	0.00	0.00
15	8	0.00	0.00	0.01	0.00	-0.02	0.00	0.00	-0.01	0.00
16	1	0.05	0.17	-0.01	-0.10	-0.08	0.03	0.00	0.08	0.12
17	1	-0.09	0.11	-0.12	-0.13	0.21	-0.20	-0.05	-0.14	-0.08
18	1	0.07	-0.34	0.35	0.61	0.05	-0.07	-0.10	0.17	-0.15
19	1	-0.09	0.53	0.26	-0.13	-0.30	-0.04	-0.10	-0.23	-0.04
20	1	0.20	-0.09	-0.11	-0.04	0.14	0.15	0.58	0.13	0.15
21	1	0.16	0.02	0.01	0.10	0.05	0.02	-0.02	-0.04	-0.05
22	1	0.23	-0.19	0.20	0.16	-0.12	0.06	-0.16	-0.28	-0.02
23	1	-0.13	0.09	0.17	-0.18	-0.35	0.20	0.10	0.52	0.01
24	1	0.01	0.03	0.02	-0.05	0.07	0.00	0.08	-0.05	0.02
25	1	0.01	0.05	0.02	0.10	-0.12	-0.01	0.05	-0.07	-0.02
26	1	0.00	-0.01	-0.06	-0.02	0.02	0.06	-0.02	0.01	-0.01

	49			50			51		
	?A			?A			?A		
Frequencies --	1368.1003			1385.6074			1386.4120		
Red. masses --	1.6112			1.3351			1.6865		
Frc consts --	1.7768			1.5102			1.9099		
IR Inten --	9.5346			6.1424			1.6486		
Raman Activ --	1.3044			1.7462			0.7324		
Depolar --	0.7476			0.7385			0.7054		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.04	-0.01	-0.01	0.02	0.00	0.00	0.04	0.04	-0.02
2	6	0.00	-0.10	-0.07	-0.01	0.05	-0.07	-0.02	-0.06	0.06

```
   3   6    -0.05   0.00   0.09    -0.06   0.00  -0.04     0.00   0.04  -
0.06
   4   6     0.05   0.04  -0.01    -0.01  -0.02  -0.02    -0.10  -0.05
0.02
   5   6    -0.02  -0.06  -0.01     0.00  -0.02   0.02     0.02   0.01
0.00
   6   6     0.04   0.05   0.01    -0.07   0.01   0.04     0.04  -0.01  -
0.07
   7   6    -0.02  -0.03  -0.05     0.00   0.00  -0.01    -0.03  -0.01
0.01
   8   6     0.00   0.02   0.03     0.03   0.00   0.02     0.08   0.09  -
0.03
   9   6     0.05  -0.01   0.02     0.01   0.01   0.01    -0.02   0.01
0.05
  10   6    -0.05  -0.04  -0.01    -0.01   0.04   0.05    -0.03  -0.01
0.05
  11   6     0.02   0.01   0.02     0.02  -0.03   0.01     0.03  -0.04
0.01
  12   8     0.00   0.02   0.00     0.00   0.01   0.00     0.00  -0.01
0.00
  13   6     0.00   0.00  -0.01     0.00   0.00   0.00     0.00   0.00  -
0.01
  14   7    -0.01   0.01   0.00     0.00   0.00   0.00     0.01   0.00
0.00
  15   8     0.00   0.01  -0.01     0.00   0.00   0.00     0.00  -0.01
0.00
  16   1     0.04   0.13  -0.02     0.00   0.02   0.15     0.00  -0.01
0.03
  17   1     0.20   0.61   0.14     0.29  -0.30   0.27    -0.09   0.26  -
0.02
  18   1     0.32   0.24  -0.09     0.42  -0.14   0.10     0.03  -0.20
0.15
  19   1    -0.31  -0.09  -0.01    -0.04   0.09   0.03     0.47   0.03  -
0.04
  20   1    -0.10  -0.03  -0.10     0.41  -0.19  -0.08    -0.16   0.23
0.13
  21   1     0.07  -0.02   0.18    -0.04  -0.01  -0.09    -0.06  -0.02
0.03
  22   1    -0.16  -0.10  -0.01    -0.23   0.04  -0.11    -0.34  -0.42  -
0.09
  23   1     0.21   0.21  -0.19     0.26  -0.25  -0.15     0.29   0.02  -
0.18
  24   1     0.02   0.04   0.02    -0.05   0.08   0.00    -0.16   0.19  -
0.01
  25   1    -0.03   0.04  -0.01    -0.12   0.12  -0.01    -0.04   0.02  -
0.01
  26   1     0.02  -0.02  -0.02     0.00  -0.01   0.01     0.00   0.00  -
0.03
                      52                    53                    54
                      ?A                    ?A                    ?A
 Frequencies --  1404.8591             1409.8711             1416.7109
 Red. masses --     1.6577                1.5499                1.4370
 Frc consts  --     1.9276                1.8152                1.6993
 IR Inten    --     2.3762                8.7016                2.4735
```

Raman Activ	--	0.5885			11.7087			1.7901		
Depolar	--	0.7223			0.7056			0.7493		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.06	0.03	0.05	-0.02	-0.11	-0.04	-0.02	0.02	0.00
2	6	-0.04	-0.06	-0.04	-0.05	0.05	-0.01	0.03	0.01	0.06
3	6	-0.02	0.06	0.02	0.01	0.00	0.01	0.01	0.00	-0.06
4	6	-0.02	-0.01	-0.03	-0.04	0.04	0.01	0.06	-0.04	-0.05
5	6	-0.01	-0.05	-0.02	0.02	0.02	-0.01	0.00	0.03	0.04
6	6	-0.04	-0.06	-0.07	0.03	-0.06	-0.01	0.02	-0.02	-0.03
7	6	0.01	0.07	0.03	-0.10	0.00	-0.04	-0.03	-0.02	-0.04
8	6	0.01	-0.08	0.02	0.01	-0.05	-0.01	0.04	-0.02	0.05
9	6	-0.06	0.02	-0.03	0.00	0.01	-0.01	0.02	0.00	0.01
10	6	0.05	-0.04	0.03	0.00	0.01	0.01	-0.05	0.01	0.04
11	6	-0.04	0.00	-0.01	0.05	0.05	0.03	-0.04	0.06	0.00
12	8	0.00	0.02	0.00	0.00	-0.01	0.00	0.00	-0.01	0.00
13	6	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.01	0.01	0.01	0.00	0.00	0.00	-0.01	0.00	0.00
16	1	-0.02	-0.20	-0.14	0.25	0.50	0.25	-0.12	-0.17	-0.02
17	1	0.19	0.29	0.21	0.09	-0.13	0.16	-0.23	-0.08	-0.22
18	1	0.13	-0.05	0.13	-0.02	0.00	0.01	-0.04	-0.12	0.04
19	1	0.09	0.17	0.02	0.20	-0.07	-0.07	-0.41	0.22	0.11
20	1	0.21	0.36	0.38	-0.08	0.15	0.18	-0.06	0.12	0.09
21	1	-0.01	0.08	-0.04	0.49	0.21	0.26	0.23	0.07	0.19
22	1	-0.02	0.43	-0.12	0.06	0.16	-0.05	-0.32	0.20	-0.16
23	1	-0.11	0.22	0.16	0.00	-0.01	0.01	0.27	-0.08	-0.20
24	1	0.11	-0.09	-0.01	0.07	0.06	0.03	0.21	-0.23	0.02
25	1	0.04	-0.06	0.03	0.07	0.05	0.05	0.15	-0.17	-0.01

```
  26   1     0.04  -0.03  -0.02     0.00   0.01   0.00    -0.01   0.01
0.02
                     55                     56                     57
                     ?A                     ?A                     ?A
 Frequencies --  1435.9662              1448.7660              1455.5723
 Red. masses --     1.4588                 1.5502                 1.4968
 Frc consts  --     1.7722                 1.9170                 1.8684
 IR Inten    --    11.0991                 1.4764                25.9740
 Raman Activ --     0.3124                 0.5923                 1.1294
 Depolar     --     0.6988                 0.3669                 0.7171
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.04  -0.04   0.12    -0.06  -0.04   0.08    -0.06  -0.02  -
0.01
   2   6     0.05   0.01  -0.02     0.05  -0.02   0.01     0.00   0.01
0.02
   3   6    -0.02   0.00  -0.02    -0.01   0.00  -0.01     0.01  -0.01
0.01
   4   6    -0.03   0.03  -0.02    -0.02   0.03  -0.04     0.05  -0.02  -
0.04
   5   6     0.00  -0.03   0.02     0.01  -0.03   0.04     0.02   0.03
0.01
   6   6    -0.02  -0.03   0.02    -0.01   0.06   0.00     0.01  -0.03
0.00
   7   6     0.04   0.02  -0.10    -0.05  -0.04   0.09     0.04   0.06  -
0.05
   8   6    -0.03   0.02   0.00     0.07  -0.04   0.00     0.04  -0.01
0.05
   9   6     0.02   0.00  -0.01    -0.06   0.03   0.02    -0.07   0.01
0.00
  10   6    -0.01   0.02   0.02     0.01  -0.01  -0.01     0.05   0.00  -
0.03
  11   6    -0.01   0.02  -0.01     0.03   0.00  -0.03     0.07  -0.08
0.02
  12   8     0.00   0.01   0.00     0.00   0.01  -0.01     0.00  -0.01
0.00
  13   6     0.00   0.00   0.00     0.00   0.00  -0.01     0.01   0.00
0.00
  14   7     0.00   0.00   0.00     0.01  -0.01   0.00     0.01  -0.01
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.19   0.12  -0.50     0.19   0.21  -0.43     0.03   0.20
0.09
  17   1    -0.08  -0.08  -0.17    -0.16   0.06  -0.24    -0.10  -0.01  -
0.09
  18   1     0.13  -0.04   0.03     0.03  -0.01   0.00    -0.09   0.06  -
0.06
  19   1     0.26  -0.06  -0.09     0.08  -0.06  -0.09    -0.27   0.17
0.08
  20   1     0.11   0.07   0.14     0.02  -0.16  -0.22    -0.10   0.11
0.12
  21   1    -0.15  -0.12   0.40     0.25   0.16  -0.50    -0.26  -0.09
0.16
```

22	1	0.05	-0.19	0.09	-0.24	0.19	-0.20	-0.36	0.07	-0.14
23	1	0.07	-0.10	-0.04	-0.05	0.03	0.04	-0.24	0.00	0.18
24	1	0.26	-0.30	0.02	-0.11	-0.02	0.00	-0.17	0.22	-0.01
25	1	-0.16	0.18	-0.01	0.00	0.09	0.05	-0.38	0.39	-0.05
26	1	0.01	-0.01	0.01	0.03	-0.02	0.00	0.01	0.01	0.01

	58			59			60		
	?A			?A			?A		
Frequencies --	1471.5772			1491.2026			1640.5276		
Red. masses --	1.7096			2.5629			1.0990		
Frc consts --	2.1813			3.3578			1.7426		
IR Inten --	13.9181			185.4008			6.1944		
Raman Activ --	7.2115			1.7186			9.6137		
Depolar --	0.7126			0.6945			0.6506		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.04	-0.02	0.00	0.02	0.00	0.06	-0.01	0.00	0.00
2 6	0.04	-0.01	0.04	0.00	-0.02	-0.04	0.00	0.00	0.00
3 6	0.00	-0.01	-0.02	-0.04	-0.10	0.07	0.00	0.00	0.00
4 6	0.02	0.00	0.00	-0.07	-0.12	-0.03	0.00	0.00	0.00
5 6	0.00	0.05	0.01	0.07	0.27	-0.04	0.00	0.00	0.00
6 6	-0.01	-0.01	-0.07	0.00	0.03	0.02	0.00	0.00	0.00
7 6	0.02	0.05	0.06	-0.01	-0.01	0.00	0.00	-0.01	0.00
8 6	-0.09	-0.06	-0.01	0.01	0.00	0.01	0.00	0.00	0.00
9 6	0.12	-0.03	-0.02	0.04	-0.03	0.01	0.00	0.00	0.00
10 6	-0.08	-0.01	0.06	0.00	0.00	-0.02	0.00	0.00	0.00
11 6	0.05	-0.06	-0.01	-0.01	0.02	-0.02	-0.06	-0.05	-0.04
12 8	0.00	-0.02	0.00	-0.01	-0.09	0.01	0.00	0.00	0.00
13 6	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14 7	-0.02	0.01	0.00	-0.01	0.01	0.00	0.00	0.00	0.00
15 8	-0.01	0.00	0.00	-0.02	-0.02	0.00	0.00	0.00	0.00
16 1	0.06	0.15	-0.05	0.05	-0.03	-0.16	-0.02	0.00	-0.01
17 1	-0.14	0.07	-0.16	0.12	0.10	0.08	-0.02	-0.01	-0.02

18	1	0.05	-0.02	-0.01	0.16	0.42	-0.36	0.00	0.00	0.00
19	1	-0.05	0.01	0.01	0.30	0.52	0.14	-0.02	-0.02	-0.01
20	1	0.10	0.20	0.15	0.03	-0.07	-0.07	-0.01	-0.02	-0.02
21	1	-0.13	0.03	-0.20	0.06	0.03	-0.04	0.00	-0.02	-0.01
22	1	0.43	0.30	0.12	-0.07	0.05	-0.04	-0.02	-0.02	-0.01
23	1	0.40	0.09	-0.28	-0.03	0.06	0.00	0.00	0.00	0.00
24	1	-0.23	0.24	-0.03	0.11	-0.12	0.00	0.52	0.45	-0.16
25	1	-0.15	0.21	0.03	0.04	0.01	0.05	0.22	0.23	0.62
26	1	-0.04	0.03	0.03	-0.12	0.13	0.02	0.00	0.00	0.00

	61	62	63
	?A	?A	?A
Frequencies --	2327.3066	2567.3306	3214.5027
Red. masses --	1.0589	12.6755	1.0584
Frc consts --	3.3792	49.2242	6.4433
IR Inten --	646.0458	13.2803	35.9735
Raman Activ --	52.4061	155.3906	126.4425
Depolar --	0.0907	0.2167	0.2036

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
2	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.04	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	-0.10	0.05	0.01	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.04	-0.04	-0.03
12	8	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.73	-0.33	-0.04	0.00	0.00	0.00

14	7	0.00	0.00	0.00	-0.53	0.25	0.03	0.00	0.00	0.00
15	8	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	0.00	0.00	0.00	0.00	0.00	0.00	-0.08	0.04	-0.02
17	1	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.01
18	1	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
19	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01
20	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.01
21	1	0.00	0.00	0.00	0.00	0.00	0.00	0.04	-0.10	-0.01
22	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01
23	1	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	1	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.10	0.68
25	1	0.00	0.00	0.00	0.00	0.00	0.00	0.46	0.40	-0.37
26	1	-0.64	-0.77	0.02	0.03	0.03	0.00	0.00	0.00	0.00

	64			65			66		
	?A			?A			?A		
Frequencies --	3260.4061			3272.7085			3282.8637		
Red. masses --	1.1071			1.0876			1.0886		
Frc consts --	6.9340			6.8633			6.9122		
IR Inten --	21.9344			14.6530			7.8911		
Raman Activ --	88.7953			52.7374			105.5011		
Depolar --	0.7486			0.5393			0.4551		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.00	0.00	0.02	-0.01	0.00	-0.06	0.03	-0.01
2 6	0.00	0.00	0.00	-0.01	0.00	0.01	0.03	0.00	-0.02
3 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4 6	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.01
5 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6 6	0.00	0.00	0.00	0.00	0.02	-0.02	0.00	0.00	0.00
7 6	0.00	0.00	0.00	0.03	-0.07	-0.01	0.01	-0.02	0.00
8 6	0.00	0.00	0.00	-0.01	0.01	0.02	0.00	0.00	0.01
9 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  10   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  11   6    -0.03  -0.02   0.09     0.00   0.00   0.00     0.00  -0.01
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.00   0.00   0.00    -0.20   0.11  -0.04     0.73  -0.40
0.16
  17   1    -0.01   0.00   0.00     0.08   0.00  -0.07    -0.30   0.00
0.26
  18   1     0.00   0.00   0.00     0.00   0.01   0.01     0.00  -0.03  -
0.04
  19   1     0.00   0.00   0.01     0.01  -0.02   0.06    -0.03   0.05  -
0.15
  20   1     0.00  -0.01   0.01    -0.03  -0.19   0.19     0.00   0.01  -
0.01
  21   1     0.00   0.01   0.00    -0.34   0.81   0.10    -0.10   0.23
0.03
  22   1    -0.01   0.00   0.01     0.10  -0.06  -0.23     0.03  -0.02  -
0.08
  23   1     0.00   0.00   0.00    -0.02   0.00  -0.03     0.00   0.00
0.00
  24   1    -0.08  -0.12  -0.70     0.01   0.01   0.06     0.01   0.01
0.07
  25   1     0.46   0.40  -0.34     0.03   0.02  -0.02     0.05   0.04  -
0.04
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     67                     68                     69
                     ?A                     ?A                     ?A
 Frequencies --  3291.8883              3296.1256              3304.8402
 Red. masses --     1.0885                 1.0891                 1.0892
 Frc consts  --     6.9497                 6.9717                 7.0092
 IR Inten    --     6.8632                28.5670                36.0530
 Raman Activ --    87.2718                53.1293               117.3461
 Depolar     --     0.6841                 0.5918                 0.3920
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.02  -0.01   0.00     0.02  -0.01   0.00    -0.02   0.01
0.00
   2   6     0.03   0.00  -0.02     0.02   0.00  -0.02    -0.04   0.00
0.04
   3   6     0.00   0.01   0.01     0.00   0.00   0.01     0.00   0.00  -
0.01
   4   6     0.00   0.01  -0.02     0.00  -0.01   0.02     0.00  -0.01
0.02
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

```
    6    6    -0.01   -0.04    0.04     0.00   -0.02    0.02     0.00   -0.03
0.03
    7    6     0.00    0.00    0.00     0.01   -0.02    0.00     0.00   -0.01
0.00
    8    6    -0.02    0.01    0.04     0.03   -0.01   -0.06     0.00    0.00
0.00
    9    6     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   10    6    -0.01    0.00   -0.01    -0.01    0.00   -0.01    -0.02    0.00  -
0.03
   11    6     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   12    8     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   13    6     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   14    7     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   15    8     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   16    1    -0.20    0.11   -0.05    -0.19    0.10   -0.04     0.19   -0.10
0.05
   17    1    -0.32    0.00    0.29    -0.23    0.00    0.20     0.51    0.00  -
0.45
   18    1     0.00   -0.06   -0.07     0.00   -0.05   -0.06    -0.01    0.05
0.06
   19    1     0.03   -0.08    0.22    -0.03    0.09   -0.24    -0.04    0.09  -
0.23
   20    1     0.07    0.46   -0.46     0.03    0.18   -0.19     0.05    0.31  -
0.31
   21    1    -0.02    0.05    0.01    -0.12    0.28    0.04    -0.05    0.12
0.02
   22    1     0.18   -0.11   -0.41    -0.30    0.18    0.68     0.02   -0.01  -
0.04
   23    1     0.12   -0.01    0.17     0.10   -0.01    0.14     0.25   -0.02
0.35
   24    1     0.00    0.00   -0.02     0.00    0.00    0.02     0.00    0.00
0.02
   25    1     0.00    0.00    0.00     0.00    0.00    0.00     0.03    0.02  -
0.02
   26    1     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
                     70                      71                      72
                     ?A                      ?A                      ?A
 Frequencies --  3313.3793               3316.6623               3335.5170
 Red. masses --     1.0897                  1.0900                  1.0910
 Frc consts  --     7.0486                  7.0648                  7.1514
 IR Inten    --    29.4114                  5.9561                 11.7831
 Raman Activ --    27.8882                259.0625                218.5246
 Depolar     --     0.4082                  0.1235                  0.0884
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
    1    6   -0.01    0.00    0.00    -0.02    0.01    0.00     0.01    0.00
0.00
```

2	6	0.00	0.00	0.00	-0.01	0.00	0.01	0.02	0.00	-0.01
3	6	0.00	0.01	0.02	0.00	-0.01	-0.02	0.00	-0.05	-0.06
4	6	-0.01	0.01	-0.03	-0.01	0.02	-0.06	0.00	0.00	0.01
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.02	-0.02	0.00	-0.02	0.02	0.00	0.01	-0.01
7	6	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
8	6	0.00	0.00	-0.01	0.01	-0.01	-0.03	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	-0.04	0.00	-0.05	0.01	0.00	0.02	-0.02	0.00	-0.02
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	0.06	-0.03	0.01	0.19	-0.10	0.04	-0.05	0.03	-0.01
17	1	-0.04	0.00	0.04	0.12	0.00	-0.11	-0.16	0.00	0.14
18	1	0.01	-0.17	-0.20	-0.01	0.17	0.20	-0.03	0.60	0.69
19	1	0.06	-0.15	0.40	0.11	-0.26	0.71	-0.01	0.03	-0.08
20	1	-0.04	-0.26	0.26	0.03	0.18	-0.18	-0.01	-0.09	0.09
21	1	0.02	-0.06	-0.01	-0.05	0.13	0.02	0.01	-0.03	0.00
22	1	-0.04	0.02	0.08	-0.13	0.08	0.29	0.02	-0.01	-0.04
23	1	0.45	-0.03	0.61	-0.15	0.01	-0.20	0.17	-0.02	0.23
24	1	0.00	0.00	0.01	0.01	0.01	0.04	0.00	0.00	-0.01
25	1	0.00	0.00	0.00	0.02	0.02	-0.01	-0.01	-0.01	0.00
26	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
 --------------------
 - Thermochemistry -
 --------------------
```

```
Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
Atom  1 has atomic number  6 and mass  12.00000
Atom  2 has atomic number  6 and mass  12.00000
Atom  3 has atomic number  6 and mass  12.00000
Atom  4 has atomic number  6 and mass  12.00000
Atom  5 has atomic number  6 and mass  12.00000
Atom  6 has atomic number  6 and mass  12.00000
Atom  7 has atomic number  6 and mass  12.00000
Atom  8 has atomic number  6 and mass  12.00000
Atom  9 has atomic number  6 and mass  12.00000
Atom 10 has atomic number  6 and mass  12.00000
Atom 11 has atomic number  6 and mass  12.00000
Atom 12 has atomic number  8 and mass  15.99491
Atom 13 has atomic number  6 and mass  12.00000
Atom 14 has atomic number  7 and mass  14.00307
Atom 15 has atomic number  8 and mass  15.99491
Atom 16 has atomic number  1 and mass   1.00783
Atom 17 has atomic number  1 and mass   1.00783
Atom 18 has atomic number  1 and mass   1.00783
Atom 19 has atomic number  1 and mass   1.00783
Atom 20 has atomic number  1 and mass   1.00783
Atom 21 has atomic number  1 and mass   1.00783
Atom 22 has atomic number  1 and mass   1.00783
Atom 23 has atomic number  1 and mass   1.00783
Atom 24 has atomic number  1 and mass   1.00783
Atom 25 has atomic number  1 and mass   1.00783
Atom 26 has atomic number  1 and mass   1.00783
Molecular mass:   201.07898 amu.
Principal axes and moments of inertia in atomic units:
                          1         2         3
    EIGENVALUES --  1774.94378 2292.82308 3062.82353
          X            0.99703   0.07659   0.00756
          Y           -0.07668   0.99698   0.01256
          Z           -0.00658  -0.01311   0.99989
THIS MOLECULE IS AN ASYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER  1.
WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
          MAY CAUSE SIGNIFICANT ERROR
ROTATIONAL TEMPERATURES (KELVIN)      0.04880     0.03778     0.02828
ROTATIONAL CONSTANTS (GHZ)            1.01679     0.78713     0.58924
   1 IMAGINARY FREQUENCIES IGNORED.
Zero-point vibrational energy     575338.3 (Joules/Mol)
                                  137.50916 (Kcal/Mol)
WARNING-- EXPLICIT CONSIDERATION OF  13 DEGREES OF FREEDOM AS
          VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
VIBRATIONAL TEMPERATURES:    190.31   235.94   265.41   495.14   573.24
         (KELVIN)            645.44   683.09   706.20   769.94   822.85
                             867.60   878.45   891.24   954.30   999.00
                            1070.90  1151.49  1156.50  1187.44  1207.38
                            1260.86  1270.62  1312.96  1331.76  1378.32
                            1413.97  1431.18  1435.27  1454.48  1487.88
                            1499.87  1519.88  1531.68  1559.14  1620.71
                            1670.32  1700.00  1750.71  1775.71  1798.70
                            1816.49  1823.47  1826.15  1871.65  1910.19
```

1954.55	1961.13	1968.38	1993.57	1994.73
2021.27	2028.48	2038.32	2066.02	2084.44
2094.23	2117.26	2145.50	2360.34	3348.46
3693.79	4624.93	4690.97	4708.67	4723.28
4736.27	4742.36	4754.90	4767.19	4771.91
4799.04				

Zero-point correction=	0.219135
(Hartree/Particle)	
Thermal correction to Energy=	0.227554
Thermal correction to Enthalpy=	0.228498
Thermal correction to Gibbs Free Energy=	0.185311
Sum of electronic and zero-point Energies=	-661.037763
Sum of electronic and thermal Energies=	-661.029344
Sum of electronic and thermal Enthalpies=	-661.028400
Sum of electronic and thermal Free Energies=	-661.071587

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	142.792	37.866	90.895
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	41.800
ROTATIONAL	0.889	2.981	30.901
VIBRATIONAL	141.015	31.904	18.194
VIBRATION 1	0.612	1.921	2.913
VIBRATION 2	0.623	1.887	2.503
VIBRATION 3	0.631	1.861	2.283
VIBRATION 4	0.723	1.587	1.193
VIBRATION 5	0.765	1.474	0.968
VIBRATION 6	0.808	1.364	0.800
VIBRATION 7	0.831	1.306	0.724
VIBRATION 8	0.847	1.270	0.681
VIBRATION 9	0.890	1.172	0.576
VIBRATION 10	0.928	1.092	0.501
VIBRATION 11	0.961	1.025	0.445
VIBRATION 12	0.970	1.009	0.432
VIBRATION 13	0.979	0.991	0.417

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.580083D-85	-85.236510	-196.264317
TOTAL V=0	0.361258D+16	15.557817	35.823198
VIB (BOT)	0.409536D-99	-99.387708	-228.848655
VIB (BOT) 1	0.154033D+01	0.187615	0.432000
VIB (BOT) 2	0.123130D+01	0.090363	0.208069
VIB (BOT) 3	0.108711D+01	0.036273	0.083522
VIB (BOT) 4	0.538151D+00	-0.269096	-0.619616
VIB (BOT) 5	0.447870D+00	-0.348848	-0.803252
VIB (BOT) 6	0.382699D+00	-0.417143	-0.960508
VIB (BOT) 7	0.353845D+00	-0.451186	-1.038895
VIB (BOT) 8	0.337558D+00	-0.471651	-1.086017
VIB (BOT) 9	0.297427D+00	-0.526619	-1.212586
VIB (BOT) 10	0.268600D+00	-0.570895	-1.314533
VIB (BOT) 11	0.246854D+00	-0.607559	-1.398957
VIB (BOT) 12	0.241906D+00	-0.616354	-1.419208
VIB (BOT) 13	0.236224D+00	-0.626676	-1.442974

```
VIB (V=0)       0.255046D+02          1.406619          3.238860
VIB (V=0)  1    0.211945D+01          0.326224          0.751158
VIB (V=0)  2    0.182895D+01          0.262201          0.603740
VIB (V=0)  3    0.169658D+01          0.229575          0.528615
VIB (V=0)  4    0.123458D+01          0.091519          0.210730
VIB (V=0)  5    0.117126D+01          0.068653          0.158079
VIB (V=0)  6    0.112965D+01          0.052944          0.121907
VIB (V=0)  7    0.111254D+01          0.046316          0.106647
VIB (V=0)  8    0.110328D+01          0.042685          0.098287
VIB (V=0)  9    0.108178D+01          0.034137          0.078604
VIB (V=0) 10    0.106758D+01          0.028400          0.065393
VIB (V=0) 11    0.105762D+01          0.024329          0.056019
VIB (V=0) 12    0.105544D+01          0.023435          0.053962
VIB (V=0) 13    0.105299D+01          0.022426          0.051637
ELECTRONIC      0.100000D+01          0.000000          0.000000
TRANSLATIONAL   0.112075D+09          8.049510         18.534683
ROTATIONAL      0.126383D+07          6.101688         14.049656
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6           0.000003590   -0.000013460   -0.000005376
   2          6           0.000004562    0.000013856    0.000002851
   3          6           0.000009222    0.000008947   -0.000000097
   4          6           0.000002846    0.000013617    0.000012025
   5          6           0.000008363    0.000078158   -0.000009060
   6          6          -0.000018970    0.000005609   -0.000009654
   7          6           0.000002767   -0.000003771   -0.000010721
   8          6          -0.000001915    0.000009513    0.000000036
   9          6          -0.000012683   -0.000038739    0.000004471
  10          6          -0.000014362    0.000008032    0.000004704
  11          6          -0.000009618   -0.000014509    0.000019826
  12          8          -0.000026536   -0.000057209    0.000007794
  13          6           0.000016257    0.000040668   -0.000023886
  14          7          -0.000000959   -0.000010828    0.000011893
  15          8           0.000022047   -0.000037870    0.000000084
  16          1           0.000001868   -0.000000202    0.000004616
  17          1          -0.000001812   -0.000002323   -0.000004370
  18          1           0.000006828    0.000002256   -0.000002032
  19          1           0.000001550    0.000003365    0.000004816
  20          1           0.000002875    0.000001010    0.000000723
  21          1          -0.000005019   -0.000005275    0.000006437
  22          1          -0.000000959   -0.000011816    0.000003976
  23          1           0.000002638   -0.000016181   -0.000004183
  24          1           0.000009211    0.000003567   -0.000004529
  25          1           0.000000360   -0.000006853   -0.000009923
  26          1          -0.000002151    0.000030437   -0.000000421
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000078158 RMS     0.000016481
-------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------
```

```
  1  C         0.000004(   1)     -0.000013(  27)     -0.000005(  53)
  2  C         0.000005(   2)      0.000014(  28)      0.000003(  54)
  3  C         0.000009(   3)      0.000009(  29)      0.000000(  55)
  4  C         0.000003(   4)      0.000014(  30)      0.000012(  56)
  5  C         0.000008(   5)      0.000078(  31)     -0.000009(  57)
  6  C        -0.000019(   6)      0.000006(  32)     -0.000010(  58)
  7  C         0.000003(   7)     -0.000004(  33)     -0.000011(  59)
  8  C        -0.000002(   8)      0.000010(  34)      0.000000(  60)
  9  C        -0.000013(   9)     -0.000039(  35)      0.000004(  61)
 10  C        -0.000014(  10)      0.000008(  36)      0.000005(  62)
 11  C        -0.000010(  11)     -0.000015(  37)      0.000020(  63)
 12  O        -0.000027(  12)     -0.000057(  38)      0.000008(  64)
 13  C         0.000016(  13)      0.000041(  39)     -0.000024(  65)
 14  N        -0.000001(  14)     -0.000011(  40)      0.000012(  66)
 15  O         0.000022(  15)     -0.000038(  41)      0.000000(  67)
 16  H         0.000002(  16)      0.000000(  42)      0.000005(  68)
 17  H        -0.000002(  17)     -0.000002(  43)     -0.000004(  69)
 18  H         0.000007(  18)      0.000002(  44)     -0.000002(  70)
 19  H         0.000002(  19)      0.000003(  45)      0.000005(  71)
 20  H         0.000003(  20)      0.000001(  46)      0.000001(  72)
 21  H        -0.000005(  21)     -0.000005(  47)      0.000006(  73)
 22  H        -0.000001(  22)     -0.000012(  48)      0.000004(  74)
 23  H         0.000003(  23)     -0.000016(  49)     -0.000004(  75)
 24  H         0.000009(  24)      0.000004(  50)     -0.000005(  76)
 25  H         0.000000(  25)     -0.000007(  51)     -0.000010(  77)
 26  H        -0.000002(  26)      0.000030(  52)      0.000000(  78)
---------------------------------------------------------------------
Internal  Forces:  Max     0.000078158 RMS     0.000016481

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   1 out of a maximum of  88
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
    Eigenvalues ---   -0.18887   0.00452   0.00670   0.00861   0.01250
    Eigenvalues ---    0.02612   0.02897   0.03330   0.04415   0.04604
    Eigenvalues ---    0.04693   0.04721   0.04824   0.05101   0.05184
    Eigenvalues ---    0.05268   0.05334   0.05386   0.05437   0.05662
    Eigenvalues ---    0.05861   0.06097   0.06809   0.07987   0.09121
    Eigenvalues ---    0.10536   0.10866   0.11789   0.13721   0.14334
    Eigenvalues ---    0.14867   0.15867   0.16105   0.18787   0.19827
    Eigenvalues ---    0.19900   0.21668   0.24555   0.24813   0.27919
    Eigenvalues ---    0.32579   0.34737   0.35528   0.37647   0.38395
    Eigenvalues ---    0.39958   0.44614   0.47796   0.49699   0.50292
    Eigenvalues ---    0.51907   0.52712   0.57874   0.59731   0.63804
    Eigenvalues ---    0.64773   0.65586   0.71612   0.72477   0.78508
    Eigenvalues ---    0.87136   0.92417   0.95181   0.95740   0.96952
    Eigenvalues ---    0.98555   0.99760   1.02525   1.05473   1.08199
    Eigenvalues ---    1.10712   3.18485
Eigenvalue   1 out of range, new value =    0.188869 Eigenvector:
                          1
          X1         -0.02278
          Y1         -0.01855
```

Z1	0.00627
X2	-0.01998
Y2	-0.01561
Z2	0.00162
X3	-0.03268
Y3	-0.00599
Z3	0.00085
X4	-0.03220
Y4	-0.01066
Z4	0.00143
X5	0.14396
Y5	-0.14630
Z5	0.00666
X6	-0.00777
Y6	-0.00484
Z6	0.00412
X7	-0.00784
Y7	-0.00540
Z7	-0.00234
X8	-0.01965
Y8	-0.02604
Z8	-0.00269
X9	-0.04445
Y9	-0.00069
Z9	-0.01793
X10	-0.02027
Y10	-0.01445
Z10	0.00240
X11	-0.00488
Y11	-0.01921
Z11	0.00331
X12	0.41770
Y12	0.02626
Z12	-0.03076
X13	-0.02010
Y13	0.05321
Z13	-0.01301
X14	-0.00087
Y14	0.09726
Z14	-0.01591
X15	-0.07737
Y15	-0.11233
Z15	0.07437
X16	-0.02198
Y16	-0.02017
Z16	0.00403
X17	-0.01314
Y17	-0.01453
Z17	0.00548
X18	-0.02469
Y18	0.00433
Z18	-0.00598
X19	-0.02323
Y19	0.00087

Z19	0.00326
X20	0.00006
Y20	-0.00537
Z20	0.00111
X21	0.00688
Y21	0.00200
Z21	-0.00005
X22	-0.01326
Y22	0.00243
Z22	-0.00598
X23	-0.00956
Y23	0.01129
Z23	-0.00336
X24	-0.00065
Y24	-0.01185
Z24	0.00169
X25	-0.00011
Y25	-0.01833
Z25	0.00291
X26	-0.64349
Y26	0.56093
Z26	-0.06161

Angle between quadratic step and forces= 70.48 degrees.
Linear search not attempted -- first point.
TrRot= -0.000002 0.000018 0.000015 0.000008 -0.000001 0.000008

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
X1	-3.95030	0.00000	0.00000	-0.00001	0.00000	-3.95030
Y1	-0.26736	-0.00001	0.00000	0.00006	0.00002	-0.26734
Z1	-0.76810	-0.00001	0.00000	0.00006	0.00007	-0.76803
X2	-3.13671	0.00000	0.00000	-0.00001	-0.00001	-3.13672
Y2	-0.27048	0.00001	0.00000	0.00014	0.00011	-0.27037
Z2	2.05038	0.00000	0.00000	0.00007	0.00009	2.05046
X3	-1.02031	0.00001	0.00000	0.00018	0.00015	-1.02015
Y3	1.75737	0.00001	0.00000	0.00001	0.00001	1.75738
Z3	2.37793	0.00000	0.00000	0.00009	0.00010	2.37804
X4	-1.64404	0.00000	0.00000	0.00006	0.00005	-1.64399
Y4	0.96819	0.00001	0.00000	-0.00001	-0.00002	0.96818
Z4	-2.05848	0.00001	0.00000	0.00011	0.00012	-2.05836
X5	-0.61919	0.00001	0.00000	0.00008	0.00003	-0.61916
Y5	2.97883	0.00008	0.00000	0.00000	0.00001	2.97884
Z5	-0.23239	-0.00001	0.00000	0.00008	0.00009	-0.23230
X6	-1.09955	-0.00002	0.00000	-0.00020	-0.00017	-1.09971
Y6	-2.43612	0.00001	0.00000	0.00002	0.00002	-2.43609
Z6	2.17187	-0.00001	0.00000	0.00000	0.00002	2.17189
X7	-0.98068	0.00000	0.00000	-0.00020	-0.00015	-0.98084
Y7	-3.40084	0.00000	0.00000	-0.00008	-0.00007	-3.40091
Z7	-0.58906	-0.00001	0.00000	0.00007	0.00008	-0.58897
X8	0.40992	0.00000	0.00000	-0.00006	-0.00005	0.40988
Y8	-1.21563	0.00001	0.00000	-0.00016	-0.00014	-1.21577
Z8	-1.93277	0.00000	0.00000	0.00000	0.00002	-1.93275
X9	2.40107	-0.00001	0.00000	0.00001	0.00001	2.40109
Y9	-0.18540	-0.00004	0.00000	-0.00021	-0.00015	-0.18556
Z9	-0.02867	0.00000	0.00000	-0.00010	-0.00008	-0.02875

X10	1.01058	-0.00001	0.00000	-0.00001	-0.00001	1.01057
Y10	-0.39761	0.00001	0.00000	-0.00019	-0.00016	-0.39777
Z10	2.53627	0.00000	0.00000	-0.00004	-0.00003	2.53624
X11	-3.73200	-0.00001	0.00000	-0.00011	-0.00007	-3.73207
Y11	-3.07729	-0.00001	0.00000	0.00006	0.00002	-3.07727
Z11	-1.50778	0.00002	0.00000	-0.00006	-0.00005	-1.50783
X12	-0.47105	-0.00003	0.00000	-0.00027	-0.00036	-0.47141
Y12	5.50462	-0.00006	0.00000	-0.00021	-0.00020	5.50442
Z12	-0.57848	0.00001	0.00000	-0.00015	-0.00013	-0.57861
X13	4.92359	0.00002	0.00000	0.00024	0.00026	4.92385
Y13	-1.20978	0.00004	0.00000	0.00034	0.00043	-1.20935
Z13	-0.20239	-0.00002	0.00000	-0.00014	-0.00012	-0.20251
X14	6.89665	0.00000	0.00000	0.00032	0.00035	6.89701
Y14	-2.06814	-0.00001	0.00000	0.00048	0.00060	-2.06754
Z14	-0.32201	0.00001	0.00000	0.00021	0.00023	-0.32178
X15	2.28506	0.00002	0.00000	0.00007	0.00003	2.28509
Y15	2.51613	-0.00004	0.00000	-0.00008	-0.00003	2.51610
Z15	-0.60002	0.00000	0.00000	0.00006	0.00008	-0.59994
X16	-5.73181	0.00000	0.00000	0.00005	0.00004	-5.73177
Y16	0.65036	0.00000	0.00000	0.00017	0.00010	0.65046
Z16	-1.15322	0.00000	0.00000	0.00009	0.00011	-1.15311
X17	-4.65946	0.00000	0.00000	-0.00006	-0.00006	-4.65951
Y17	-0.30576	0.00000	0.00000	0.00018	0.00013	-0.30563
Z17	3.40355	0.00000	0.00000	0.00001	0.00003	3.40357
X18	-1.11300	0.00001	0.00000	0.00044	0.00039	-1.11261
Y18	3.09862	0.00000	0.00000	0.00001	0.00002	3.09864
Z18	3.90383	0.00000	0.00000	0.00010	0.00011	3.90395
X19	-1.94821	0.00000	0.00000	0.00011	0.00008	-1.94813
Y19	1.67851	0.00000	0.00000	0.00012	0.00011	1.67862
Z19	-3.94378	0.00000	0.00000	0.00016	0.00017	-3.94361
X20	-1.29335	0.00000	0.00000	-0.00020	-0.00014	-1.29349
Y20	-3.87514	0.00000	0.00000	0.00008	0.00007	-3.87506
Z20	3.60137	0.00000	0.00000	0.00006	0.00008	3.60145
X21	-0.14055	-0.00001	0.00000	-0.00036	-0.00028	-0.14083
Y21	-5.24506	-0.00001	0.00000	-0.00018	-0.00017	-5.24522
Z21	-0.83990	0.00001	0.00000	0.00025	0.00026	-0.83964
X22	1.21275	0.00000	0.00000	-0.00020	-0.00017	1.21258
Y22	-1.66554	-0.00001	0.00000	-0.00043	-0.00040	-1.66593
Z22	-3.75297	0.00000	0.00000	0.00001	0.00003	-3.75294
X23	2.22224	0.00000	0.00000	0.00008	0.00008	2.22232
Y23	-0.46740	-0.00002	0.00000	-0.00063	-0.00058	-0.46798
Z23	4.17125	0.00000	0.00000	-0.00013	-0.00011	4.17113
X24	-3.94730	0.00001	0.00000	0.00028	0.00033	-3.94697
Y24	-3.39740	0.00000	0.00000	0.00041	0.00037	-3.39704
Z24	-3.51982	0.00000	0.00000	-0.00018	-0.00016	-3.51998
X25	-5.04559	0.00000	0.00000	-0.00030	-0.00023	-5.04582
Y25	-4.27327	-0.00001	0.00000	-0.00013	-0.00019	-4.27346
Z25	-0.48709	-0.00001	0.00000	-0.00054	-0.00053	-0.48762
X26	2.28122	0.00000	0.00000	-0.00002	-0.00010	2.28113
Y26	4.64978	0.00003	0.00000	0.00002	0.00008	4.64986
Z26	-0.60199	0.00000	0.00000	-0.00049	-0.00047	-0.60247

Item	Value	Threshold	Converged?
Maximum Force	0.000078	0.000450	YES
RMS Force	0.000016	0.000300	YES

```
Maximum Displacement     0.000604     0.001800     YES
RMS     Displacement     0.000200     0.001200     YES
Predicted change in Energy=-4.361354D-08
Optimization completed.
   -- Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1\1\GINC-PELICAN\Freq\RHF\3-21+G*\C12H11N1O2\SINGH\22-Apr-2002\0\\#N R
HF/3-21+G* FREQ\\Freq calc of output str of mech1str5ts\\0,1\C,-2.0904
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,-0.5399230283,0.9299590849,1.258348\C,-0.8699860283,0.5123460849,-1.0
89299\C,-0.3276610283,1.5763280849,-0.122975\C,-0.5818550283,-1.289136
9151,1.149305\C,-0.5189560283,-1.7996469151,-0.311715\C,0.2169209717,-
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739717,-0.2104049151,1.342136\C,-1.9748880283,-1.6284309151,-0.797885\
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.107102\N,3.6495519717,-1.0944139151,-0.1704\O,1.2092029717,1.33147908
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743750283,-2.7755639151,-0.444455\H,0.6417599717,-0.8813639151,-1.9859
85\H,1.1759579717,-0.2473399151,2.207329\H,-2.0888230283,-1.7978289151
,-1.862608\H,-2.6700100283,-2.2613169151,-0.257757\H,1.2071709717,2.46
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065369,0.00019707,-0.00049373,-0.00050833,-0.00019557,-0.00001785,-0.0
0013379,-0.00632762,-0.00085130,-0.00178360,-0.00142161,-0.00718973,-0
.03473793,0.00153217,0.00071521,-0.00057504,0.00020211,0.00024470,-0.0
0027668,0.00010132,-0.00039101,-0.00200837,-0.06166510,-0.00555697,-0.
02473498,-0.00000789,0.00002257,0.00009591,-0.00005842,0.00006558,0.00
005233,0.00002078,-0.00001349,0.00000820,-0.00001051,0.00009752,0.0001
4256,-0.00015780,-0.00038995,0.00005388,0.00000471,-0.00024386,-0.0003
2527,0.00010600,0.00010435,-0.00000942,0.00020805,-0.00021666,-0.00011

613,-0.00002885,-0.00006804,-0.00046823,0.00102816,0.00063557,0.000566
37,-0.00054721,-0.00027601,0.00027265,-0.00027915,-0.00047716,0.000044
95,0.06379910,-0.00538213,-0.00285991,-0.03585940,-0.00102819,-0.00655
449,-0.00145364,-0.00029324,-0.00004634,-0.00185500,0.00098039,0.00201
795,-0.00021322,0.00033547,-0.00017865,-0.00074790,0.00282115,-0.00015
003,-0.00009363,0.00125098,0.00077941,0.01025703,-0.00064309,0.0002628
9,-0.00049951,-0.00007402,-0.00024696,-0.00000214,-0.00022324,-0.00001
973,0.00065294,-0.00591718,-0.06471471,-0.03953764,0.00003877,0.000061
43,0.00023353,0.00001208,0.00004029,0.00009709,-0.00000379,-0.00001909
,-0.00001522,0.00000024,0.00004249,0.00024667,0.00072748,0.00095881,0.
00052719,-0.00004929,-0.00002865,-0.00047893,-0.00049135,-0.00024123,0
.00002341,-0.00033922,-0.00055254,0.00031405,-0.00021274,0.00000223,-0
.00031185,-0.00050478,-0.00013517,0.00002534,-0.00022809,0.00017562,-0
.00014357,0.00011173,0.00012341,-0.00000200,0.00621258,0.06719106,-0.0
0036833,0.00209109,-0.00599207,-0.00075629,-0.00082821,0.00076046,0.00
001822,0.00007492,-0.00022895,-0.00010690,0.00038753,0.00071142,-0.000
08192,-0.00015754,-0.00041193,-0.00119502,-0.00062797,0.00067215,0.002
14814,-0.00133669,-0.00812685,0.00027730,-0.00005282,0.00047570,-0.000
05873,-0.00014660,-0.00019612,0.00006477,-0.00009309,-0.00037294,-0.02
779433,-0.04219041,-0.33204429,0.00000736,-0.00013608,0.00017083,-0.00
001245,0.00000220,0.00005430,-0.00006130,0.00002415,0.00000236,-0.0002
0269,-0.00017710,0.00028779,0.00044853,-0.00074693,-0.00001617,0.00007
250,0.00006935,-0.00003637,-0.00012984,-0.00010939,0.00007454,-0.00030
902,-0.00037864,0.00034783,0.00008181,0.00006308,-0.00004154,-0.000666
73,0.00053754,-0.00001725,-0.00044468,-0.00027630,0.00035730,-0.000150
89,-0.00012600,0.00005479,0.03116894,0.04691026,0.36111092,0.00574222,
0.00640267,-0.00432784,0.00027071,-0.00078909,-0.00028579,0.00000225,0
.00009880,-0.00019954,-0.00019377,0.00231783,0.00051826,0.00009747,-0.
00004106,-0.00007070,0.00085301,0.00052613,0.00113236,-0.01986958,-0.0
2196159,0.01840494,-0.00560686,0.00048083,-0.00357720,-0.00046394,-0.0
0039919,0.00134320,-0.00006864,0.00009930,0.00032569,-0.17245172,-0.10
456748,0.08936234,0.00020662,-0.00003877,-0.00003509,0.00013148,-0.000
10951,-0.00019315,-0.00015718,0.00010138,0.00003846,0.00025111,-0.0016
5753,-0.00030387,0.00016919,-0.00086244,-0.00043551,0.00008126,-0.0002
1980,-0.00011467,0.00003536,-0.00000674,-0.00000979,-0.00010163,-0.000
16299,0.00009386,-0.00018413,0.00003871,-0.00080803,0.00055447,0.00080
992,0.00047536,-0.00010436,-0.00010105,0.00017290,0.00009025,0.0000812
5,-0.00009431,0.00334699,0.00289808,-0.00196824,0.18761294,-0.02478875
,-0.01737225,0.01907960,0.00057024,0.00104584,0.00112968,0.00007490,-0
.00010418,0.00009340,-0.00007014,-0.00648602,-0.00367712,-0.00024124,0
.00030488,0.00236180,-0.00083181,0.00028473,-0.00036308,0.00789351,0.0
0583872,-0.00494293,0.00260463,-0.00059534,0.00095471,0.00003209,0.000
05786,-0.00011456,0.00012401,0.00005809,-0.00020111,-0.10460780,-0.152
81943,0.08091888,-0.00038709,-0.00049994,-0.00048214,-0.00008418,0.000
04992,-0.00010936,-0.00004125,-0.00000630,0.00000902,-0.00105305,0.000
50515,-0.00054082,0.00084572,0.00061890,0.00052719,0.00006318,-0.00023
051,-0.00079446,0.00007898,0.00008060,-0.00009267,-0.00013266,-0.00007
627,0.00016764,-0.00022463,0.00011028,-0.00008670,-0.00081527,0.000162
38,-0.00053641,-0.00020679,-0.00011206,0.00010290,-0.00000240,0.000018
51,-0.00000993,0.00437046,0.00406917,-0.00290778,0.11666076,0.16529567
,-0.00613157,-0.00475207,0.00310457,-0.00006301,-0.00038261,0.00118309
,0.00018296,0.00031414,-0.00002841,-0.00099963,-0.00136882,0.00023537,
-0.00045929,-0.00064815,0.00053921,-0.00044153,0.00003355,0.00116308,-
0.00709860,-0.00735968,0.00445339,-0.00229135,-0.00092227,-0.00021921,

-0.00029014,-0.00037228,0.00053308,0.00021400,0.00011194,0.00018272,0.
09233797,0.08373562,-0.13308970,0.00008644,0.00022776,-0.00012827,-0.0
0001497,0.00007014,-0.00004127,0.00002218,-0.00001568,0.00001599,-0.00
003976,-0.00033831,-0.00032453,0.00001404,0.00077161,0.00012572,0.0001
0244,-0.00017289,0.00013054,0.00005112,0.00000327,0.00003150,-0.000225
95,-0.00033094,0.00012664,-0.00019402,0.00010023,0.00006778,0.00086984
,0.00000237,0.00023210,-0.00035429,-0.00021518,0.00012555,0.00002186,0
.00005392,0.00001129,0.02416877,0.02199129,-0.01755274,-0.09931920,-0.
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00093685,-0.00040779,-0.00219295,0.00282902,-0.00006559,-0.00420010,0.
00150188,0.00054453,-0.02317355,-0.08774134,0.01080211,-0.00001917,-0.
00004562,0.00075697,-0.00102464,0.00056213,-0.00103582,0.00037817,-0.0
0348403,0.00249587,-0.01377965,0.01603040,-0.00604142,-0.00038080,-0.0
0149261,-0.00123345,-0.00031465,-0.00067347,0.00027185,0.04665468,0.01
279835,-0.00552952,0.00025570,0.00240158,-0.00028662,-0.00054260,-0.00
043727,0.00008250,-0.01179059,-0.08821812,0.00829254,-0.00039495,-0.00
011797,0.00007522,0.00000599,0.00015020,0.00002882,-0.00018528,-0.0000
5734,0.00082137,-0.00029935,-0.00021524,-0.00054263,-0.00035928,-0.000
00674,-0.00004902,-0.00008124,0.00009297,-0.00003372,-0.00052645,0.000
24203,-0.00018561,-0.00052624,0.00058076,0.00007614,0.00002525,0.00000
140,0.00001980,-0.00024349,0.00016858,-0.00014833,0.01445186,0.0006266
8,0.00111212,0.00022037,0.00028992,0.00079001,-0.00050384,0.00495725,-
0.00469666,0.00113345,0.00549622,-0.00453239,0.00027800,-0.08238265,0.
05361071,-0.00075031,-0.00034106,-0.00004951,-0.00156572,0.00201230,-0
.00084678,0.00168508,-0.00271566,0.00533387,-0.00463449,0.00934369,-0.
01641845,0.00931088,-0.00093562,0.00333079,0.00383312,0.00032494,0.000
68932,-0.00059164,-0.09380355,-0.03215498,0.00763424,0.00281753,0.0015
2060,-0.00057636,-0.00244086,0.00043931,0.00022341,0.00552189,-0.08804
497,-0.01713460,0.00056649,-0.00004795,-0.00005425,0.00041549,0.000048
78,0.00000013,0.00043205,0.00024082,-0.00129723,0.00055593,0.00058089,
0.00073333,0.00073045,0.00037497,0.00000351,-0.00006924,-0.00007658,0.
00010606,0.00088223,-0.00002241,0.00048458,0.00077646,-0.00037542,-0.0
0066236,-0.00000225,0.00002272,0.00013141,0.00040156,-0.00019840,0.000
00189,0.14653981,0.07936958,-0.00027096,-0.00016564,0.00013224,0.00049
355,0.00023909,0.00054353,-0.00149080,0.00090116,-0.00038401,0.0006992
0,-0.00121512,-0.00043386,0.01423371,0.00214398,0.02445540,0.00024684,
-0.00010310,-0.00103462,-0.00075895,0.00001814,-0.00102289,-0.00130770
,-0.00385113,0.00119312,0.00174440,-0.00587027,-0.01814002,0.00065493,
0.00562668,-0.00075003,-0.00007359,-0.00030623,-0.00000568,0.00329786,
0.00094873,-0.02641513,0.00060663,-0.00025156,0.00050871,-0.00003800,0
.00005892,-0.00010718,-0.00952298,0.00039641,0.00576085,-0.00004996,-0
.00000503,0.00003035,-0.00017738,-0.00018143,-0.00011320,0.00056343,-0
.00009963,-0.00066454,-0.00041888,-0.00028556,-0.00055060,0.00025019,-
0.00000271,0.00004651,-0.00001642,-0.00003699,-0.00005346,0.00015870,-
0.00026950,-0.00018148,-0.00001341,0.00033151,-0.00031818,0.00002326,-
0.00006514,-0.00004316,-0.00012444,0.00005309,0.00002483,-0.00870922,0
.00199133,0.01752251\\-0.00000359,0.00001346,0.00000538,-0.00000456,-0
.00001386,-0.00000285,-0.00000922,-0.00000895,0.00000010,-0.00000285,-
0.00001362,-0.00001203,-0.00000836,-0.00007816,0.00000906,0.00001897,-
0.00000561,0.00000965,-0.00000277,0.00000377,0.00001072,0.00000191,-0.
00000951,-0.00000004,0.00001268,0.00003874,-0.00000447,0.00001436,-0.0
0000803,-0.00000470,0.00000962,0.00001451,-0.00001983,0.00002654,0.000
05721,-0.00000779,-0.00001626,-0.00004067,0.00002389,0.00000096,0.0000
1083,-0.00001189,-0.00002205,0.00003787,-0.00000008,-0.00000187,0.0000

```
 0020,-0.00000462,0.00000181,0.00000232,0.00000437,-0.00000683,-0.00000
 226,0.00000203,-0.00000155,-0.00000337,-0.00000482,-0.00000287,-0.0000
 0101,-0.00000072,0.00000502,0.00000527,-0.00000644,0.00000096,0.000011
 82,-0.00000398,-0.00000264,0.00001618,0.00000418,-0.00000921,-0.000003
 57,0.00000453,-0.00000036,0.00000685,0.00000992,0.00000215,-0.00003044
 ,0.00000042\\\@


 HOW IS IT THAT THE SKY FEEDS THE STARS?

                             -- LUCRETIUS
 Job cpu time:  0 days  2 hours 24 minutes 35.2 seconds.
 File lengths (MBytes):  RWF=  252 Int=    0 D2E=    0 Chk=    6 Scr=
1
 Normal termination of Gaussian 98.
```

```
 Entering Gaussian System, Link 0=g98
 Input=mech1str5F.gjf
 Output=mech1str5F.out
 Initial command:
 /usr/g98/l1.exe /usr/scratch/Singh/Gau-15958.inp -
scrdir=/usr/scratch/Singh/
 Default is to use a total of   2 processors:
                                2 via shared-memory
                                1 via Linda
 Entering Link 1 = /usr/g98/l1.exe PID=     18492.
```

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

Cite this work as:
Gaussian 98, Revision A.7,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe,
P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres,
C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 1998.

```
**********************************************
Gaussian 98:  DEC-AXP-OSF/1-G98RevA.7 11-Apr-1999
                  22-Apr-2002
**********************************************
%nproc=2
Will use up to    2 processors via shared memory.
%chk=mech1str5tsF
%nosave
-------------------
#N RHF/3-21+G* FREQ
-------------------
1/10=4,30=1,38=1/1,3;
2/17=6,18=5/2;
3/5=5,7=11,11=1,25=1,30=1/1,2,3;
4/7=1/1;
5/5=2,38=4/2;
8/6=4,11=11/1;
10/13=10/2;
11/6=2,8=1,9=11,15=111,16=11/1,2,10;
```

```
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;
-------------------------------------
Freq calc of output str of mech1str5ts
-------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                    -2.09041  -0.14148  -0.40646
C                    -1.65988  -0.14313   1.08501
C                    -0.53992   0.92996   1.25835
C                    -0.86999   0.51235  -1.0893
C                    -0.32766   1.57633  -0.12298
C                    -0.58186  -1.28914   1.14931
C                    -0.51896  -1.79965  -0.31172
C                     0.21692  -0.64328  -1.02278
C                     1.27059  -0.09811  -0.01517
C                     0.53477  -0.21041   1.34214
C                    -1.97489  -1.62843  -0.79789
O                    -0.24927   2.91292  -0.30612
C                     2.60545  -0.64019  -0.1071
N                     3.64955  -1.09441  -0.1704
O                     1.2092    1.33148  -0.31752
H                    -3.03314   0.34416  -0.61026
H                    -2.46568  -0.1618    1.80108
H                    -0.58898   1.63972   2.06582
H                    -1.03095   0.88823  -2.08696
H                    -0.68441  -2.05064   1.90576
H                    -0.07438  -2.77556  -0.44446
H                     0.64176  -0.88136  -1.98598
H                     1.17596  -0.24734   2.20733
H                    -2.08882  -1.79783  -1.86261
H                    -2.67001  -2.26132  -0.25776
H                     1.20717   2.46056  -0.31856

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  88 maximum allowed number of steps= 156.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

--------------------------------------------------------------------------
                          Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
--------------------------------------------------------------------------
  1   1  C     0  -2.090408         -0.141479         -0.406460
  2   2  C     0  -1.659875         -0.143131          1.085012
  3   3  C     0  -0.539923          0.929959          1.258348
  4   4  C     0  -0.869986          0.512346         -1.089299
  5   5  C     0  -0.327661          1.576328         -0.122975
  6   6  C     0  -0.581855         -1.289137          1.149305
```

7	7	C	0	-0.518956	-1.799647	-0.311715
8	8	C	0	0.216921	-0.643284	-1.022779
9	9	C	0	1.270594	-0.098112	-0.015174
10	10	C	0	0.534774	-0.210405	1.342136
11	11	C	0	-1.974888	-1.628431	-0.797885
12	12	O	0	-0.249269	2.912917	-0.306116
13	13	C	0	2.605453	-0.640189	-0.107102
14	14	N	0	3.649552	-1.094414	-0.170400
15	15	O	0	1.209203	1.331479	-0.317519
16	16	H	0	-3.033144	0.344156	-0.610258
17	17	H	0	-2.465678	-0.161801	1.801080
18	18	H	0	-0.588976	1.639719	2.065820
19	19	H	0	-1.030947	0.888229	-2.086960
20	20	H	0	-0.684409	-2.050635	1.905763
21	21	H	0	-0.074375	-2.775564	-0.444455
22	22	H	0	0.641760	-0.881364	-1.985985
23	23	H	0	1.175958	-0.247340	2.207329
24	24	H	0	-2.088823	-1.797829	-1.862608
25	25	H	0	-2.670010	-2.261317	-0.257757
26	26	H	0	1.207171	2.460559	-0.318561

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.090408	-0.141479	-0.406460
2	6	0	-1.659875	-0.143131	1.085012
3	6	0	-0.539923	0.929959	1.258348
4	6	0	-0.869986	0.512346	-1.089299
5	6	0	-0.327661	1.576328	-0.122975
6	6	0	-0.581855	-1.289137	1.149305
7	6	0	-0.518956	-1.799647	-0.311715
8	6	0	0.216921	-0.643284	-1.022779
9	6	0	1.270594	-0.098112	-0.015174
10	6	0	0.534774	-0.210405	1.342136
11	6	0	-1.974888	-1.628431	-0.797885
12	8	0	-0.249269	2.912917	-0.306116
13	6	0	2.605453	-0.640189	-0.107102
14	7	0	3.649552	-1.094414	-0.170400
15	8	0	1.209203	1.331479	-0.317519
16	1	0	-3.033144	0.344156	-0.610258
17	1	0	-2.465678	-0.161801	1.801080
18	1	0	-0.588976	1.639719	2.065820
19	1	0	-1.030947	0.888229	-2.086960
20	1	0	-0.684409	-2.050635	1.905763
21	1	0	-0.074375	-2.775564	-0.444455
22	1	0	0.641760	-0.881364	-1.985985
23	1	0	1.175958	-0.247340	2.207329
24	1	0	-2.088823	-1.797829	-1.862608
25	1	0	-2.670010	-2.261317	-0.257757
26	1	0	1.207171	2.460559	-0.318561

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.552369	0.000000			
3	C	2.514671	1.560724	0.000000		
4	C	1.543757	2.404413	2.407237	0.000000	
5	C	2.477600	2.488085	1.539773	1.536215	0.000000
6	C	2.452194	1.574672	2.222169	2.887855	3.145505
7	C	2.286473	2.448793	3.149014	2.464380	3.386654
8	C	2.440374	2.866234	2.872533	1.587852	2.456195
9	C	3.383980	3.130509	2.440647	2.471535	2.317281
10	C	3.154983	2.210684	1.569211	2.899585	2.466325
11	C	1.541942	2.418812	3.582259	2.426655	3.665971
12	O	3.567800	3.642043	2.542469	2.600270	1.351353
13	C	4.731748	4.456593	3.771367	3.791006	3.676460
14	N	5.823311	5.538142	4.867351	4.883879	4.790964
15	O	3.614547	3.517553	2.388308	2.364244	1.568359
16	H	1.079873	2.235454	3.170332	2.221941	3.012529
17	H	2.239302	1.078156	2.279261	3.369718	3.360684
18	H	3.396930	2.299427	1.076186	3.362248	2.205250
19	H	2.237596	3.394210	3.381410	1.078204	2.196663
20	H	3.311810	2.294284	3.053516	3.946354	4.171080
21	H	3.317263	3.432606	4.104531	3.443715	4.371095
22	H	3.241461	3.908137	3.899098	2.243178	3.232775
23	H	4.184764	3.051623	2.287104	3.953576	3.319179
24	H	2.205417	3.407416	4.424962	2.724056	4.184848
25	H	2.202672	2.703722	4.125541	3.409509	4.498031
26	H	4.201471	4.119365	2.807439	2.950280	1.782085

		6	7	8	9	10
6	C	0.000000				
7	C	1.548921	0.000000			
8	C	2.402731	1.544119	0.000000		
9	C	2.491208	2.487096	1.556505	0.000000	
10	C	1.564515	2.524136	2.425126	1.548009	0.000000
11	C	2.418101	1.544479	2.413528	3.672556	3.590110
12	O	4.459386	4.720278	3.657527	3.385399	3.617540
13	C	3.486922	3.338883	2.558038	1.443657	2.563731
14	N	4.436704	4.230104	3.565533	2.583825	3.573665
15	O	3.496726	3.576383	2.319850	1.462502	2.363623
16	H	3.431111	3.317553	3.421715	4.367137	4.104804
17	H	2.290084	3.306988	3.924582	4.154824	3.035738
18	H	3.068916	4.181724	3.924413	3.287642	2.282431
19	H	3.926324	3.261642	2.243922	3.249963	3.926471
20	H	1.078251	2.237762	3.371853	3.365172	2.278273
21	H	2.237649	1.080595	2.228437	3.026875	3.184809
22	H	3.390215	2.234656	1.079322	2.212015	3.396766
23	H	2.301013	3.409981	3.392657	2.229517	1.077516
24	H	3.406074	2.206752	2.711963	4.193773	4.435489
25	H	2.699139	2.200701	3.396713	4.501851	4.127534
26	H	4.406298	4.596620	3.333221	2.577375	3.216222

		11	12	13	14	15
11	C	0.000000				
12	O	4.882974	0.000000			
13	C	4.736383	4.562193	0.000000		
14	N	5.684473	5.592667	1.140381	0.000000	

15	O	4.373815	2.151329	2.425132	3.444112	0.000000
16	H	2.246377	3.800131	5.745944	6.849919	4.365548
17	H	3.024318	4.336662	5.439337	6.492499	4.497010
18	H	4.560961	2.713395	4.485972	5.517362	3.001460
19	H	2.980993	2.807452	4.413536	5.432416	2.888886
20	H	3.025443	5.451477	4.106601	4.899799	4.468495
21	H	2.247838	5.692850	3.443125	4.094997	4.304821
22	H	2.969265	4.244109	2.728453	3.519737	2.828859
23	H	4.567992	4.282044	2.748523	3.534091	2.978025
24	H	1.084118	5.291290	5.143749	6.023895	4.801754
25	H	1.084194	5.712707	5.520984	6.426987	5.287726
26	H	5.203373	1.525123	3.408012	4.315670	1.129082

		16	17	18	19	20
16	H	0.000000				
17	H	2.528351	0.000000			
18	H	3.848874	2.614875	0.000000		
19	H	2.546656	4.275263	4.243307	0.000000	
20	H	4.193083	2.598379	3.695056	4.969793	0.000000
21	H	4.302843	4.194343	5.104999	4.127497	2.534006
22	H	4.110893	4.951344	4.928255	2.437130	4.274532
23	H	5.099530	3.665224	2.587665	4.959926	2.608406
24	H	2.654849	4.030039	5.431282	2.895573	4.029505
25	H	2.654169	2.947631	4.994777	3.994014	2.944116
26	H	4.748107	4.985927	3.095997	3.257089	5.373692

		21	22	23	24	25
21	H	0.000000				
22	H	2.545026	0.000000			
23	H	3.871332	4.274487	0.000000		
24	H	2.650495	2.882918	5.443087	0.000000	
25	H	2.652664	3.982319	4.992416	1.768657	0.000000
26	H	5.392142	3.777359	3.703216	5.601922	6.110020

		26
26	H	0.000000

Interatomic angles:

C1-C2-C3=107.7574	C2-C1-C4=101.898	C1-C4-C3= 75.5519
C3-C2-C4= 71.1711	C2-C1-C5= 72.1508	C1-C5-C3= 73.3525
C2-C3-C5=106.7331	C1-C4-C5=107.1089	C2-C4-C5= 74.6899
C3-C5-C4=102.9966	C1-C2-C6=103.2893	C1-C6-C3= 64.8731
C3-C2-C6= 90.2633	C4-C1-C6= 89.5707	C4-C2-C6= 90.5971
C4-C3-C6= 77.0744	C5-C1-C6= 79.2928	C5-C2-C6= 98.987
C5-C3-C6=112.1963	C5-C4-C6= 84.7915	C2-C1-C7= 76.6326
C3-C1-C7= 81.8247	C3-C2-C7=101.1935	C4-C1-C7= 77.4167
C4-C2-C7= 61.0245	C3-C4-C7= 80.5321	C5-C1-C7= 90.5207
C5-C2-C7= 86.6233	C5-C4-C7=113.6413	C1-C7-C6= 76.8297
C2-C6-C7=103.2474	C3-C6-C7=112.003	C4-C7-C6= 89.0046
C2-C1-C8= 88.8658	C3-C1-C8= 70.8434	C3-C2-C8= 74.4416
C1-C4-C8=102.3787	C2-C4-C8= 89.3458	C3-C4-C8= 89.5157
C1-C8-C5= 60.7928	C2-C5-C8= 70.8565	C3-C5-C8= 88.8459
C5-C4-C8=103.6545	C1-C8-C6= 60.833	C2-C6-C8= 89.7167
C3-C6-C8= 76.6829	C4-C8-C6= 90.3403	C5-C8-C6= 80.6785
C1-C7-C8= 76.4296	C2-C7-C8= 88.7453	C3-C8-C7= 85.3481
C4-C8-C7=103.7748	C5-C8-C7=113.7275	C6-C7-C8=101.9403
C1-C3-C9= 86.1275	C2-C3-C9=100.6464	C1-C4-C9=112.8208
C2-C4-C9= 79.8739	C4-C3-C9= 61.2987	C1-C5-C9= 89.7157

C2-C5-C9= 81.2193 C3-C5-C9= 75.5234 C4-C5-C9= 76.8374
C1-C6-C9= 86.3958 C2-C6-C9= 98.1657 C6-C3-C9= 64.3894
C4-C9-C6= 71.1683 C5-C9-C6= 81.6247 C1-C7-C9= 90.19
C2-C7-C9= 78.7222 C3-C9-C7= 79.4341 C7-C4-C9= 60.5135
C5-C9-C7= 89.5724 C6-C7-C9= 72.017 C1-C8-C9=113.8618
C2-C8-C9= 84.6114 C3-C9-C8= 89.0345 C4-C8-C9=103.6262
C5-C9-C8= 75.8817 C6-C8-C9= 74.5728 C7-C8-C9=106.6669
C1-C2-C10=112.7746 C1-C3-C10= 98.5103 C2-C3-C10= 89.8694
C1-C4-C10= 84.6363 C4-C2-C10= 77.7218 C4-C3-C10= 91.1406
C1-C5-C10= 79.3082 C2-C10-C5= 64.0053 C5-C3-C10=104.9841
C4-C5-C10= 89.7345 C1-C6-C10=101.2198 C2-C6-C10= 89.5328
C3-C10-C6= 90.3256 C4-C6-C10= 74.7301 C5-C10-C6=100.1784
C1-C7-C10= 81.8052 C7-C2-C10= 65.3687 C3-C10-C7= 97.8547
C4-C7-C10= 71.0658 C5-C10-C7= 85.4643 C7-C6-C10=108.3323
C1-C8-C10= 80.8475 C2-C10-C8= 76.2252 C3-C10-C8= 89.3058
C4-C8-C10= 90.0378 C5-C8-C10= 60.693 C8-C6-C10= 71.8691
C7-C8-C10= 75.3491 C2-C10-C9=111.5736 C3-C10-C9=103.062
C4-C9-C10= 89.272 C5-C9-C10= 76.4298 C6-C10-C9=106.332
C7-C9-C10= 73.3154 C8-C9-C10=102.7337 C2-C1-C11=102.8318
C3-C1-C11=122.1912 C3-C2-C11=127.0213 C4-C1-C11=103.7044
C4-C2-C11= 60.4122 C3-C4-C11= 95.6447 C5-C1-C11=130.1171
C5-C2-C11= 96.6704 C5-C4-C11=134.1234 C1-C11-C6= 72.7485
C2-C6-C11= 71.0254 C3-C6-C11=100.9823 C4-C11-C6= 73.1789
C1-C11-C7= 95.6021 C2-C11-C7= 72.5585 C4-C11-C7= 72.9254
C6-C7-C11=102.8323 C1-C11-C8= 72.4264 C2-C11-C8= 72.7596
C3-C8-C11= 84.8527 C4-C8-C11= 71.2973 C5-C8-C11= 97.6647
C6-C8-C11= 60.2736 C8-C7-C11=102.7837 C9-C4-C11= 97.1381
C9-C6-C11= 96.8374 C9-C7-C11=129.7897 C9-C8-C11=134.2192
C10-C2-C11=101.6038 C10-C4-C11= 84.2604 C10-C6-C11=127.3846
C10-C7-C11=122.004 C10-C8-C11= 95.7978 C1-C3-O12= 89.7378
C2-C3-O12=123.3632 C1-C4-O12=116.5188 C2-C4-O12= 93.3095
C4-C3-O12= 63.3127 C1-C5-O12=135.3592 C2-C5-O12=141.2959
C3-C5-O12=123.009 C4-C5-O12=128.3353 C6-C3-O12=138.6613
C6-C4-O12=108.5788 C7-C4-O12=137.4829 C8-C3-O12= 84.7439
C8-C4-O12=119.7278 C8-C5-O12=146.2321 C9-C3-O12= 85.5636
C9-C4-O12= 83.7067 C9-C5-O12=132.9209 C10-C3-O12=121.4228
C10-C4-O12= 82.0623 C10-C5-O12=140.9648 C11-C4-O12=152.4938
C1-C8-C13=142.3895 C2-C8-C13=110.3623 C3-C8-C13= 87.7702
C4-C8-C13=130.7887 C5-C8-C13= 94.2896 C6-C8-C13= 89.2633
C7-C8-C13=106.3231 C3-C9-C13=151.3191 C4-C9-C13=149.9847
C5-C9-C13=154.9711 C6-C9-C13=122.5341 C7-C9-C13=113.6299
C8-C9-C13=116.9488 C2-C10-C13=137.8318 C3-C10-C13=130.1503
C4-C10-C13= 87.654 C5-C10-C13= 93.9035 C6-C10-C13=113.0292
C7-C10-C13= 82.0241 C10-C8-C13= 61.8572 C10-C9-C13=117.9114
C11-C8-C13=144.5969 C3-C9-N14=151.2552 C4-C9-N14=150.0605
C5-C9-N14=155.6237 C6-C9-N14=121.8954 C7-C9-N14=113.0491
C8-C9-N14=116.7006 C10-C9-N14=117.5388 C8-C13-N14=146.569
C9-C13-N14=178.5171 C10-C13-N14=146.8916 C1-C3-O15= 94.9544
C2-C3-O15=124.6003 C1-C4-O15=134.2335 C2-C4-O15= 95.0578
C3-O15-C4= 60.8614 C1-C5-O15=125.0822 C2-C5-O15=118.4909
C3-C5-O15=100.418 C4-C5-O15= 99.1943 C6-C3-O15= 98.588
C6-C4-O15= 82.8388 C7-C4-O15= 95.5535 C1-C8-O15= 98.7776
C2-C8-O15= 84.7197 C3-O15-C8= 75.1804 C4-C8-O15= 71.6992
C5-O15-C8= 75.6088 C6-C8-O15= 95.5195 C7-C8-O15=134.5339

C3-O15-C9= 74.3357 C4-O15-C9= 76.4514 C5-O15-C9= 99.6771
C6-C9-O15=122.1916 C7-C9-O15=127.8718 C8-C9-O15=100.3772
C2-C10-O15=100.4715 C3-C10-O15= 71.5705 C4-O15-C10= 75.6565
C5-O15-C10= 74.6411 C6-C10-O15=124.534 C7-C10-O15= 94.0009
C8-O15-C10= 62.362 C10-C9-O15=103.4278 C11-C4-O15=131.826
C11-C8-O15=135.0378 C3-O15-O12= 67.8881 C4-O15-O12= 70.1363
O12-C5-O15= 94.632 C8-O15-O12=109.7174 C9-O15-O12=138.238
C10-O15-O12=106.4017 C3-O15-C13=103.1631 C4-O15-C13=104.6531
C5-O15-C13=132.8705 C8-O15-C13= 65.2012 C13-C9-O15=113.1219
C10-O15-C13= 64.7224 O12-O15-C13=170.9328 N14-C9-O15=113.7749
N14-C13-O15=147.7951 C2-C1-H16=115.0822 C3-C1-H16=118.1385
C3-C2-H16=112.0349 C4-C1-H16=114.5958 C2-H16-C4= 65.2877
C3-C4-H16= 86.3511 C5-C1-H16=109.3241 C5-C2-H16= 79.0528
C3-C5-H16= 81.3503 C5-C4-H16=105.0996 C6-C1-H16=150.1425
C6-C2-H16=127.6013 C6-C4-H16= 83.2688 C7-C1-H16=159.0605
C7-C2-H16= 90.0645 C7-C4-H16= 89.9789 C8-C1-H16=150.4845
C8-C2-H16= 83.258 C8-C4-H16=127.0336 C8-C5-H16= 76.7173
C9-C4-H16=136.9524 C9-C5-H16=109.3531 C10-C2-H16=134.8049
C10-C4-H16=105.7832 C10-C5-H16= 96.5355 C11-C1-H16=116.819
C2-H16-C11= 65.3249 C4-H16-C11= 65.7845 C5-H16-C11= 87.1108
C6-C11-H16= 94.6414 C7-C11-H16=121.0068 C8-C11-H16= 94.426
O12-C4-H16=103.7298 O12-C5-H16=115.7677 O15-C4-H16=144.293
O15-C5-H16=142.7615 C1-C2-H17=115.5211 C1-H17-C3= 67.6243
C3-C2-H17=118.3242 C4-C1-H17=124.9161 C4-C2-H17=148.3043
C4-C3-H17= 91.9071 C5-C1-H17= 90.7292 C5-C2-H17=137.2737
C5-C3-H17=122.0839 C1-H17-C6= 65.5463 C6-C2-H17=118.1605
C6-C3-H17= 61.1451 C4-C6-H17= 80.2973 C7-C1-H17= 93.8846
C7-C2-H17=135.6696 C7-C6-H17=117.6525 C8-C1-H17=113.9256
C8-C2-H17=167.1048 C8-C3-H17= 98.5902 C8-C6-H17=113.4804
C9-C3-H17=123.3153 C9-C6-H17=120.6217 C10-C2-H17=131.6205
C10-C3-H17=102.582 C10-C6-H17=102.2754 C11-C1-H17=104.7176
C11-C2-H17=114.1444 C11-C6-H17= 79.8845 O12-C3-H17=128.0753
O15-C3-H17=148.9177 H16-C1-H17= 92.5119 H16-C2-H17= 92.7692
C3-H17-H16= 82.3385 C4-H16-H17= 90.1296 C5-H16-H17= 74.0986
C6-H17-H16= 90.6703 C11-H16-H17= 78.3579 C1-C2-H18=122.5578
C1-C3-H18=138.5585 C2-C3-H18=120.2701 C4-C2-H18= 91.2237
C4-C3-H18=147.1295 C1-C5-H18= 92.8194 C2-H18-C5= 67.0167
C5-C3-H18=113.7364 C4-C5-H18=127.0428 C6-C2-H18=103.1809
C6-C3-H18=133.9922 C7-C2-H18=123.4216 C8-C2-H18= 98.2804
C8-C3-H18=165.7075 C8-C5-H18=114.5733 C9-C3-H18=134.6785
C9-C5-H18= 93.229 C2-C10-H18= 61.5386 C10-C3-H18=118.0622
C4-C10-H18= 79.9388 C5-H18-C10= 66.6502 C6-C10-H18=104.2754
C7-C10-H18=120.8355 C8-C10-H18=112.9143 C9-C10-H18=116.9515
C11-C2-H18=150.3198 C2-H18-O12= 92.8231 O12-C3-H18= 87.2787
C4-O12-H18= 78.4755 O12-C5-H18= 96.4857 C10-H18-O12= 92.3811
C13-C10-H18=135.4617 C2-H18-O15= 81.992 O15-C3-H18=114.6818
C4-O15-H18= 76.5807 O15-C5-H18=104.1063 C8-O15-H18= 94.1614
C9-O15-H18= 87.7865 O15-C10-H18= 80.4642 O15-O12-H18= 75.2016
C13-O15-H18=111.071 H16-C2-H18=116.1398 H16-C5-H18= 93.7776
C1-H17-H18= 88.4689 H17-C2-H18= 94.4857 H17-C3-H18= 95.6662
C5-H18-H17= 87.9801 C6-H17-H18= 77.1489 C10-H18-H17= 76.2786
O12-H18-H17=108.9428 O15-H18-H17=106.1904 H16-H17-H18= 96.8789
C2-C1-H19=126.2097 C3-C1-H19= 90.5271 C1-C4-H19=116.0345
C2-C4-H19=151.9751 C3-C4-H19=149.5853 C1-H19-C5= 67.9302

C2-C5-H19= 92.6467 C3-C5-H19=128.788 C5-C4-H19=113.1593
C6-C1-H19=113.6141 C6-C4-H19=161.7393 C7-C1-H19= 92.26
C7-C4-H19=129.8131 C1-H19-C8= 65.9865 C2-C8-H19= 82.2715
C3-C8-H19= 81.7371 C8-C4-H19=113.2457 C5-H19-C8= 67.1534
C6-C8-H19=115.2969 C7-C8-H19=117.6773 C9-C4-H19=128.1365
C9-C5-H19= 92.0667 C9-C8-H19=116.3856 C10-C4-H19=159.2487
C10-C5-H19=114.5915 C10-C8-H19=114.4271 C11-C1-H19=102.5711
C2-C11-H19= 77.1129 C11-C4-H19=110.5298 C5-H19-C11= 88.8086
C6-C11-H19= 92.7134 C7-C11-H19= 86.0555 C11-C8-H19= 79.4995
C1-H19-O12= 89.2729 C3-O12-H19= 78.23 O12-C4-H19= 89.5694
O12-C5-H19=101.96 C8-H19-O12= 92.0947 C11-H19-O12=115.0059
C13-C8-H19=133.4876 C1-H19-O15= 88.7255 C3-O15-H19= 79.0729
O15-C4-H19=108.2133 O15-C5-H19= 98.8544 O15-C8-H19= 78.5248
C9-O15-H19= 90.5267 C10-O15-H19= 96.2418 C11-H19-O15= 96.3277
O15-O12-H19= 69.8338 C13-O15-H19=112.0152 H16-C1-H19= 93.7075
C2-H16-H19= 90.191 H16-C4-H19= 94.6198 C5-H19-H16= 78.4746
C8-H19-H16= 90.94 C11-H16-H19= 76.6319 O12-H19-H16= 90.2955
O15-H19-H16=106.6946 H17-C1-H19=145.4772 H17-H16-H19=114.7916
H18-C5-H19=149.1454 H18-O12-H19=100.4423 H18-O15-H19= 92.1521
C1-C2-H20=117.5489 C3-C2-H20=103.1099 C4-C2-H20=114.2351
C5-C2-H20=121.3728 C1-C6-H20=135.8166 C2-C6-H20=118.5229
C3-C6-H20=132.2701 C4-C6-H20=167.1366 C1-C7-H20= 94.1051
C2-H20-C7= 65.3981 C4-C7-H20=114.0392 C7-C6-H20=115.648
C8-C2-H20= 80.7695 C8-C6-H20=148.8338 C8-C7-H20=125.1385
C9-C6-H20=137.4174 C9-C7-H20= 90.6751 C2-C10-H20= 61.4517
C3-C10-H20=103.5151 C4-C10-H20= 98.5996 C5-C10-H20=123.0244
C10-C6-H20=117.928 C7-H20-C10= 67.9565 C8-C10-H20= 91.5434
C9-C10-H20=121.9971 C11-C2-H20= 79.8229 C11-C6-H20=114.2707
C11-C7-H20=104.7536 C13-C10-H20=115.8908 O15-C10-H20=148.5744
H16-C2-H20=135.5379 C1-H17-H20= 86.0681 H17-C2-H20= 93.7715
C3-H17-H20= 77.2077 H17-C6-H20= 93.9996 C7-H20-H17= 85.9418
C10-H20-H17= 76.6866 H16-H17-H20=109.74 H18-C2-H20=107.0994
H18-C10-H20=108.2298 H18-H17-H20= 90.2711 C1-C6-H21= 89.916
C2-C6-H21=127.5626 C3-C6-H21=133.9502 C4-C6-H21= 83.3904
C1-C7-H21=158.8484 C2-C7-H21=150.772 C4-C7-H21=150.1265
C6-C7-H21=115.4827 C1-C8-H21= 90.4366 C2-C8-H21= 83.7151
C3-C8-H21=106.4705 C4-C8-H21=128.1545 C5-C8-H21=137.7851
C6-H21-C8= 65.0941 C8-C7-H21=115.0684 C9-C6-H21= 79.3981
C9-C7-H21=109.6629 C9-C8-H21=104.8109 C10-C6-H21=112.578
C10-C7-H21=118.5131 C10-C8-H21= 86.2646 C1-C11-H21=121.0347
C2-C11-H21= 94.6384 C4-C11-H21= 94.8256 C6-H21-C11= 65.2436
C11-C7-H21=116.6979 C8-H21-C11= 65.2543 C13-C8-H21= 91.7372
O15-C8-H21=142.3288 H16-C11-H21=146.4391 H17-C6-H21=135.7477
H19-C8-H21=134.7044 H19-C11-H21=103.362 C2-H20-H21= 90.4822
H20-C6-H21= 92.9874 H20-C7-H21= 92.9148 C8-H21-H20= 89.9101
C10-H20-H21= 82.6921 C11-H21-H20= 78.2461 H17-H20-H21=109.6107
C1-C4-H22=116.5161 C2-C4-H22=114.4251 C3-C4-H22=113.9053
C5-C4-H22=116.3499 C6-C4-H22= 81.6655 C1-C7-H22= 91.6005
C2-C7-H22=113.0395 C4-H22-C7= 66.7819 C6-C7-H22=126.325
C1-C8-H22=130.0081 C2-C8-H22=162.2699 C3-C8-H22=158.9396
C4-C8-H22=113.1157 C5-C8-H22=127.8457 C6-C8-H22=151.4397
C7-C8-H22=115.6804 C3-C9-H22=113.7763 C4-H22-C9= 67.3833
C5-C9-H22= 91.0509 C6-C9-H22= 92.0509 C7-H22-C9= 68.0149
C9-C8-H22=112.8618 C10-C4-H22= 81.5951 C10-C7-H22= 90.8791

C10-C8-H22=149.0977 C10-C9-H22=128.3444 C1-C11-H22= 85.697
C2-C11-H22= 92.4193 C11-C4-H22= 78.857 C6-C11-H22= 77.246
C11-C7-H22=102.0193 C11-C8-H22=110.5225 C9-H22-C11= 89.0322
O12-C4-H22=122.2163 C4-H22-C13= 98.9078 C7-H22-C13= 83.9275
C13-C8-H22= 87.2593 C13-C9-H22= 94.1959 C10-C13-H22= 79.7928
C11-H22-C13=112.3918 N14-C9-H22= 94.1106 N14-C13-H22=125.8393
C3-O15-H22= 96.3586 O15-C4-H22= 75.7046 C5-O15-H22= 89.9266
C7-H22-O15= 89.0682 O15-C8-H22=106.9006 O15-C9-H22= 98.6269
C10-O15-H22= 81.177 C11-H22-O15= 97.9079 O12-O15-H22=116.2418
O15-C13-H22= 66.281 H16-C4-H22=134.0474 H16-C11-H22=103.1579
H18-O15-H22=115.3722 C1-H19-H22= 87.6912 H19-C4-H22= 86.9809
C5-H19-H22= 88.319 C7-H22-H19= 88.4481 H19-C8-H22= 86.9169
C9-H22-H19= 88.5631 C11-H22-H19= 66.0731 O12-H19-H22=107.8346
C13-H22-H19=117.2785 O15-H22-H19= 66.0543 H16-H19-H22=111.1283
H20-C7-H22=145.7849 C4-H22-H21= 91.7574 C6-H21-H22= 90.0469
H21-C7-H22= 93.7491 H21-C8-H22= 94.1282 C9-H22-H21= 78.6897
C11-H21-H22= 76.2815 C13-H22-H21= 81.4427 O15-H22-H21=106.3438
H19-H22-H21=111.8627 H20-H21-H22=114.6195 C1-C3-H23=121.1951
C2-C3-H23=103.3277 C4-C3-H23=114.7224 C5-C3-H23=119.0053
C1-C6-H23=123.3521 C2-C6-H23=102.2546 C6-C3-H23= 61.3456
C4-C6-H23= 98.6396 C7-C6-H23=123.4986 C8-C3-H23= 81.3676
C8-C6-H23= 92.2927 C3-H23-C9= 65.4032 C4-C9-H23=114.3934
C5-C9-H23= 93.7534 C6-H23-C9= 66.6947 C7-C9-H23= 92.4371
C8-C9-H23=126.3799 C2-C10-H23=133.2494 C3-C10-H23=118.38
C4-C10-H23=165.9639 C5-C10-H23=135.2272 C6-C10-H23=120.0025
C7-C10-H23=138.8455 C8-C10-H23=148.7475 C9-C10-H23=115.0666
C11-C6-H23=150.9127 O12-C3-H23=124.8218 C3-H23-C13= 96.5677
C6-H23-C13= 86.871 C8-C13-H23= 79.3952 C13-C9-H23= 94.4502
C13-C10-H23= 88.1394 N14-C9-H23= 94.1955 N14-C13-H23=125.4403
O15-C3-H23= 79.0977 C4-O15-H23= 94.7762 C5-O15-H23= 88.0894
C6-H23-O15= 81.8782 C8-O15-H23= 78.5613 O15-C9-H23=105.648
O15-C10-H23=114.6059 O12-O15-H23=112.1885 O15-C13-H23= 69.9656
H17-C3-H23=106.769 H17-C6-H23=105.9421 C2-H18-H23= 77.0297
H18-C3-H23= 93.5754 C5-H18-H23= 87.2771 C6-H23-H18= 77.5249
C9-H23-H18= 85.7348 H18-C10-H23= 93.7941 O12-H18-H23=107.734
C13-H23-H18=114.3883 O15-H23-H18= 64.8261 H17-H18-H23= 89.5778
H19-O15-H23=115.4227 C2-H20-H23= 76.6917 C3-H23-H20= 76.8685
H20-C6-H23= 94.0041 C7-H20-H23= 89.0999 C9-H23-H20= 87.782
H20-C10-H23= 95.2847 C13-H23-H20=100.0656 O15-H23-H20=106.0491
H17-H20-H23= 89.4865 H18-H23-H20= 90.6522 H21-C6-H23=117.065
H21-H20-H23= 97.6607 H22-C9-H23=148.4723 H22-C13-H23=102.6023
H22-O15-H23= 94.7669 C2-C1-H24=129.2985 C3-C1-H24=139.1717
C4-C1-H24= 91.4594 C2-C4-H24= 83.0231 C3-C4-H24=119.0339
C5-C1-H24=126.5665 C5-C4-H24=157.5024 C6-C1-H24= 93.8392
C6-C4-H24= 74.6727 C1-H24-C7= 62.4258 C2-C7-H24= 93.9481
C4-C7-H24= 71.1037 C6-C7-H24=129.3274 C8-C1-H24= 71.2244
C2-C8-H24= 75.2445 C3-C8-H24=104.7777 C4-C8-H24= 73.4342
C5-C8-H24=108.0385 C6-C8-H24= 83.2733 C8-C7-H24= 90.8465
C9-C4-H24=107.5433 C9-C7-H24=126.52 C9-C8-H24=157.6879
C10-C4-H24=104.0889 C10-C7-H24=139.1953 C10-C8-H24=119.3019
C1-C11-H24=113.0864 C2-C11-H24=150.9444 C4-C11-H24= 93.8852
C6-C11-H24=150.8465 C7-C11-H24=113.0102 C8-C11-H24= 93.8822
O12-C4-H24=167.2248 C13-C8-H24=154.8557 O15-C4-H24=141.2591
O15-C8-H24=145.1054 H16-C1-H24=102.3436 C2-H16-H24= 87.8998

C4-H16-H24= 67.2373 C5-H16-H24= 94.9831 C7-H24-H16= 85.5368
C8-H24-H16= 79.2138 H16-C11-H24= 99.7721 H17-C1-H24=130.1057
H17-H16-H24=102.0404 H19-C1-H24= 81.3384 H19-C4-H24= 88.0619
C5-H19-H24=109.7719 C7-H24-H19= 78.189 H19-C8-H24= 70.7851
C11-H24-H19= 83.8433 O12-H19-H24=136.1846 O15-H19-H24=112.2206
H19-H16-H24= 67.616 H20-C7-H24=130.0846 C1-H24-H21= 85.6598
C4-H24-H21= 79.6819 C6-H21-H24= 87.9184 H21-C7-H24=101.9522
C8-H21-H24= 66.8912 H21-C11-H24= 99.412 H16-H24-H21=108.3952
H19-H24-H21= 96.0838 H20-H21-H24=101.9903 C1-H24-H22= 77.8886
H22-C4-H24= 70.1932 H22-C7-H24= 80.9449 H22-C8-H24= 87.9593
C9-H22-H24=110.1021 C11-H24-H22= 83.847 C13-H22-H24=132.8678
O15-H22-H24=114.4199 H16-H24-H22= 95.774 H19-H22-H24= 65.3244
H22-H21-H24= 67.3702 C2-C1-H25= 90.4063 C3-C1-H25=121.8435
C3-C2-H25=149.5317 C4-C1-H25=130.2021 C4-C2-H25= 83.5234
C5-C1-H25=147.86 C5-C2-H25=120.0222 C6-C1-H25= 70.6483
C2-C6-H25= 73.2147 C3-C6-H25=113.5696 C4-C6-H25= 75.1314
C1-H25-C7= 62.5646 C2-C7-H25= 70.8844 C4-C7-H25= 93.7452
C6-C7-H25= 90.3623 C8-C1-H25= 93.896 C8-C2-H25= 75.0906
C8-C6-H25= 83.2666 C8-C7-H25=129.3614 C9-C6-H25=120.2516
C9-C7-H25=147.5543 C10-C2-H25=113.88 C10-C6-H25=149.8552
C10-C7-H25=121.6051 C1-C11-H25=112.8564 C2-C11-H25= 93.1038
C4-C11-H25=150.0797 C6-C11-H25= 92.8714 C7-C11-H25=112.5106
C8-C11-H25=150.1041 H16-C1-H25=102.4639 C2-H16-H25= 66.5001
C4-H16-H25= 88.2661 C5-H16-H25=104.9015 C6-H25-H16= 79.718
C7-H25-H16= 85.6723 H16-C11-H25= 99.7264 H17-C1-H25= 83.1435
H17-C2-H25= 92.1232 C3-H17-H25=103.4989 H17-C6-H25= 71.8972
C7-H25-H17= 78.4599 C11-H25-H17= 83.5545 H17-H16-H25= 69.2793
H18-C2-H25=173.3481 H18-H17-H25=127.6755 H19-C1-H25=128.1827
H19-C11-H25=155.6804 H19-H16-H25=100.3213 C1-H25-H20= 78.6545
H20-C2-H25= 71.6485 H20-C6-H25= 92.1645 H20-C7-H25= 83.1024
C10-H20-H25=103.7044 C11-H25-H20= 83.7953 H16-H25-H20= 96.8703
H17-H20-H25= 63.9006 C1-H25-H21= 85.6609 C2-H25-H21= 79.7033
C6-H21-H25= 66.3704 H21-C7-H25=102.4561 C8-H21-H25= 87.7464
H21-C11-H25= 99.5465 H16-H25-H21=108.3506 H17-H25-H21= 96.8581
H20-H21-H25= 69.1269 H22-C7-H25=127.7541 H22-C11-H25=155.6731
H22-H21-H25=100.0019 H23-C6-H25=173.6048 H23-H20-H25=127.9846
C1-H25-H24= 66.4264 C2-H25-H24= 97.0403 C4-H24-H25= 96.4122
C6-H25-H24= 97.1468 C7-H25-H24= 66.521 C8-H24-H25= 96.3125
H24-C11-H25=109.31 H16-H25-H24= 70.5612 H17-H25-H24=115.1094
H19-H24-H25=115.6869 H20-H25-H24=115.2412 H21-H24-H25= 70.5843
H22-H24-H25=115.6822 C1-C3-H26=104.1307 C2-C3-H26=139.3788
C1-C4-H26=136.1136 C2-C4-H26=100.0829 C4-C3-H26= 68.4153
C1-C5-H26=160.7729 C2-C5-H26=149.0182 C3-C5-H26=115.1804
C4-C5-H26=125.3565 C6-C3-H26=121.9123 C6-C4-H26= 98.0003
C7-C4-H26=115.8998 C8-C3-H26= 71.8554 C8-C4-H26= 89.2963
C8-C5-H26=102.546 C3-C9-H26= 67.9754 C4-C9-H26= 71.4778
C9-C5-H26= 76.6805 C6-C9-H26=120.7535 C7-C9-H26=130.3488
C8-C9-H26=104.7649 C10-C3-H26= 89.9996 C10-C4-H26= 66.6992
C10-C5-H26= 97.0933 C10-C9-H26= 99.4117 C11-C4-H26=150.6628
C3-O12-H26= 83.273 C4-O12-H26= 87.2303 C5-O12-H26= 76.2987
C9-H26-O12=108.481 C13-C9-H26=112.8314 N14-C9-H26=113.4768
C3-O15-H26= 99.6372 C4-O15-H26=110.1563 C5-O15-H26= 80.9227
C8-O15-H26=148.2328 C9-O15-H26=167.894 C10-O15-H26=130.7283
O12-H26-O15=107.3564 C13-O15-H26=144.5014 H16-C4-H26=132.7726

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    H16-C5-H26=163.4691     H17-C3-H26=157.0265     H18-C3-H26= 95.1775
    H18-C5-H26=101.3455    H18-O12-H26= 89.2847    H18-O15-H26= 84.0856
    H19-C4-H26= 96.6972     H19-C5-H26=109.4535    H19-O12-H26= 92.6829
   H19-O15-H26= 98.7122     H22-C4-H26= 92.3054     H22-C9-H26=103.8658
   H22-O15-H26=141.3827     H23-C3-H26= 92.6836     H23-C9-H26=100.5296
   H23-O15-H26=122.0675     H24-C4-H26=161.6586
 Stoichiometry    C12H11NO2
 Framework group  C1[X(C12H11NO2)]
 Deg. of freedom   72
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -2.092005   -0.095578   -0.411596
    2          6             0       -1.665516   -0.101788    1.081026
    3          6             0       -0.522029    0.946295    1.253711
    4          6             0       -0.855324    0.528105   -1.093376
    5          6             0       -0.291591    1.582899   -0.129233
    6          6             0       -0.613872   -1.271651    1.152127
    7          6             0       -0.558723   -1.788522   -0.306968
    8          6             0        0.204982   -0.651572   -1.019991
    9          6             0        1.268084   -0.126874   -0.011422
   10          6             0        0.526370   -0.217785    1.344279
   11          6             0       -2.009134   -1.586112   -0.797633
   12          8             0       -0.182502    2.916729   -0.316721
   13          6             0        2.590573   -0.699316   -0.097910
   14          7             0        3.624290   -1.177255   -0.156849
   15          8             0        1.239843    1.302682   -0.318806
   16          1             0       -3.022977    0.410543   -0.619584
   17          1             0       -2.473403   -0.099744    1.794984
   18          1             0       -0.557121    1.659781    2.058622
   19          1             0       -1.005134    0.904067   -2.092743
   20          1             0       -0.735603   -2.028004    1.910900
   21          1             0       -0.135991   -2.774698   -0.435182
   22          1             0        0.626840   -0.902541   -1.981233
   23          1             0        1.164292   -0.266207    2.211315
   24          1             0       -2.124092   -1.756585   -1.862075
   25          1             0       -2.719805   -2.201237   -0.257221
   26          1             0        1.263359    2.431508   -0.323706
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.0167878      0.7871262      0.5892410
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,C-12,O-16,C-
12,N-14,
 O-16,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1
 Standard basis: 3-21+G* (6D, 7F)
 There are   217 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    131072 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
```

```
  217 basis functions      318 primitive gaussians
   53 alpha electrons       53 beta electrons
      nuclear repulsion energy      1060.0790644747 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis=   217 RedAO= T  NBF=   217
 NBsUse=   217 1.00D-04 NBFU=   217
 Projected INDO Guess.
 Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 SCF Done:  E(RHF) =  -661.256897752     A.U. after   18 cycles
            Convg  =    0.7268D-08             -V/T =  2.0018
            S**2   =   0.0000
 Range of M.O.s used for correlation:     1   217
 NBasis=   217 NAE=    53 NBE=    53 NFC=     0 NFV=     0
 NROrb=    217 NOA=    53 NOB=    53 NVA=   164 NVB=   164

 **** Warning!!: The largest alpha MO coefficient is  0.10281511D+03

          Differentiating once with respect to electric field.
                with respect to dipole field.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2
JSym2E=2.
          There are   3 degrees of freedom in the 1st order CPHF.
   3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
   3 vectors were produced by pass  1.
   3 vectors were produced by pass  2.
   3 vectors were produced by pass  3.
   3 vectors were produced by pass  4.
   3 vectors were produced by pass  5.
   3 vectors were produced by pass  6.
   3 vectors were produced by pass  7.
   3 vectors were produced by pass  8.
   3 vectors were produced by pass  9.
   3 vectors were produced by pass 10.
   3 vectors were produced by pass 11.
   2 vectors were produced by pass 12.
   1 vectors were produced by pass 13.
 Inv2:  IOpt= 1 Iter= 1 AM= 7.79D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension  39 with in-core refinement.
 G2DrvN: will do   13 atoms at a time, making    2 passes doing MaxLOS=1.
 FoFDir used for L=0 through L=1.
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 1 Meth= 1.
 IRaf=       0 NMat=  41 IRICut=      41 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
          There are  81 degrees of freedom in the 1st order CPHF.
```

```
 78 vectors were produced by pass  0.
 AX will form  39 AO Fock derivatives at one time.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  1.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  2.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  3.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  4.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  5.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 78 vectors were produced by pass  6.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 46 vectors were produced by pass  7.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
  3 vectors were produced by pass  8.
 Inv2:  IOpt= 1 Iter= 1 AM= 5.31D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension 595 with in-core refinement.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.
 PrRfSu:  requested number of processors reduced to:   1 ShMem   1 Linda.

 ********************************************************************

           Population analysis using the SCF density.

 ********************************************************************

 Alpha  occ. eigenvalues --  -20.55086 -20.41754 -15.55182 -11.33540 -
11.31239
 Alpha  occ. eigenvalues --  -11.26167 -11.22743 -11.22606 -11.21088 -
11.21022
 Alpha  occ. eigenvalues --  -11.20642 -11.20482 -11.20388 -11.20222 -
11.19542
 Alpha  occ. eigenvalues --   -1.48023  -1.30309  -1.28691  -1.26004  -
1.12490
 Alpha  occ. eigenvalues --   -1.10396  -1.06913  -0.99074  -0.94356  -
0.90875
 Alpha  occ. eigenvalues --   -0.85680  -0.82071  -0.81021  -0.77953  -
0.74530
 Alpha  occ. eigenvalues --   -0.74190  -0.69459  -0.67128  -0.65980  -
0.63362
 Alpha  occ. eigenvalues --   -0.63182  -0.60454  -0.58866  -0.55332  -
0.54762
 Alpha  occ. eigenvalues --   -0.53466  -0.53184  -0.52552  -0.51541  -
0.50661
```

```
 Alpha  occ. eigenvalues --   -0.49448  -0.48431  -0.47486  -0.47106  -
0.46552
 Alpha  occ. eigenvalues --   -0.44369  -0.41556  -0.38217
 Alpha virt. eigenvalues --    0.04928   0.06224   0.06629   0.07097
0.08363
 Alpha virt. eigenvalues --    0.08582   0.08803   0.09327   0.09598
0.11414
 Alpha virt. eigenvalues --    0.11918   0.12126   0.13038   0.13362
0.13451
 Alpha virt. eigenvalues --    0.14166   0.14761   0.15351   0.16544
0.17159
 Alpha virt. eigenvalues --    0.17608   0.18145   0.18429   0.19064
0.19309
 Alpha virt. eigenvalues --    0.19651   0.19846   0.20234   0.21962
0.23376
 Alpha virt. eigenvalues --    0.23714   0.24161   0.24303   0.24622
0.25029
 Alpha virt. eigenvalues --    0.25056   0.25425   0.25649   0.26474
0.26561
 Alpha virt. eigenvalues --    0.27351   0.27677   0.28391   0.28966
0.29184
 Alpha virt. eigenvalues --    0.29480   0.30109   0.30626   0.31626
0.32729
 Alpha virt. eigenvalues --    0.32912   0.34172   0.35430   0.35648
0.36218
 Alpha virt. eigenvalues --    0.36595   0.37344   0.38659   0.39561
0.39868
 Alpha virt. eigenvalues --    0.41830   0.42518   0.43212   0.43986
0.45271
 Alpha virt. eigenvalues --    0.45289   0.45788   0.46962   0.48148
0.48681
 Alpha virt. eigenvalues --    0.49431   0.50190   0.51720   0.51993
0.53187
 Alpha virt. eigenvalues --    0.53679   0.54179   0.55101   0.55520
0.55795
 Alpha virt. eigenvalues --    0.57018   0.57982   0.59069   0.59422
0.60561
 Alpha virt. eigenvalues --    0.61080   0.62484   0.62835   0.65445
0.67853
 Alpha virt. eigenvalues --    0.71627   0.73089   0.99872   1.07926
1.09902
 Alpha virt. eigenvalues --    1.10709   1.11149   1.12100   1.13784
1.14379
 Alpha virt. eigenvalues --    1.15158   1.15714   1.16652   1.17490
1.17832
 Alpha virt. eigenvalues --    1.19439   1.19525   1.20225   1.21045
1.21280
 Alpha virt. eigenvalues --    1.23509   1.24139   1.25933   1.28181
1.29886
 Alpha virt. eigenvalues --    1.30938   1.31589   1.34554   1.36402
1.37881
 Alpha virt. eigenvalues --    1.39032   1.43898   1.45028   1.47208
1.48560
```

```
 Alpha virt. eigenvalues --    1.49568   1.50187   1.50980   1.52599
1.55557
 Alpha virt. eigenvalues --    1.56770   1.56918   1.59115   1.60408
1.66829
 Alpha virt. eigenvalues --    1.69023   1.72810   1.74523   1.76412
1.80687
 Alpha virt. eigenvalues --    1.85947   1.92970   1.98588   2.05377
2.10411
 Alpha virt. eigenvalues --    2.15207   2.23343   2.25798   2.31442
2.36254
 Alpha virt. eigenvalues --    2.39258   2.39738   2.49076   2.53276
2.62534
 Alpha virt. eigenvalues --    2.78897   2.93915   3.15053   3.18680
3.48847
 Alpha virt. eigenvalues --    3.63124   3.79584   3.93564   4.08521
          Condensed to atoms (all electrons):
               1         2         3         4         5         6
  1  C   13.822302  -6.213738   2.205413  -7.093227   0.470716   3.685909
  2  C   -6.213738  19.027183 -11.921231   1.354348   5.561698  -9.734794
  3  C    2.205413 -11.921231  35.309100  12.928828 -30.342271   7.968111
  4  C   -7.093227   1.354348  12.928828  33.004382 -28.952468  -1.859996
  5  C    0.470716   5.561698 -30.342271 -28.952468  63.535009  -1.885365
  6  C    3.685909  -9.734794   7.968111  -1.859996  -1.885365  18.275825
  7  C   -1.333115   2.572037  -0.500294   3.032853  -1.471736  -5.495044
  8  C    4.347578  -1.509713  -9.030028 -19.874223  23.697986   3.938205
  9  C   -1.245440  -2.825574  18.903533  19.290957 -31.988269   1.248690
 10  C   -2.509627   9.247593 -20.314880  -7.608364  22.660347  -9.066289
 11  C   -3.138652   0.652398   0.446546   2.458422  -0.705341  -0.395989
 12  O   -0.006399  -0.192772   1.121218   1.167542  -2.432681   0.047002
 13  C    2.249444  -0.296694  -0.253672  -1.432727 -12.922604  -0.531130
 14  N   -0.073798   0.014178   0.084513   0.178677   0.184976  -0.085350
 15  O   -0.001046   0.000107  -0.737483  -0.728346   1.647546   0.146272
 16  H    0.465750  -0.085844   0.023834  -0.082093   0.014504   0.032396
 17  H   -0.071574   0.535994  -0.143101  -0.005998   0.054993  -0.111087
 18  H    0.017510  -0.082413   0.539721   0.021474  -0.081723   0.032634
 19  H   -0.034155  -0.005238   0.051889   0.580138  -0.167734   0.006039
 20  H    0.006651  -0.121455   0.074493  -0.000372   0.001414   0.580968
 21  H   -0.044733   0.042688  -0.005352   0.076547   0.012110  -0.108915
 22  H    0.024708   0.001722  -0.017084  -0.136373   0.057048   0.009657
 23  H   -0.002066   0.041276  -0.066301  -0.007508   0.039498  -0.064841
 24  H   -0.076743   0.026837   0.004779   0.019383  -0.017965   0.034420
 25  H   -0.029171  -0.004022  -0.010578  -0.023930   0.015836   0.029508
 26  H    0.019446  -0.013823   0.167543   0.148693  -0.467827  -0.002084
               7         8         9        10        11        12
  1  C   -1.333115   4.347578  -1.245440  -2.509627  -3.138652  -0.006399
  2  C    2.572037  -1.509713  -2.825574   9.247593   0.652398  -0.192772
  3  C   -0.500294  -9.030028  18.903533 -20.314880   0.446546   1.121218
  4  C    3.032853 -19.874223  19.290957  -7.608364   2.458422   1.167542
  5  C   -1.471736  23.697986 -31.988269  22.660347  -0.705341  -2.432681
  6  C   -5.495044   3.938205   1.248690  -9.066289  -0.395989   0.047002
  7  C   12.552052  -5.523389   0.178170   2.129955  -1.540201   0.072527
  8  C   -5.523389  34.913180 -23.489166  12.606313  -1.653919  -0.793367
  9  C    0.178170 -23.489166  90.352744 -22.689570   1.473815   1.146936
 10  C    2.129955  12.606313 -22.689570  36.335217   0.465425  -0.678932
```

11	C	-1.540201	-1.653919	1.473815	0.465425	10.824364	0.013392
12	O	0.072527	-0.793367	1.146936	-0.678932	0.013392	9.113750
13	C	0.364406	-11.841246	-47.479430	-14.755925	-1.947834	0.359469
14	N	0.173086	0.155505	2.958816	0.539831	0.056041	-0.001526
15	O	0.082297	1.324158	-2.189465	1.290402	-0.062413	-0.346350
16	H	-0.023903	0.035598	-0.006253	-0.013128	-0.005217	0.000852
17	H	0.004526	0.015336	-0.033055	0.099789	0.022237	0.000070
18	H	0.000777	0.013565	-0.027341	-0.055629	0.001143	-0.001822
19	H	0.016778	-0.137875	0.031664	-0.009107	0.021121	0.004814
20	H	-0.111767	0.030820	0.031671	-0.119756	0.018469	-0.000051
21	H	0.473870	-0.123517	0.087543	0.039443	0.027560	-0.000050
22	H	-0.062435	0.602049	-0.128019	0.075457	0.009896	0.000126
23	H	0.008982	0.083958	-0.063696	0.593019	-0.002315	0.000169
24	H	-0.084659	0.058917	-0.029550	0.005749	0.379073	0.000103
25	H	-0.097388	0.086593	-0.028874	0.007925	0.368211	-0.000034
26	H	-0.002402	-0.160631	0.316629	-0.166819	0.003245	0.231722

		13	14	15	16	17	18
1	C	2.249444	-0.073798	-0.001046	0.465750	-0.071574	0.017510
2	C	-0.296694	0.014178	0.000107	-0.085844	0.535994	-0.082413
3	C	-0.253672	0.084513	-0.737483	0.023834	-0.143101	0.539721
4	C	-1.432727	0.178677	-0.728346	-0.082093	-0.005998	0.021474
5	C	-12.922604	0.184976	1.647546	0.014504	0.054993	-0.081723
6	C	-0.531130	-0.085350	0.146272	0.032396	-0.111087	0.032634
7	C	0.364406	0.173086	0.082297	-0.023903	0.004526	0.000777
8	C	-11.841246	0.155505	1.324158	0.035598	0.015336	0.013565
9	C	-47.479430	2.958816	-2.189465	-0.006253	-0.033055	-0.027341
10	C	-14.755925	0.539831	1.290402	-0.013128	0.099789	-0.055629
11	C	-1.947834	0.056041	-0.062413	-0.005217	0.022237	0.001143
12	O	0.359469	-0.001526	-0.346350	0.000852	0.000070	-0.001822
13	C	98.260186	-4.675115	-1.771844	-0.006428	-0.003807	-0.025048
14	N	-4.675115	8.150748	0.006464	0.000021	0.000005	0.000120
15	O	-1.771844	0.006464	9.724960	-0.000751	0.000066	0.005297
16	H	-0.006428	0.000021	-0.000751	0.372684	-0.000621	-0.000013
17	H	-0.003807	0.000005	0.000066	-0.000621	0.366714	-0.000570
18	H	-0.025048	0.000120	0.005297	-0.000013	-0.000570	0.337955
19	H	-0.009536	-0.000034	0.004357	-0.000595	-0.000015	-0.000009
20	H	-0.029987	-0.000232	-0.000135	-0.000009	-0.000456	-0.000067
21	H	-0.128683	0.002481	-0.000596	-0.000012	-0.000012	0.000000
22	H	-0.087838	-0.000324	0.008018	-0.000016	0.000000	0.000000
23	H	-0.209683	0.001665	0.012330	0.000000	-0.000069	-0.000665
24	H	-0.003310	0.000067	0.000072	-0.000213	-0.000028	0.000000
25	H	0.003709	-0.000018	0.000244	-0.000407	0.000123	0.000000
26	H	0.210930	-0.004324	-0.109153	-0.000002	0.000001	0.000290

		19	20	21	22	23	24
1	C	-0.034155	0.006651	-0.044733	0.024708	-0.002066	-0.076743
2	C	-0.005238	-0.121455	0.042688	0.001722	0.041276	0.026837
3	C	0.051889	0.074493	-0.005352	-0.017084	-0.066301	0.004779
4	C	0.580138	-0.000372	0.076547	-0.136373	-0.007508	0.019383
5	C	-0.167734	0.001414	0.012110	0.057048	0.039498	-0.017965
6	C	0.006039	0.580968	-0.108915	0.009657	-0.064841	0.034420
7	C	0.016778	-0.111767	0.473870	-0.062435	0.008982	-0.084659
8	C	-0.137875	0.030820	-0.123517	0.602049	0.083958	0.058917
9	C	0.031664	0.031671	0.087543	-0.128019	-0.063696	-0.029550
10	C	-0.009107	-0.119756	0.039443	0.075457	0.593019	0.005749

11	C	0.021121	0.018469	0.027560	0.009896	-0.002315	0.379073
12	O	0.004814	-0.000051	-0.000050	0.000126	0.000169	0.000103
13	C	-0.009536	-0.029987	-0.128683	-0.087838	-0.209683	-0.003310
14	N	-0.000034	-0.000232	0.002481	-0.000324	0.001665	0.000067
15	O	0.004357	-0.000135	-0.000596	0.008018	0.012330	0.000072
16	H	-0.000595	-0.000009	-0.000012	-0.000016	0.000000	-0.000213
17	H	-0.000015	-0.000456	-0.000012	0.000000	-0.000069	-0.000028
18	H	-0.000009	-0.000067	0.000000	0.000000	-0.000665	0.000000
19	H	0.344684	0.000000	-0.000018	-0.000558	0.000000	0.000070
20	H	0.000000	0.366518	-0.000209	-0.000018	-0.000297	-0.000028
21	H	-0.000018	-0.000209	0.372831	-0.000258	-0.000027	-0.000244
22	H	-0.000558	-0.000018	-0.000258	0.353628	-0.000016	0.000027
23	H	0.000000	-0.000297	-0.000027	-0.000016	0.350691	0.000000
24	H	0.000070	-0.000028	-0.000244	0.000027	0.000000	0.429813
25	H	-0.000023	0.000060	-0.000449	-0.000025	0.000001	-0.015537
26	H	0.000205	0.000000	0.000000	-0.000055	-0.000080	0.000000

		25	26
1	C	-0.029171	0.019446
2	C	-0.004022	-0.013823
3	C	-0.010578	0.167543
4	C	-0.023930	0.148693
5	C	0.015836	-0.467827
6	C	0.029508	-0.002084
7	C	-0.097388	-0.002402
8	C	0.086593	-0.160631
9	C	-0.028874	0.316629
10	C	0.007925	-0.166819
11	C	0.368211	0.003245
12	O	-0.000034	0.231722
13	C	0.003709	0.210930
14	N	-0.000018	-0.004324
15	O	0.000244	-0.109153
16	H	-0.000407	-0.000002
17	H	0.000123	0.000001
18	H	0.000000	0.000290
19	H	-0.000023	0.000205
20	H	0.000060	0.000000
21	H	-0.000449	0.000000
22	H	-0.000025	-0.000055
23	H	0.000001	-0.000080
24	H	-0.015537	0.000000
25	H	0.429328	0.000000
26	H	0.000000	0.267316

Total atomic charges:

		1
1	C	0.558055
2	C	-0.070747
3	C	-0.487245
4	C	-0.456619
5	C	-0.517698
6	C	-0.694751
7	C	0.584014
8	C	-1.772685
9	C	2.202533

```
10  C   -2.108440
11  C   -1.789475
12  O   -0.825709
13  C    2.964396
14  N   -0.666474
15  O   -0.305006
16  H    0.279866
17  H    0.270540
18  H    0.304814
19  H    0.303136
20  H    0.273773
21  H    0.278001
22  H    0.290683
23  H    0.285973
24  H    0.268966
25  H    0.268916
26  H    0.561181
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  C    0.837922
 2  C    0.199794
 3  C   -0.182431
 4  C   -0.153483
 5  C   -0.517698
 6  C   -0.420978
 7  C    0.862015
 8  C   -1.482003
 9  C    2.202533
10  C   -1.822467
11  C   -1.251593
12  O   -0.825709
13  C    2.964396
14  N   -0.666474
15  O    0.256175
16  H    0.000000
17  H    0.000000
18  H    0.000000
19  H    0.000000
20  H    0.000000
21  H    0.000000
22  H    0.000000
23  H    0.000000
24  H    0.000000
25  H    0.000000
26  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  2162.6291
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=    -3.3419    Y=    -4.5758    Z=     1.2907  Tot=     5.8114
Quadrupole moment (Debye-Ang):
  XX=  -101.5566   YY=  -107.5372   ZZ=   -83.2855
  XY=    10.7413   XZ=     1.0384   YZ=     2.7728
```

```
 Octapole moment (Debye-Ang**2):
  XXX=   -83.8577  YYY=   -55.9204  ZZZ=     0.0133  XYY=     5.6070
  XXY=    34.5448  XXZ=     4.4098  XZZ=    -1.7007  YZZ=     1.7818
  YYZ=     8.7937  XYZ=    -1.7666
 Hexadecapole moment (Debye-Ang**3):
 XXXX= -1749.1412 YYYY= -1236.3411 ZZZZ=  -471.2319 XXXY=   131.0021
 XXXZ=    12.2396 YYYX=    81.5819 YYYZ=    19.2427 ZZZX=     2.5667
 ZZZY=     1.4407 XXYY=  -437.0466 XXZZ=  -316.5426 YYZZ=  -251.8104
 XXYZ=    -8.4711 YYXZ=    -6.9307 ZZXY=     2.0150
 N-N= 1.060079064475D+03 E-N=-3.663972689242D+03  KE= 6.600482073076D+02
  Exact polarizability: 129.634  -5.439 117.219   0.557   0.672  98.557
 Approx polarizability: 116.889  -7.947 109.553  -0.512  -0.358  95.099
 Full mass-weighted force constant matrix:
 Low frequencies ----1746.1312   -1.1392   -0.0017   -0.0004    0.0006
0.6892
 Low frequencies ---    0.9479  132.2759  163.9862
 ******    1 imaginary frequencies (negative Signs) ******
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                      1                      2                      3
                     ?A                     ?A                     ?A
 Frequencies -- -1746.1312               132.2759               163.9862
 Red. masses --     1.0958                 7.8843                 7.9092
 Frc consts  --     1.9684                 0.0813                 0.1253
 IR Inten    --  1025.3312                 6.0832                 4.3685
 Raman Activ --    13.4087                 2.8525                 2.0870
 Depolar     --     0.7452                 0.7254                 0.7499
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.00   0.00   0.00    -0.03   0.09   0.00    -0.06   0.02
0.09
   2   6     0.00   0.00   0.00    -0.05   0.05   0.00     0.08  -0.02
0.05
   3   6     0.00   0.00   0.00     0.02  -0.04   0.02     0.11  -0.04  -
0.04
   4   6     0.00   0.00   0.00     0.04  -0.03   0.02    -0.12   0.02  -
0.02
   5   6    -0.03   0.05   0.00     0.09  -0.06   0.02    -0.02  -0.01  -
0.05
   6   6     0.00   0.00   0.00    -0.14  -0.03   0.01     0.07  -0.03  -
0.07
   7   6     0.00   0.00   0.00    -0.17  -0.04   0.02    -0.06   0.00  -
0.09
   8   6     0.00   0.00   0.00    -0.05  -0.11   0.02    -0.09   0.00  -
0.11
   9   6     0.01  -0.01   0.01    -0.02  -0.16   0.02    -0.01  -0.01  -
0.16
  10   6     0.00   0.00   0.00    -0.05  -0.13   0.02     0.08  -0.03  -
0.13
  11   6     0.00   0.00   0.00    -0.15   0.08   0.00    -0.11   0.03
0.06
  12   8    -0.05  -0.01   0.00     0.13  -0.06  -0.10     0.04   0.01
0.19
```

13	6	0.00	0.00	0.00	0.08	0.08	-0.01	0.02	0.02	0.05
14	7	0.00	0.00	0.00	0.26	0.48	-0.08	0.08	0.10	0.47
15	8	0.01	0.01	-0.01	0.00	-0.13	0.09	-0.01	-0.05	-0.30
16	1	0.00	0.00	0.00	0.03	0.17	-0.02	-0.07	0.03	0.19
17	1	0.00	0.00	0.00	-0.06	0.11	-0.01	0.15	-0.02	0.13
18	1	0.00	0.00	0.00	0.08	-0.05	0.03	0.18	-0.03	-0.04
19	1	0.00	0.00	0.00	0.08	-0.01	0.02	-0.20	0.02	-0.01
20	1	0.00	0.00	0.00	-0.21	-0.02	0.01	0.13	-0.05	-0.07
21	1	0.00	0.00	0.00	-0.26	-0.08	0.03	-0.10	-0.01	-0.15
22	1	0.01	0.00	0.00	-0.07	-0.16	0.02	-0.16	0.03	-0.15
23	1	0.00	0.00	0.00	-0.07	-0.18	0.02	0.14	-0.06	-0.18
24	1	0.00	0.00	0.00	-0.16	0.09	0.00	-0.22	0.05	0.07
25	1	0.00	0.00	0.00	-0.21	0.14	-0.01	-0.06	0.03	0.12
26	1	0.76	-0.65	0.07	0.15	-0.16	-0.23	-0.04	-0.01	0.26

	4	5	6
	?A	?A	?A
Frequencies --	184.4695	344.1383	398.4251
Red. masses --	4.2193	6.1555	2.6133
Frc consts --	0.0846	0.4295	0.2444
IR Inten --	25.8610	4.0365	12.9379
Raman Activ --	1.4394	1.4763	0.3614
Depolar --	0.7396	0.7465	0.5840

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	-0.03	-0.08	-0.06	-0.14	0.05	0.02	-0.01	-0.08
2	6	-0.05	0.04	-0.06	-0.02	-0.11	0.02	-0.01	0.04	-0.08
3	6	-0.04	0.02	-0.08	-0.10	0.02	0.01	-0.01	0.00	-0.04
4	6	0.00	-0.04	-0.07	-0.13	0.06	0.04	0.04	-0.01	-0.08
5	6	-0.01	-0.02	-0.08	0.01	0.13	0.02	0.03	0.01	0.00
6	6	-0.06	0.04	0.06	0.06	-0.04	-0.01	0.00	0.02	-0.04
7	6	0.01	-0.02	0.09	0.10	0.00	-0.04	0.00	-0.01	-0.01
8	6	0.02	-0.04	0.07	-0.07	0.09	-0.03	0.00	-0.01	-0.08

9	6	-0.01	0.01	0.09	-0.10	0.00	-0.02	0.00	-0.01	-0.06
10	6	-0.04	0.05	0.06	-0.05	0.04	-0.01	-0.01	-0.01	-0.05
11	6	0.03	-0.06	0.01	0.09	-0.16	0.01	-0.07	-0.09	0.20
12	8	0.10	0.03	0.28	0.40	0.13	-0.09	0.00	0.04	0.08
13	6	-0.01	0.01	0.01	-0.13	-0.02	-0.01	0.01	0.01	-0.04
14	7	0.01	0.07	-0.16	-0.08	0.10	0.02	0.00	-0.02	0.02
15	8	0.03	-0.06	-0.19	-0.04	-0.07	0.05	0.00	0.05	0.16
16	1	-0.02	-0.07	-0.13	-0.14	-0.27	0.09	0.02	-0.01	-0.12
17	1	-0.07	0.10	-0.09	0.00	-0.18	0.05	-0.03	0.03	-0.11
18	1	-0.09	0.10	-0.14	-0.16	-0.05	0.08	-0.01	-0.02	-0.03
19	1	0.05	-0.12	-0.11	-0.21	0.04	0.04	0.06	0.03	-0.07
20	1	-0.10	0.09	0.09	0.12	-0.07	-0.03	-0.02	0.03	-0.03
21	1	0.03	-0.02	0.15	0.23	0.06	-0.07	0.02	-0.01	0.01
22	1	0.07	-0.08	0.11	-0.08	0.17	-0.05	0.00	-0.06	-0.07
23	1	-0.10	0.09	0.10	-0.01	0.09	-0.03	0.00	-0.01	-0.07
24	1	0.09	-0.13	0.01	0.08	-0.15	0.01	-0.39	-0.43	0.29
25	1	0.01	-0.03	0.01	0.16	-0.23	0.02	0.07	0.10	0.61
26	1	-0.01	-0.01	0.72	0.31	-0.17	-0.17	0.05	0.03	-0.01

	7			8			9		
	?A			?A			?A		
Frequencies --	448.6085			474.7717			490.8366		
Red. masses --	3.2913			8.7270			7.5639		
Frc consts --	0.3903			1.1590			1.0737		
IR Inten --	52.6424			7.3039			25.0147		
Raman Activ --	0.6364			6.8580			3.0687		
Depolar --	0.5502			0.1650			0.4743		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	-0.03	-0.06	-0.20	-0.07	0.05	0.05	0.03	0.02
2 6	-0.03	0.06	-0.02	-0.17	0.00	0.03	0.04	-0.10	0.00
3 6	0.03	0.01	0.02	-0.16	0.05	-0.03	-0.04	-0.05	0.01
4 6	0.03	0.00	0.02	-0.18	0.04	0.06	0.05	-0.08	0.00

```
   5   6     0.04   0.03   0.08    -0.14   0.06   0.01     0.05   0.05  -
0.05
   6   6    -0.06   0.06   0.09    -0.08   0.08  -0.03     0.02  -0.12  -
0.03
   7   6    -0.02  -0.05   0.16    -0.03   0.08  -0.02    -0.09  -0.12  -
0.03
   8   6    -0.04  -0.09   0.00    -0.02   0.07   0.00     0.08  -0.14
0.07
   9   6    -0.02  -0.05  -0.16     0.21  -0.01  -0.02     0.07   0.09
0.08
  10   6     0.03  -0.01  -0.07    -0.06   0.06  -0.03     0.01  -0.05
0.04
  11   6     0.10  -0.04  -0.09    -0.04  -0.06  -0.02    -0.15   0.07
0.00
  12   8     0.00   0.07   0.10     0.04   0.04   0.00     0.15   0.15  -
0.03
  13   6     0.02   0.03  -0.17     0.43  -0.09  -0.02     0.20   0.41
0.05
  14   7     0.01  -0.03   0.08     0.41  -0.22  -0.03    -0.08  -0.18  -
0.02
  15   8    -0.11   0.02   0.04     0.01  -0.01   0.02    -0.28   0.05  -
0.07
  16   1     0.01  -0.08  -0.13    -0.24  -0.15   0.01     0.11   0.16
0.08
  17   1    -0.07   0.13  -0.06    -0.11  -0.02   0.10     0.02  -0.15  -
0.02
  18   1     0.07  -0.04   0.07    -0.15   0.03  -0.01    -0.09  -0.08
0.04
  19   1     0.09   0.04   0.03    -0.22   0.00   0.05     0.07  -0.20  -
0.05
  20   1    -0.06   0.14   0.17    -0.03   0.04  -0.05     0.04  -0.10
0.00
  21   1     0.02  -0.05   0.26     0.03   0.10   0.04    -0.25  -0.18  -
0.09
  22   1    -0.19  -0.23  -0.03    -0.15   0.12  -0.07     0.15  -0.12
0.10
  23   1     0.12   0.00  -0.14    -0.20   0.11   0.08    -0.06  -0.08
0.09
  24   1     0.39   0.05  -0.14    -0.03  -0.02  -0.02    -0.22   0.07
0.01
  25   1    -0.06  -0.08  -0.35     0.04  -0.18  -0.04    -0.18   0.15
0.04
  26   1     0.07  -0.02  -0.42    -0.06   0.00  -0.02     0.18  -0.04  -
0.04
                     10                     11                     12
                     ?A                     ?A                     ?A
 Frequencies --   535.1356               571.9128               603.0171
 Red. masses --     3.1628                 3.7361                 6.5102
 Frc consts  --     0.5336                 0.7200                 1.3948
 IR Inten    --     1.4433                 8.0841                22.1988
 Raman Activ --     1.3351                 1.6156                 8.3763
 Depolar     --     0.7389                 0.5229                 0.1914
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
```

1	6	0.04	0.03	-0.10	-0.08	-0.02	-0.01	-0.01	0.00
0.13									
2	6	-0.06	0.02	-0.06	-0.02	0.12	0.00	-0.06	0.14
0.11									
3	6	-0.01	0.00	0.16	0.16	-0.06	0.00	-0.04	0.13
0.01									
4	6	0.06	0.06	0.10	-0.09	0.04	-0.01	0.01	-0.13
0.02									
5	6	0.01	0.01	0.17	0.05	-0.06	-0.05	0.02	-0.18
0.03									
6	6	-0.05	0.02	-0.06	-0.14	0.01	-0.01	0.01	0.20 -
0.11									
7	6	0.06	0.03	-0.04	0.04	0.09	0.01	0.10	0.09 -
0.13									
8	6	0.03	0.03	0.02	-0.04	0.11	0.02	0.12	-0.07 -
0.20									
9	6	0.00	-0.01	0.00	0.02	0.03	0.04	-0.02	-0.03 -
0.06									
10	6	-0.03	-0.02	0.05	0.02	-0.19	0.07	-0.07	0.12 -
0.08									
11	6	0.04	-0.04	0.06	0.08	-0.09	0.02	0.08	0.05
0.01									
12	8	-0.01	-0.02	-0.02	0.01	-0.07	-0.07	0.06	-0.22
0.11									
13	6	0.01	-0.02	0.03	0.04	0.20	-0.10	0.02	0.14
0.11									
14	7	0.01	0.00	-0.02	-0.06	-0.04	0.05	-0.08	-0.02 -
0.04									
15	8	-0.06	-0.05	-0.22	0.01	-0.01	0.01	-0.15	-0.14
0.08									
16	1	0.04	-0.01	-0.19	-0.14	-0.16	-0.07	0.03	0.01 -
0.02									
17	1	-0.12	-0.05	-0.13	0.03	0.27	0.06	0.01	0.07
0.18									
18	1	-0.07	-0.09	0.24	0.26	-0.03	-0.03	0.09	0.29 -
0.13									
19	1	0.20	0.22	0.14	-0.09	0.06	0.00	-0.15	-0.06
0.07									
20	1	-0.12	0.00	-0.08	-0.31	-0.05	-0.09	0.09	0.13 -
0.18									
21	1	0.09	0.04	-0.01	0.19	0.14	0.06	0.04	0.04
0.06									
22	1	0.03	0.10	0.00	-0.03	0.13	0.02	0.17	-0.01 -
0.19									
23	1	-0.03	-0.14	0.05	-0.01	-0.34	0.08	-0.06	0.06 -
0.09									
24	1	-0.15	-0.26	0.12	0.07	-0.11	0.02	0.00	0.24 -
0.02									
25	1	0.13	0.07	0.32	0.16	-0.16	0.04	0.20	-0.14 -
0.06									
26	1	-0.04	-0.05	-0.53	0.03	0.00	0.41	0.09	-0.22 -
0.21									

	13	14	15
	?A	?A	?A

Frequencies --		610.5575			619.4439			663.2744		
Red. masses --		9.3468			5.6892			4.9516		
Frc consts --		2.0529			1.2862			1.2835		
IR Inten --		63.9170			6.7031			9.0581		
Raman Activ --		1.8937			7.4185			1.1023		
Depolar --		0.6582			0.2667			0.6718		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.05	-0.05	0.00	-0.06	-0.12	0.08	-0.12	-0.01	-0.16
2	6	-0.16	-0.10	0.03	-0.01	0.11	0.05	0.13	0.00	-0.14
3	6	-0.14	0.00	0.09	0.17	0.06	0.01	0.09	-0.02	-0.02
4	6	0.09	-0.08	0.12	-0.01	-0.08	0.09	-0.13	0.11	-0.06
5	6	-0.03	-0.01	0.13	0.09	0.11	0.03	0.01	-0.06	0.07
6	6	-0.03	0.01	0.00	-0.12	0.02	-0.10	0.14	0.06	0.02
7	6	-0.09	-0.07	0.04	-0.05	-0.13	-0.07	-0.08	0.01	0.06
8	6	0.00	-0.05	0.01	0.03	-0.09	-0.04	-0.16	0.03	0.01
9	6	0.06	0.19	-0.12	0.00	-0.01	0.00	0.01	0.02	0.03
10	6	-0.06	0.11	-0.10	-0.05	-0.07	-0.12	0.17	0.09	0.04
11	6	-0.13	-0.05	-0.04	-0.04	-0.18	-0.06	-0.10	-0.07	-0.08
12	8	0.08	-0.19	-0.01	-0.06	0.18	0.02	0.01	-0.13	0.04
13	6	0.01	0.31	-0.16	-0.02	-0.02	0.31	0.05	0.10	0.23
14	7	-0.14	-0.02	0.05	-0.03	0.02	-0.11	-0.03	-0.02	-0.07
15	8	0.47	0.05	-0.05	0.12	0.13	-0.03	0.00	-0.06	0.05
16	1	0.03	0.05	-0.08	-0.05	-0.15	-0.01	-0.19	-0.08	-0.01
17	1	-0.18	-0.19	0.00	0.09	0.21	0.15	0.17	-0.03	-0.09
18	1	-0.18	-0.07	0.15	0.35	-0.01	0.08	-0.04	-0.01	-0.04
19	1	0.13	0.01	0.15	-0.08	-0.13	0.08	0.04	0.28	-0.03
20	1	0.13	0.07	0.08	-0.13	0.06	-0.06	0.09	0.16	0.12
21	1	-0.13	-0.09	0.09	-0.02	-0.14	0.08	-0.02	0.04	-0.01
22	1	-0.11	-0.07	-0.04	0.03	-0.01	-0.07	-0.20	-0.02	0.01
23	1	-0.06	0.14	-0.10	-0.07	-0.22	-0.12	0.23	0.15	0.00

24	1	-0.08	-0.03	-0.04	-0.04	-0.01	-0.09	0.10	-0.17	-0.09
25	1	-0.18	-0.02	-0.07	-0.01	-0.30	-0.15	-0.19	-0.03	-0.15
26	1	0.03	0.01	-0.01	0.01	0.15	-0.27	0.02	-0.10	-0.44

	16	17	18
	?A	?A	?A
Frequencies --	694.3433	744.3176	800.3281
Red. masses --	5.7168	1.9945	5.3959
Frc consts --	1.6239	0.6510	2.0363
IR Inten --	3.6223	98.2289	102.4796
Raman Activ --	6.4080	1.5266	2.1593
Depolar --	0.4071	0.7453	0.6322

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.08	0.08	0.02	-0.04	-0.01	0.05	0.12	0.02	0.06
2	6	-0.10	-0.07	0.07	-0.02	-0.03	0.00	0.17	0.08	-0.07
3	6	-0.05	-0.17	-0.08	-0.02	-0.05	-0.13	0.00	0.15	-0.03
4	6	-0.01	0.14	-0.08	0.00	-0.01	-0.02	-0.09	0.10	-0.06
5	6	-0.06	0.01	-0.03	0.14	-0.04	-0.04	-0.21	0.13	0.02
6	6	-0.05	-0.11	0.13	-0.03	-0.07	0.04	-0.03	-0.07	-0.02
7	6	0.04	0.08	0.17	0.02	0.05	-0.02	0.04	-0.16	-0.07
8	6	-0.02	0.02	-0.10	0.00	0.05	0.04	-0.03	-0.07	-0.02
9	6	-0.01	-0.01	-0.13	0.01	-0.02	0.03	-0.06	-0.10	0.04
10	6	-0.10	-0.11	-0.20	-0.05	0.02	0.07	-0.08	-0.03	0.09
11	6	0.18	0.13	0.12	0.00	0.01	0.01	0.10	0.03	0.04
12	8	0.01	-0.01	-0.01	-0.02	0.00	0.08	-0.07	0.07	0.04
13	6	0.05	0.09	0.28	-0.01	0.01	-0.04	0.07	0.15	-0.07
14	7	-0.02	-0.03	-0.09	-0.01	0.00	0.01	-0.02	-0.04	0.02
15	8	0.05	-0.02	-0.03	0.04	0.04	-0.03	0.15	-0.22	0.03
16	1	0.02	-0.01	0.04	-0.04	-0.01	0.07	0.02	-0.12	0.20
17	1	-0.19	0.07	-0.04	0.02	0.09	0.06	0.15	0.11	-0.10
18	1	0.12	-0.28	0.02	-0.06	0.04	-0.21	-0.09	0.16	-0.04
19	1	-0.09	0.19	-0.05	-0.06	-0.08	-0.04	-0.17	0.04	-0.07

```
  20   1     0.12  -0.15   0.12    -0.04  -0.14  -0.04    -0.27  -0.01
0.01
  21   1     0.03   0.08   0.12     0.04   0.07  -0.09    -0.02  -0.18  -
0.14
  22   1    -0.20  -0.21  -0.12     0.05   0.05   0.06     0.00   0.02  -
0.04
  23   1    -0.04   0.05  -0.24    -0.10   0.16   0.12    -0.14   0.01
0.14
  24   1     0.26   0.04   0.13    -0.04   0.04   0.01     0.02   0.14
0.04
  25   1     0.11   0.20   0.11     0.06  -0.04   0.02     0.04   0.09
0.02
  26   1    -0.03  -0.02  -0.08     0.10   0.00  -0.85    -0.29  -0.10  -
0.41
                     19                    20                    21
                     ?A                    ?A                    ?A
 Frequencies --   803.8146              825.3193              839.1783
 Red. masses --     4.0219                4.7479                3.1342
 Frc consts  --     1.5311                1.9054                1.3004
 IR Inten    --    31.1082               15.0037                9.2860
 Raman Activ --     7.5779               12.7648                1.1002
 Depolar     --     0.0465                0.0359                0.7351
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.11  -0.02   0.04    -0.01   0.06   0.04     0.11  -0.06  -
0.06
   2   6     0.01  -0.04   0.04     0.02   0.02  -0.16    -0.02   0.06
0.14
   3   6    -0.06   0.10   0.07     0.00   0.02  -0.20     0.07   0.04  -
0.08
   4   6     0.04   0.11  -0.01     0.00   0.07   0.30     0.10   0.04
0.04
   5   6     0.25  -0.06  -0.02     0.13  -0.04   0.02    -0.09   0.02
0.02
   6   6    -0.01  -0.03   0.09     0.04  -0.03  -0.12    -0.01  -0.10
0.16
   7   6    -0.03  -0.06  -0.03     0.05  -0.15   0.00    -0.05   0.00  -
0.09
   8   6    -0.14   0.00  -0.22    -0.10   0.01   0.18     0.01   0.13
0.04
   9   6    -0.06  -0.08  -0.03     0.00  -0.04   0.01    -0.01  -0.01
0.01
  10   6    -0.09   0.06   0.15    -0.09   0.06  -0.18    -0.02   0.05  -
0.08
  11   6     0.00  -0.09  -0.02     0.09   0.04   0.05    -0.08  -0.10  -
0.10
  12   8    -0.06  -0.01  -0.03    -0.03  -0.06  -0.02     0.01  -0.03
0.00
  13   6     0.06   0.04   0.02     0.01   0.02  -0.01     0.01   0.02  -
0.01
  14   7     0.04  -0.04  -0.01     0.00  -0.01   0.00     0.00  -0.01
0.00
  15   8     0.00   0.06  -0.04    -0.05   0.00   0.02    -0.05  -0.07
0.01
```

16	1	0.09	-0.03	0.12	-0.04	-0.03	0.00	0.18	0.05	-0.10
17	1	-0.08	-0.08	-0.06	0.11	0.03	-0.06	-0.11	0.38	0.05
18	1	-0.23	0.22	-0.04	0.00	-0.05	-0.15	0.34	0.04	-0.06
19	1	-0.10	0.38	0.11	0.16	0.04	0.27	0.17	0.08	0.04
20	1	-0.01	-0.05	0.08	0.07	0.14	0.05	0.23	-0.16	0.14
21	1	0.06	-0.02	-0.06	0.03	-0.14	-0.12	0.09	0.08	-0.20
22	1	-0.18	-0.05	-0.23	-0.31	0.25	0.04	0.03	0.24	0.02
23	1	-0.01	0.06	0.09	-0.22	0.18	-0.08	-0.03	0.34	-0.06
24	1	0.04	-0.04	-0.03	0.03	0.01	0.06	-0.23	-0.19	-0.07
25	1	-0.09	-0.04	-0.08	0.05	0.11	0.08	-0.05	0.00	0.07
26	1	0.10	0.11	0.52	0.04	0.03	0.42	-0.09	-0.06	0.03

	22			23			24		
	?A			?A			?A		
Frequencies --	876.3470			883.1277			912.5566		
Red. masses --	4.2355			3.5977			2.6968		
Frc consts --	1.9165			1.6532			1.3232		
IR Inten --	10.2978			0.2380			7.2939		
Raman Activ --	4.5091			14.4764			0.4972		
Depolar --	0.2494			0.0157			0.7291		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.20	-0.05	0.10	0.13	-0.04	0.08	-0.04	-0.04	0.05
2	6	0.14	0.06	-0.11	0.13	-0.14	-0.03	-0.01	0.03	-0.11
3	6	-0.02	-0.03	0.00	-0.05	0.02	-0.06	-0.05	-0.12	-0.06
4	6	-0.06	-0.03	-0.01	0.12	-0.04	0.04	0.00	-0.05	0.11
5	6	-0.09	-0.03	0.03	-0.01	0.02	-0.03	0.02	0.02	0.05
6	6	-0.17	-0.02	0.02	-0.07	0.14	-0.08	-0.06	0.04	0.12
7	6	0.00	-0.11	0.02	-0.05	0.22	0.08	0.04	0.05	-0.05
8	6	0.00	0.10	-0.03	-0.07	0.08	0.06	0.09	-0.01	-0.08
9	6	0.04	0.19	-0.05	-0.02	-0.07	-0.01	-0.01	-0.09	-0.05
10	6	-0.01	-0.01	0.00	-0.01	-0.06	-0.06	0.14	0.04	0.04
11	6	-0.04	-0.01	0.01	-0.07	-0.09	-0.04	-0.04	0.04	-0.01

12	8	0.10	-0.16	0.02	-0.03	0.05	0.01	-0.03	0.07	-0.03
13	6	-0.02	-0.09	0.03	0.02	0.04	0.02	0.00	0.03	0.03
14	7	0.04	0.01	-0.01	-0.01	-0.01	-0.01	-0.03	0.00	-0.01
15	8	-0.06	0.14	-0.01	0.01	-0.08	0.00	0.02	-0.06	0.00
16	1	0.21	0.03	0.26	0.24	0.23	0.28	0.00	0.01	0.02
17	1	0.02	0.18	-0.25	0.12	-0.32	-0.04	0.03	0.29	-0.08
18	1	-0.18	-0.07	0.02	-0.13	0.00	-0.05	-0.36	-0.32	0.09
19	1	-0.28	-0.03	0.03	0.07	-0.13	0.02	-0.07	-0.03	0.13
20	1	-0.46	0.14	0.13	-0.15	0.09	-0.16	-0.30	0.03	0.07
21	1	0.08	-0.08	0.06	0.25	0.32	0.28	0.00	0.02	0.00
22	1	0.00	0.17	-0.05	-0.18	-0.06	0.05	0.08	0.11	-0.12
23	1	0.00	-0.02	-0.01	-0.07	-0.19	-0.03	0.35	0.37	-0.09
24	1	-0.09	0.19	-0.02	0.00	-0.09	-0.04	-0.16	0.12	-0.01
25	1	-0.15	0.06	-0.07	-0.05	-0.12	-0.04	0.06	-0.04	0.03
26	1	0.10	0.01	-0.15	-0.07	-0.03	-0.03	-0.05	0.00	0.24

	25	26	27
	?A	?A	?A
Frequencies --	925.6229	957.9829	982.7641
Red. masses --	2.8257	2.1281	2.2284
Frc consts --	1.4264	1.1507	1.2681
IR Inten --	10.0214	4.3779	7.0740
Raman Activ --	1.8475	2.7024	3.9333
Depolar --	0.6045	0.7375	0.0809

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.06	-0.03	0.06	-0.09	0.05	0.01	0.03	-0.02	0.03
2	6	0.05	-0.06	0.02	0.12	0.06	0.05	0.01	0.11	-0.08
3	6	0.01	-0.04	-0.08	-0.06	0.01	-0.02	0.03	-0.12	0.02
4	6	0.01	0.22	-0.05	0.10	0.01	-0.02	0.02	-0.07	-0.04
5	6	0.02	0.00	0.05	-0.04	0.01	0.05	0.00	0.02	0.07
6	6	-0.03	0.07	-0.01	-0.06	-0.13	-0.05	0.12	-0.01	-0.04
7	6	-0.04	-0.04	0.06	-0.03	0.07	-0.01	-0.01	0.06	0.03

8	6	0.21	-0.03	-0.05	-0.03	-0.09	0.02	-0.05	0.02	-0.05
9	6	0.04	0.00	0.07	0.01	0.04	-0.05	-0.01	0.01	0.07
10	6	-0.05	0.00	-0.05	0.00	0.04	0.02	-0.13	0.03	0.00
11	6	-0.06	-0.06	0.00	0.05	-0.05	0.01	-0.05	-0.03	0.08
12	8	-0.01	-0.02	-0.02	0.02	-0.03	-0.01	0.00	0.02	-0.02
13	6	-0.03	-0.02	-0.06	-0.01	-0.02	0.01	0.01	0.00	-0.04
14	7	-0.02	0.02	0.02	0.01	0.00	0.00	0.02	-0.01	0.01
15	8	-0.03	-0.02	-0.02	-0.02	0.03	0.00	0.00	-0.02	-0.01
16	1	-0.14	-0.09	0.27	-0.09	0.05	0.05	0.07	0.04	0.00
17	1	0.15	-0.05	0.13	0.30	0.20	0.25	-0.02	0.33	-0.12
18	1	0.04	-0.12	-0.01	-0.25	-0.03	0.01	0.04	-0.38	0.25
19	1	0.06	0.51	0.05	0.34	0.12	-0.02	-0.04	-0.01	-0.01
20	1	0.01	0.15	0.07	-0.22	-0.29	-0.24	0.33	-0.07	-0.07
21	1	-0.14	-0.12	0.29	-0.04	0.07	-0.08	0.04	0.09	-0.02
22	1	0.43	-0.04	0.04	-0.14	-0.32	0.03	0.03	-0.05	0.00
23	1	-0.21	0.05	0.06	0.05	0.22	0.00	-0.32	0.12	0.14
24	1	-0.01	-0.02	-0.01	0.10	-0.07	0.01	0.26	0.26	-0.01
25	1	-0.08	-0.08	-0.06	0.18	-0.21	-0.01	-0.17	-0.20	-0.28
26	1	-0.01	0.00	0.03	0.01	0.01	0.14	-0.02	0.00	0.04

	28	29	30
	?A	?A	?A
Frequencies --	994.7261	997.5654	1010.9207
Red. masses --	2.7742	2.2117	5.7400
Frc consts --	1.6173	1.2968	3.4562
IR Inten --	2.8023	1.7894	1.7811
Raman Activ --	8.3195	7.2309	0.3323
Depolar --	0.0485	0.5044	0.6311

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.06	0.22	0.03	0.05	-0.02	-0.03	-0.12	-0.14	-0.13
2	6	-0.02	0.01	0.00	0.02	-0.10	-0.01	0.13	-0.07	-0.12
3	6	0.02	-0.03	0.03	0.15	-0.06	0.03	0.12	0.22	-0.06

```
   4   6    -0.03   0.00  -0.02    -0.08  -0.02   0.00    -0.04  -0.11
0.14
   5   6    -0.01   0.00  -0.02     0.00   0.00   0.02    -0.03   0.01
0.09
   6   6     0.00  -0.04   0.01    -0.09   0.02  -0.02     0.07  -0.13
0.12
   7   6     0.24  -0.07   0.05    -0.01   0.06  -0.02     0.11   0.14
0.13
   8   6     0.01  -0.03   0.00    -0.02  -0.09   0.00     0.14   0.01  -
0.10
   9   6    -0.01   0.01  -0.04    -0.01   0.00   0.02     0.02   0.02  -
0.13
  10   6    -0.05   0.02   0.01    -0.06   0.16   0.02    -0.21  -0.12
0.07
  11   6    -0.12  -0.09  -0.09     0.05   0.04  -0.05    -0.13   0.15  -
0.01
  12   8    -0.01   0.01   0.00     0.01   0.00  -0.01     0.02  -0.01  -
0.01
  13   6     0.00   0.00   0.01     0.01   0.00  -0.02    -0.01  -0.01
0.02
  14   7     0.00   0.00   0.00     0.01   0.00   0.01    -0.01   0.01  -
0.01
  15   8     0.00  -0.02   0.01     0.00   0.02   0.02    -0.01   0.03  -
0.01
  16   1     0.07   0.55   0.17     0.03  -0.03   0.05    -0.11  -0.11  -
0.08
  17   1     0.00  -0.06   0.02    -0.04  -0.23  -0.07     0.21   0.00  -
0.02
  18   1     0.11  -0.03   0.03     0.45  -0.16   0.13     0.08   0.31  -
0.14
  19   1    -0.02  -0.06  -0.04    -0.19  -0.04   0.01     0.04   0.07
0.20
  20   1    -0.07   0.00   0.04    -0.21  -0.06  -0.12     0.02  -0.24
0.00
  21   1     0.59   0.05   0.19    -0.05   0.04   0.07     0.02   0.11
0.07
  22   1    -0.05  -0.04  -0.03    -0.04  -0.22   0.03    -0.06  -0.09  -
0.17
  23   1    -0.02   0.10   0.00    -0.12   0.52   0.08    -0.26  -0.19
0.10
  24   1    -0.17  -0.12  -0.08    -0.14  -0.15   0.01    -0.05   0.03
0.00
  25   1    -0.10  -0.09  -0.04     0.15   0.14   0.20    -0.17   0.22
0.01
  26   1    -0.02  -0.01   0.00     0.01   0.01   0.08     0.01   0.00
0.13
                      31                     32                     33
                      ?A                     ?A                     ?A
 Frequencies --  1034.1343              1042.4705              1056.3764
 Red. masses --     2.1246                 1.8752                 2.0908
 Frc consts  --     1.3387                 1.2007                 1.3746
 IR Inten    --     1.8405                 1.5321                 2.9809
 Raman Activ --     2.1060                 6.6059                 9.1208
 Depolar     --     0.6682                 0.7339                 0.5274
```

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.09	0.04	-0.05	-0.06	0.03	-0.03	-0.05	0.06	-0.07
2	6	-0.03	0.03	0.07	-0.02	-0.06	0.02	0.14	0.00	0.07
3	6	-0.03	-0.05	-0.10	0.05	-0.01	-0.02	-0.04	-0.08	0.02
4	6	-0.06	0.01	0.12	0.09	-0.05	0.01	-0.02	-0.08	0.00
5	6	-0.05	0.00	-0.01	-0.04	0.00	-0.01	0.01	0.00	0.00
6	6	0.04	0.01	-0.08	-0.05	-0.01	-0.04	0.01	0.09	0.07
7	6	-0.04	0.00	0.06	-0.01	-0.08	0.04	-0.03	-0.03	-0.02
8	6	-0.01	-0.06	-0.09	-0.01	0.11	-0.09	-0.01	0.05	-0.03
9	6	0.07	0.03	0.03	-0.01	0.00	0.00	-0.06	-0.04	0.01
10	6	0.06	-0.02	0.09	0.02	0.04	0.04	-0.10	-0.01	-0.02
11	6	0.01	-0.03	-0.04	0.00	0.00	0.12	0.07	0.02	-0.07
12	8	0.01	0.02	0.00	0.01	0.02	0.00	0.01	0.00	0.00
13	6	-0.03	-0.01	0.00	0.00	0.00	0.01	0.02	0.01	-0.01
14	7	-0.02	0.02	0.00	0.00	0.00	0.00	0.02	-0.01	0.00
15	8	0.01	0.00	0.00	-0.01	-0.03	0.00	0.01	0.03	-0.01
16	1	0.19	0.14	-0.24	0.01	0.07	-0.23	0.00	0.14	-0.07
17	1	0.06	0.21	0.17	0.10	-0.32	0.16	0.37	0.06	0.33
18	1	-0.11	0.04	-0.19	0.22	0.06	-0.07	-0.20	-0.23	0.13
19	1	-0.33	0.05	0.18	0.18	-0.02	0.01	0.00	-0.19	-0.04
20	1	0.13	-0.21	-0.29	-0.35	0.02	-0.06	0.06	0.29	0.27
21	1	-0.08	-0.05	0.33	-0.07	-0.10	0.03	-0.15	-0.09	-0.02
22	1	-0.09	0.02	-0.15	0.02	0.39	-0.15	0.04	0.27	-0.07
23	1	-0.10	-0.03	0.21	0.03	0.25	0.05	-0.17	-0.11	0.02
24	1	0.10	-0.29	-0.01	0.36	0.13	0.05	-0.02	-0.31	0.00
25	1	-0.13	0.22	0.06	-0.21	-0.06	-0.23	0.15	0.12	0.17
26	1	-0.01	-0.01	-0.06	-0.04	-0.03	-0.03	0.02	0.02	-0.03

	34			35			36		
	?A			?A			?A		
Frequencies --	1064.5738			1083.6626			1126.4565		
Red. masses --	1.8026			2.4612			7.1241		
Frc consts --	1.2037			1.7029			5.3261		
IR Inten --	1.8494			3.4969			40.7417		
Raman Activ --	5.6199			0.8605			5.5279		
Depolar --	0.7268			0.6710			0.7252		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.01	-0.11	-0.02	-0.03	0.03	0.06	-0.03	-0.02	0.02
2 6	0.01	0.02	0.09	-0.06	-0.05	-0.05	0.02	0.00	0.00
3 6	-0.02	-0.06	-0.02	0.06	-0.04	-0.09	0.02	-0.04	0.10
4 6	0.06	0.03	-0.04	0.10	0.01	0.03	0.01	-0.03	-0.04
5 6	-0.01	0.00	0.01	-0.11	0.01	0.01	0.21	-0.06	-0.05
6 6	-0.02	0.07	-0.04	0.04	0.11	0.09	-0.06	-0.06	0.00
7 6	0.11	-0.06	0.00	0.00	0.00	-0.10	-0.05	-0.04	0.04
8 6	-0.09	-0.02	0.01	-0.08	-0.08	-0.06	0.00	0.09	0.00
9 6	0.00	0.01	0.00	0.08	0.07	0.00	0.23	0.40	-0.13
10 6	0.00	0.01	0.02	-0.01	-0.07	0.10	-0.06	0.09	-0.02
11 6	-0.05	0.09	-0.02	0.04	-0.02	-0.01	0.04	0.02	-0.06
12 8	0.00	0.01	-0.01	0.03	0.01	0.00	-0.11	0.15	0.00
13 6	0.00	0.00	0.00	-0.02	-0.02	0.01	-0.05	-0.07	0.02
14 7	0.00	0.00	0.00	-0.02	0.02	0.00	-0.01	0.03	-0.01
15 8	0.00	0.00	0.00	-0.01	0.02	0.00	-0.03	-0.34	0.06
16 1	-0.12	-0.43	-0.20	0.01	0.14	0.16	-0.09	-0.12	0.06
17 1	0.16	0.05	0.26	-0.10	-0.07	-0.10	0.07	0.11	0.06
18 1	-0.04	-0.08	-0.01	0.18	0.04	-0.16	-0.29	0.02	0.04
19 1	0.22	0.08	-0.04	0.24	0.12	0.05	-0.12	-0.05	-0.03
20 1	-0.04	0.07	-0.04	0.03	0.30	0.28	0.00	0.12	0.20
21 1	0.41	0.05	0.14	-0.09	-0.02	-0.27	-0.18	-0.08	-0.11
22 1	-0.17	-0.09	0.00	-0.29	-0.18	-0.13	-0.21	-0.02	-0.07

```
  23   1    -0.07  -0.02   0.07    -0.24  -0.15   0.27    -0.16  -0.17
0.05
  24   1    -0.31   0.28  -0.02    -0.09   0.05   0.00    -0.11  -0.17  -
0.01
  25   1    -0.18   0.28   0.03     0.26  -0.22   0.05     0.10   0.12
0.15
  26   1     0.00   0.00   0.01    -0.03  -0.02  -0.04    -0.03  -0.21
0.06
                     37                    38                    39
                     ?A                    ?A                    ?A
 Frequencies --  1160.9361             1181.5624             1216.8079
 Red. masses --     2.0427                2.2095                2.5872
 Frc consts  --     1.6221                1.8174                2.2569
 IR Inten    --     6.2682                6.4947               29.5190
 Raman Activ --     2.7612                2.1387                6.5335
 Depolar     --     0.6898                0.5233                0.0874
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.01   0.02  -0.06    -0.07   0.00   0.04     0.01   0.01  -
0.04
   2   6     0.02  -0.02   0.03     0.00  -0.03  -0.03     0.07   0.05
0.04
   3   6    -0.06   0.07  -0.04    -0.02   0.08  -0.01    -0.10   0.04
0.06
   4   6    -0.04  -0.06   0.00     0.05  -0.09  -0.04    -0.06   0.02  -
0.01
   5   6     0.04  -0.01   0.08     0.00   0.00   0.05     0.02  -0.02  -
0.05
   6   6    -0.04  -0.03   0.05    -0.05  -0.04   0.00    -0.01  -0.01
0.01
   7   6     0.04   0.03  -0.03     0.01  -0.03   0.06     0.00   0.01  -
0.01
   8   6    -0.05  -0.03  -0.05    -0.09   0.02  -0.11     0.04   0.01
0.00
   9   6     0.05   0.05   0.16     0.01   0.02   0.16     0.26  -0.15  -
0.01
  10   6     0.06  -0.04  -0.12     0.08  -0.01  -0.08     0.03  -0.02  -
0.03
  11   6    -0.01   0.00   0.05     0.06   0.06  -0.06    -0.02  -0.01
0.02
  12   8    -0.01   0.02  -0.01     0.00   0.00   0.00    -0.01   0.00
0.01
  13   6    -0.01  -0.01  -0.03     0.00   0.00  -0.03    -0.05   0.01
0.01
  14   7     0.00   0.01   0.01     0.00   0.00   0.01    -0.09   0.04
0.00
  15   8     0.00  -0.01  -0.01    -0.01   0.00  -0.01    -0.01   0.03  -
0.01
  16   1     0.13   0.15  -0.30    -0.17  -0.01   0.44    -0.09  -0.11
0.11
  17   1     0.13  -0.16   0.15    -0.17   0.21  -0.22    -0.11  -0.14  -
0.16
  18   1     0.05   0.00   0.02     0.06  -0.04   0.10     0.18  -0.16
0.26
```

19	1	-0.34	0.25	0.15	0.26	0.04	-0.02	0.14	-0.22	-0.13
20	1	-0.19	0.17	0.22	0.20	-0.20	-0.11	-0.08	0.03	0.04
21	1	0.22	0.14	-0.34	0.02	-0.07	0.43	0.02	0.03	-0.10
22	1	0.14	-0.37	0.12	0.01	0.24	-0.12	-0.40	0.13	-0.23
23	1	-0.02	0.05	-0.06	0.00	0.03	-0.01	-0.37	0.27	0.28
24	1	0.11	0.09	0.02	-0.14	-0.13	-0.01	0.06	0.01	0.00
25	1	-0.06	-0.05	-0.08	0.14	0.16	0.17	-0.09	0.00	-0.07
26	1	0.02	-0.01	-0.01	-0.01	0.00	-0.05	0.01	0.05	0.01

	40	41	42
	?A	?A	?A
Frequencies --	1234.1843	1250.1693	1262.5332
Red. masses --	2.2030	3.9469	2.1141
Frc consts --	1.9771	3.6345	1.9855
IR Inten --	7.0833	39.4466	90.5494
Raman Activ --	0.3534	3.0529	5.0586
Depolar --	0.4862	0.6088	0.7495

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.02	0.03	-0.11	0.04	0.01	0.00	0.00	0.04	-0.01
2	6	0.07	-0.10	0.07	-0.07	-0.03	0.04	-0.02	-0.08	-0.01
3	6	0.03	-0.03	0.00	-0.02	0.06	-0.12	0.03	0.10	-0.04
4	6	-0.10	-0.01	0.02	-0.08	-0.09	-0.19	0.01	0.07	0.00
5	6	0.01	-0.06	0.02	0.06	-0.01	0.32	0.07	0.16	-0.02
6	6	-0.12	0.06	0.04	0.02	0.06	-0.04	-0.01	0.04	0.07
7	6	0.04	0.01	-0.10	-0.01	-0.08	-0.01	0.00	0.01	-0.06
8	6	0.00	-0.08	0.04	-0.03	0.10	0.11	-0.02	-0.06	0.00
9	6	0.01	0.02	-0.01	0.03	-0.05	-0.16	0.00	0.07	0.01
10	6	-0.01	0.06	-0.02	0.04	-0.08	0.06	0.01	-0.06	0.01
11	6	-0.02	-0.01	0.11	0.03	0.02	-0.01	0.00	-0.02	0.04
12	8	0.00	0.04	-0.01	-0.01	0.03	-0.05	-0.02	-0.11	0.02
13	6	0.00	0.00	0.00	0.00	0.01	0.04	0.00	-0.01	0.00
14	7	0.00	0.00	0.00	-0.02	0.01	-0.01	0.01	0.00	0.00

15	8	0.02	0.00	0.01	0.00	0.00	-0.02	-0.03	-0.03	0.01
16	1	0.02	0.12	0.14	0.15	0.24	0.11	0.03	-0.04	-0.31
17	1	-0.18	0.32	-0.22	0.02	0.03	0.14	0.09	0.02	0.11
18	1	-0.20	0.17	-0.20	0.06	0.08	-0.14	-0.11	-0.37	0.37
19	1	0.31	0.09	-0.01	-0.10	-0.01	-0.16	-0.11	-0.43	-0.17
20	1	0.34	-0.16	-0.11	0.04	-0.06	-0.16	0.09	-0.21	-0.16
21	1	0.06	-0.01	0.07	-0.13	-0.14	0.13	-0.01	-0.04	0.27
22	1	-0.01	0.26	-0.06	0.20	0.03	0.23	-0.03	0.16	-0.07
23	1	0.00	-0.26	-0.05	-0.24	0.31	0.29	0.00	0.07	0.02
24	1	0.20	0.22	0.04	-0.09	0.05	0.00	-0.08	0.22	0.00
25	1	-0.09	-0.16	-0.17	0.17	-0.09	0.05	0.02	-0.14	-0.06
26	1	0.04	-0.03	0.02	0.04	0.01	0.30	-0.06	0.07	0.01

	43			44			45		
	?A			?A			?A		
Frequencies --	1267.3852			1269.2438			1300.8679		
Red. masses --	1.6353			1.3781			1.6606		
Frc consts --	1.5476			1.3081			1.6557		
IR Inten --	1.7517			7.7813			1.4101		
Raman Activ --	5.3384			11.2785			0.6981		
Depolar --	0.6119			0.7003			0.5958		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.02	0.01	-0.03	-0.01	0.01	0.01	-0.01	0.13	0.04
2 6	0.06	0.07	0.02	0.01	-0.02	-0.03	0.02	0.00	-0.03
3 6	-0.09	-0.03	0.01	0.05	-0.01	0.03	0.02	-0.01	0.00
4 6	-0.04	-0.01	0.02	0.01	0.00	-0.02	0.00	-0.04	0.02
5 6	0.02	-0.06	-0.03	-0.03	-0.01	0.00	-0.02	-0.02	0.03
6 6	0.07	0.01	0.04	-0.04	-0.07	-0.02	0.00	-0.01	0.03
7 6	0.00	0.02	-0.01	-0.03	-0.01	0.05	-0.13	0.01	-0.06
8 6	-0.02	-0.04	0.02	0.01	0.05	-0.01	0.03	0.00	-0.02
9 6	-0.05	0.08	0.01	0.04	-0.08	0.01	0.01	0.01	-0.03
10 6	-0.03	-0.09	-0.01	0.01	0.07	-0.01	-0.01	-0.03	0.00

11	6	-0.01	-0.01	-0.01	0.02	0.00	0.00	0.07	-0.07	0.01
12	8	0.00	0.04	0.00	0.01	0.01	0.00	0.00	0.02	-0.01
13	6	0.01	-0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00
14	7	0.02	-0.01	0.00	-0.02	0.01	0.00	0.00	0.00	0.00
15	8	0.02	-0.01	0.00	0.00	0.01	0.00	0.00	0.01	0.00
16	1	0.03	-0.03	-0.15	0.12	0.09	-0.40	-0.27	-0.41	-0.11
17	1	-0.07	-0.31	-0.14	0.08	-0.04	0.04	-0.01	-0.15	-0.08
18	1	0.28	0.07	-0.06	-0.19	0.09	-0.07	-0.10	0.14	-0.14
19	1	0.14	0.20	0.07	-0.15	0.08	0.03	0.02	-0.11	0.00
20	1	-0.15	-0.08	-0.09	0.25	0.04	0.14	0.17	0.00	0.07
21	1	-0.17	-0.09	0.35	0.00	-0.03	0.25	0.48	0.24	0.18
22	1	0.01	0.22	-0.03	-0.12	-0.06	-0.04	0.19	-0.06	0.07
23	1	0.05	0.33	-0.05	-0.07	-0.18	0.03	-0.04	0.16	0.04
24	1	-0.27	0.27	-0.03	-0.37	0.37	-0.02	-0.10	0.11	-0.01
25	1	0.24	-0.28	0.01	0.33	-0.32	0.05	-0.25	0.29	-0.01
26	1	0.05	-0.04	-0.05	-0.02	0.00	0.00	0.01	-0.02	0.02

	46			47			48		
	?A			?A			?A		
Frequencies --	1327.6566			1358.4909			1363.0636		
Red. masses --	1.5893			1.6516			1.4935		
Frc consts --	1.6505			1.7958			1.6349		
IR Inten --	5.4758			9.7182			8.4440		
Raman Activ --	2.5157			1.4563			1.8136		
Depolar --	0.7007			0.5329			0.6010		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.05	-0.01	-0.01	-0.03	0.01	-0.05	-0.03	-0.04	-0.04
2	6	0.03	-0.02	0.01	0.07	-0.02	0.03	0.04	0.04	0.02
3	6	-0.01	0.06	0.00	-0.12	-0.04	-0.03	0.01	-0.02	0.02
4	6	0.02	-0.05	0.03	0.03	0.02	0.05	0.03	0.03	0.03
5	6	-0.01	-0.01	-0.13	0.04	0.06	0.03	0.01	0.04	0.00
6	6	-0.03	0.04	-0.01	-0.01	-0.04	-0.03	-0.10	0.02	-0.06

7	6	-0.03	-0.06	-0.02	-0.02	0.00	0.02	0.02	-0.03	0.00
8	6	-0.01	0.05	0.03	0.01	0.01	-0.04	0.03	0.04	-0.02
9	6	-0.01	-0.01	-0.08	-0.06	0.02	-0.04	-0.04	0.02	0.02
10	6	0.03	-0.02	0.04	0.07	0.07	0.04	0.01	-0.09	0.03
11	6	0.03	0.02	0.02	0.00	0.01	0.01	-0.02	0.03	0.02
12	8	0.00	0.00	0.02	-0.01	-0.02	0.00	0.00	-0.02	0.00
13	6	0.00	0.00	0.02	0.01	0.00	0.01	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.01	-0.01	0.00	0.01	0.00	0.00
15	8	0.00	0.00	0.01	0.00	-0.02	0.00	0.00	-0.01	0.00
16	1	0.05	0.17	-0.01	-0.10	-0.08	0.03	0.00	0.08	0.12
17	1	-0.09	0.11	-0.12	-0.13	0.21	-0.20	-0.05	-0.14	-0.08
18	1	0.07	-0.34	0.35	0.61	0.05	-0.07	-0.10	0.17	-0.15
19	1	-0.09	0.53	0.26	-0.13	-0.30	-0.04	-0.10	-0.23	-0.04
20	1	0.20	-0.09	-0.11	-0.04	0.14	0.15	0.58	0.13	0.15
21	1	0.16	0.02	0.01	0.10	0.05	0.02	-0.02	-0.04	-0.05
22	1	0.23	-0.19	0.20	0.16	-0.12	0.06	-0.16	-0.28	-0.02
23	1	-0.13	0.09	0.17	-0.18	-0.35	0.20	0.10	0.52	0.01
24	1	0.01	0.03	0.02	-0.05	0.07	0.00	0.08	-0.05	0.02
25	1	0.01	0.05	0.02	0.10	-0.12	-0.01	0.05	-0.07	-0.02
26	1	0.00	-0.01	-0.06	-0.02	0.02	0.06	-0.02	0.01	-0.01

	49			50			51		
	?A			?A			?A		
Frequencies --	1368.1003			1385.6074			1386.4120		
Red. masses --	1.6112			1.3351			1.6865		
Frc consts --	1.7768			1.5102			1.9099		
IR Inten --	9.5346			6.1424			1.6486		
Raman Activ --	1.3044			1.7462			0.7324		
Depolar --	0.7476			0.7385			0.7054		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.04	-0.01	-0.01	0.02	0.00	0.00	0.04	0.04	-0.02
2	6	0.00	-0.10	-0.07	-0.01	0.05	-0.07	-0.02	-0.06	0.06

```
   3   6    -0.05   0.00   0.09    -0.06   0.00  -0.04     0.00   0.04  -
0.06
   4   6     0.05   0.04  -0.01    -0.01  -0.02  -0.02    -0.10  -0.05
0.02
   5   6    -0.02  -0.06  -0.01     0.00  -0.02   0.02     0.02   0.01
0.00
   6   6     0.04   0.05   0.01    -0.07   0.01   0.04     0.04  -0.01  -
0.07
   7   6    -0.02  -0.03  -0.05     0.00   0.00  -0.01    -0.03  -0.01
0.01
   8   6     0.00   0.02   0.03     0.03   0.00   0.02     0.08   0.09  -
0.03
   9   6     0.05  -0.01   0.02     0.01   0.01   0.01    -0.02   0.01
0.05
  10   6    -0.05  -0.04  -0.01    -0.01   0.04   0.05    -0.03  -0.01
0.05
  11   6     0.02   0.01   0.02     0.02  -0.03   0.01     0.03  -0.04
0.01
  12   8     0.00   0.02   0.00     0.00   0.01   0.00     0.00  -0.01
0.00
  13   6     0.00   0.00  -0.01     0.00   0.00   0.00     0.00   0.00  -
0.01
  14   7    -0.01   0.01   0.00     0.00   0.00   0.00     0.01   0.00
0.00
  15   8     0.00   0.01  -0.01     0.00   0.00   0.00     0.00  -0.01
0.00
  16   1     0.04   0.13  -0.02     0.00   0.02   0.15     0.00  -0.01
0.03
  17   1     0.20   0.61   0.14     0.29  -0.30   0.27    -0.09   0.26  -
0.02
  18   1     0.32   0.24  -0.09     0.42  -0.14   0.10     0.03  -0.20
0.15
  19   1    -0.31  -0.09  -0.01    -0.04   0.09   0.03     0.47   0.03  -
0.04
  20   1    -0.10  -0.03  -0.10     0.41  -0.19  -0.08    -0.16   0.23
0.13
  21   1     0.07  -0.02   0.18    -0.04  -0.01  -0.09    -0.06  -0.02
0.03
  22   1    -0.16  -0.10  -0.01    -0.23   0.04  -0.11    -0.34  -0.42  -
0.09
  23   1     0.21   0.21  -0.19     0.26  -0.25  -0.15     0.29   0.02  -
0.18
  24   1     0.02   0.04   0.02    -0.05   0.08   0.00    -0.16   0.19  -
0.01
  25   1    -0.03   0.04  -0.01    -0.12   0.12  -0.01    -0.04   0.02  -
0.01
  26   1     0.02  -0.02  -0.02     0.00  -0.01   0.01     0.00   0.00  -
0.03
                      52                    53                    54
                      ?A                    ?A                    ?A
 Frequencies --  1404.8591             1409.8711             1416.7109
 Red. masses --     1.6577                1.5499                1.4370
 Frc consts  --     1.9276                1.8152                1.6993
 IR Inten    --     2.3762                8.7016                2.4735
```

Raman Activ	--	0.5885			11.7087			1.7901		
Depolar	--	0.7223			0.7056			0.7493		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.06	0.03	0.05	-0.02	-0.11	-0.04	-0.02	0.02	0.00
2	6	-0.04	-0.06	-0.04	-0.05	0.05	-0.01	0.03	0.01	0.06
3	6	-0.02	0.06	0.02	0.01	0.00	0.01	0.01	0.00	-0.06
4	6	-0.02	-0.01	-0.03	-0.04	0.04	0.01	0.06	-0.04	-0.05
5	6	-0.01	-0.05	-0.02	0.02	0.02	-0.01	0.00	0.03	0.04
6	6	-0.04	-0.06	-0.07	0.03	-0.06	-0.01	0.02	-0.02	-0.03
7	6	0.01	0.07	0.03	-0.10	0.00	-0.04	-0.03	-0.02	-0.04
8	6	0.01	-0.08	0.02	0.01	-0.05	-0.01	0.04	-0.02	0.05
9	6	-0.06	0.02	-0.03	0.00	0.01	-0.01	0.02	0.00	0.01
10	6	0.05	-0.04	0.03	0.00	0.01	0.01	-0.05	0.01	0.04
11	6	-0.04	0.00	-0.01	0.05	0.05	0.03	-0.04	0.06	0.00
12	8	0.00	0.02	0.00	0.00	-0.01	0.00	0.00	-0.01	0.00
13	6	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.01	0.01	0.01	0.00	0.00	0.00	-0.01	0.00	0.00
16	1	-0.02	-0.20	-0.14	0.25	0.50	0.25	-0.12	-0.17	-0.02
17	1	0.19	0.29	0.21	0.09	-0.13	0.16	-0.23	-0.08	-0.22
18	1	0.13	-0.05	0.13	-0.02	0.00	0.01	-0.04	-0.12	0.04
19	1	0.09	0.17	0.02	0.20	-0.07	-0.07	-0.41	0.22	0.11
20	1	0.21	0.36	0.38	-0.08	0.15	0.18	-0.06	0.12	0.09
21	1	-0.01	0.08	-0.04	0.49	0.21	0.26	0.23	0.07	0.19
22	1	-0.02	0.43	-0.12	0.06	0.16	-0.05	-0.32	0.20	-0.16
23	1	-0.11	0.22	0.16	0.00	-0.01	0.01	0.27	-0.08	-0.20
24	1	0.11	-0.09	-0.01	0.07	0.06	0.03	0.21	-0.23	0.02
25	1	0.04	-0.06	0.03	0.07	0.05	0.05	0.15	-0.17	-0.01

```
  26   1     0.04  -0.03  -0.02     0.00   0.01   0.00    -0.01   0.01
0.02
                     55                     56                     57
                     ?A                     ?A                     ?A
 Frequencies --  1435.9662              1448.7660              1455.5723
 Red. masses --     1.4588                 1.5502                 1.4968
 Frc consts  --     1.7722                 1.9170                 1.8684
 IR Inten    --    11.0991                 1.4764                25.9740
 Raman Activ --     0.3124                 0.5923                 1.1294
 Depolar     --     0.6988                 0.3669                 0.7171
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6    -0.04  -0.04   0.12    -0.06  -0.04   0.08    -0.06  -0.02  -
0.01
   2   6     0.05   0.01  -0.02     0.05  -0.02   0.01     0.00   0.01
0.02
   3   6    -0.02   0.00  -0.02    -0.01   0.00  -0.01     0.01  -0.01
0.01
   4   6    -0.03   0.03  -0.02    -0.02   0.03  -0.04     0.05  -0.02  -
0.04
   5   6     0.00  -0.03   0.02     0.01  -0.03   0.04     0.02   0.03
0.01
   6   6    -0.02  -0.03   0.02    -0.01   0.06   0.00     0.01  -0.03
0.00
   7   6     0.04   0.02  -0.10    -0.05  -0.04   0.09     0.04   0.06  -
0.05
   8   6    -0.03   0.02   0.00     0.07  -0.04   0.00     0.04  -0.01
0.05
   9   6     0.02   0.00  -0.01    -0.06   0.03   0.02    -0.07   0.01
0.00
  10   6    -0.01   0.02   0.02     0.01  -0.01  -0.01     0.05   0.00  -
0.03
  11   6    -0.01   0.02  -0.01     0.03   0.00  -0.03     0.07  -0.08
0.02
  12   8     0.00   0.01   0.00     0.00   0.01  -0.01     0.00  -0.01
0.00
  13   6     0.00   0.00   0.00     0.00   0.00  -0.01     0.01   0.00
0.00
  14   7     0.00   0.00   0.00     0.01  -0.01   0.00     0.01  -0.01
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.19   0.12  -0.50     0.19   0.21  -0.43     0.03   0.20
0.09
  17   1    -0.08  -0.08  -0.17    -0.16   0.06  -0.24    -0.10  -0.01  -
0.09
  18   1     0.13  -0.04   0.03     0.03  -0.01   0.00    -0.09   0.06  -
0.06
  19   1     0.26  -0.06  -0.09     0.08  -0.06  -0.09    -0.27   0.17
0.08
  20   1     0.11   0.07   0.14     0.02  -0.16  -0.22    -0.10   0.11
0.12
  21   1    -0.15  -0.12   0.40     0.25   0.16  -0.50    -0.26  -0.09
0.16
```

22	1	0.05	-0.19	0.09	-0.24	0.19	-0.20	-0.36	0.07	-0.14
23	1	0.07	-0.10	-0.04	-0.05	0.03	0.04	-0.24	0.00	0.18
24	1	0.26	-0.30	0.02	-0.11	-0.02	0.00	-0.17	0.22	-0.01
25	1	-0.16	0.18	-0.01	0.00	0.09	0.05	-0.38	0.39	-0.05
26	1	0.01	-0.01	0.01	0.03	-0.02	0.00	0.01	0.01	0.01

	58			59			60		
	?A			?A			?A		
Frequencies --	1471.5772			1491.2026			1640.5276		
Red. masses --	1.7096			2.5629			1.0990		
Frc consts --	2.1813			3.3578			1.7426		
IR Inten --	13.9181			185.4008			6.1944		
Raman Activ --	7.2115			1.7186			9.6137		
Depolar --	0.7126			0.6945			0.6506		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.04	-0.02	0.00	0.02	0.00	0.06	-0.01	0.00	0.00
2 6	0.04	-0.01	0.04	0.00	-0.02	-0.04	0.00	0.00	0.00
3 6	0.00	-0.01	-0.02	-0.04	-0.10	0.07	0.00	0.00	0.00
4 6	0.02	0.00	0.00	-0.07	-0.12	-0.03	0.00	0.00	0.00
5 6	0.00	0.05	0.01	0.07	0.27	-0.04	0.00	0.00	0.00
6 6	-0.01	-0.01	-0.07	0.00	0.03	0.02	0.00	0.00	0.00
7 6	0.02	0.05	0.06	-0.01	-0.01	0.00	0.00	-0.01	0.00
8 6	-0.09	-0.06	-0.01	0.01	0.00	0.01	0.00	0.00	0.00
9 6	0.12	-0.03	-0.02	0.04	-0.03	0.01	0.00	0.00	0.00
10 6	-0.08	-0.01	0.06	0.00	0.00	-0.02	0.00	0.00	0.00
11 6	0.05	-0.06	-0.01	-0.01	0.02	-0.02	-0.06	-0.05	-0.04
12 8	0.00	-0.02	0.00	-0.01	-0.09	0.01	0.00	0.00	0.00
13 6	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14 7	-0.02	0.01	0.00	-0.01	0.01	0.00	0.00	0.00	0.00
15 8	-0.01	0.00	0.00	-0.02	-0.02	0.00	0.00	0.00	0.00
16 1	0.06	0.15	-0.05	0.05	-0.03	-0.16	-0.02	0.00	-0.01
17 1	-0.14	0.07	-0.16	0.12	0.10	0.08	-0.02	-0.01	-0.02

18	1	0.05	-0.02	-0.01	0.16	0.42	-0.36	0.00	0.00	0.00
19	1	-0.05	0.01	0.01	0.30	0.52	0.14	-0.02	-0.02	-0.01
20	1	0.10	0.20	0.15	0.03	-0.07	-0.07	-0.01	-0.02	-0.02
21	1	-0.13	0.03	-0.20	0.06	0.03	-0.04	0.00	-0.02	-0.01
22	1	0.43	0.30	0.12	-0.07	0.05	-0.04	-0.02	-0.02	-0.01
23	1	0.40	0.09	-0.28	-0.03	0.06	0.00	0.00	0.00	0.00
24	1	-0.23	0.24	-0.03	0.11	-0.12	0.00	0.52	0.45	-0.16
25	1	-0.15	0.21	0.03	0.04	0.01	0.05	0.22	0.23	0.62
26	1	-0.04	0.03	0.03	-0.12	0.13	0.02	0.00	0.00	0.00

	61	62	63
	?A	?A	?A
Frequencies --	2327.3066	2567.3306	3214.5027
Red. masses --	1.0589	12.6755	1.0584
Frc consts --	3.3792	49.2242	6.4433
IR Inten --	646.0458	13.2803	35.9735
Raman Activ --	52.4061	155.3906	126.4425
Depolar --	0.0907	0.2167	0.2036

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
2	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	6	0.04	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	6	0.00	0.00	0.00	-0.10	0.05	0.01	0.00	0.00	0.00
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.04	-0.04	-0.03
12	8	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.73	-0.33	-0.04	0.00	0.00	0.00

14	7	0.00	0.00	0.00	-0.53	0.25	0.03	0.00	0.00	0.00
15	8	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	0.00	0.00	0.00	0.00	0.00	0.00	-0.08	0.04	-0.02
17	1	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.01
18	1	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
19	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01
20	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.01
21	1	0.00	0.00	0.00	0.00	0.00	0.00	0.04	-0.10	-0.01
22	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01
23	1	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	1	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.10	0.68
25	1	0.00	0.00	0.00	0.00	0.00	0.00	0.46	0.40	-0.37
26	1	-0.64	-0.77	0.02	0.03	0.03	0.00	0.00	0.00	0.00

	64			65			66		
	?A			?A			?A		
Frequencies --	3260.4061			3272.7085			3282.8637		
Red. masses --	1.1071			1.0876			1.0886		
Frc consts --	6.9340			6.8633			6.9122		
IR Inten --	21.9344			14.6530			7.8911		
Raman Activ --	88.7953			52.7374			105.5011		
Depolar --	0.7486			0.5393			0.4551		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.00	0.00	0.02	-0.01	0.00	-0.06	0.03	-0.01
2 6	0.00	0.00	0.00	-0.01	0.00	0.01	0.03	0.00	-0.02
3 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4 6	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.01
5 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6 6	0.00	0.00	0.00	0.00	0.02	-0.02	0.00	0.00	0.00
7 6	0.00	0.00	0.00	0.03	-0.07	-0.01	0.01	-0.02	0.00
8 6	0.00	0.00	0.00	-0.01	0.01	0.02	0.00	0.00	0.01
9 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
  10   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  11   6    -0.03  -0.02   0.09     0.00   0.00   0.00     0.00  -0.01
0.00
  12   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  13   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  14   7     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  15   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
  16   1     0.00   0.00   0.00    -0.20   0.11  -0.04     0.73  -0.40
0.16
  17   1    -0.01   0.00   0.00     0.08   0.00  -0.07    -0.30   0.00
0.26
  18   1     0.00   0.00   0.00     0.00   0.01   0.01     0.00  -0.03  -
0.04
  19   1     0.00   0.00   0.01     0.01  -0.02   0.06    -0.03   0.05  -
0.15
  20   1     0.00  -0.01   0.01    -0.03  -0.19   0.19     0.00   0.01  -
0.01
  21   1     0.00   0.01   0.00    -0.34   0.81   0.10    -0.10   0.23
0.03
  22   1    -0.01   0.00   0.01     0.10  -0.06  -0.23     0.03  -0.02  -
0.08
  23   1     0.00   0.00   0.00    -0.02   0.00  -0.03     0.00   0.00
0.00
  24   1    -0.08  -0.12  -0.70     0.01   0.01   0.06     0.01   0.01
0.07
  25   1     0.46   0.40  -0.34     0.03   0.02  -0.02     0.05   0.04  -
0.04
  26   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
                     67                     68                     69
                     ?A                     ?A                     ?A
 Frequencies --  3291.8883              3296.1256              3304.8402
 Red. masses --     1.0885                 1.0891                 1.0892
 Frc consts  --     6.9497                 6.9717                 7.0092
 IR Inten    --     6.8632                28.5670                36.0530
 Raman Activ --    87.2718                53.1293               117.3461
 Depolar     --     0.6841                 0.5918                 0.3920
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
   1   6     0.02  -0.01   0.00     0.02  -0.01   0.00    -0.02   0.01
0.00
   2   6     0.03   0.00  -0.02     0.02   0.00  -0.02    -0.04   0.00
0.04
   3   6     0.00   0.01   0.01     0.00   0.00   0.01     0.00   0.00  -
0.01
   4   6     0.00   0.01  -0.02     0.00  -0.01   0.02     0.00  -0.01
0.02
   5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00   0.00
0.00
```

```
    6    6    -0.01   -0.04    0.04     0.00   -0.02    0.02     0.00   -0.03
0.03
    7    6     0.00    0.00    0.00     0.01   -0.02    0.00     0.00   -0.01
0.00
    8    6    -0.02    0.01    0.04     0.03   -0.01   -0.06     0.00    0.00
0.00
    9    6     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   10    6    -0.01    0.00   -0.01    -0.01    0.00   -0.01    -0.02    0.00  -
0.03
   11    6     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   12    8     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   13    6     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   14    7     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   15    8     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
   16    1    -0.20    0.11   -0.05    -0.19    0.10   -0.04     0.19   -0.10
0.05
   17    1    -0.32    0.00    0.29    -0.23    0.00    0.20     0.51    0.00  -
0.45
   18    1     0.00   -0.06   -0.07     0.00   -0.05   -0.06    -0.01    0.05
0.06
   19    1     0.03   -0.08    0.22    -0.03    0.09   -0.24    -0.04    0.09  -
0.23
   20    1     0.07    0.46   -0.46     0.03    0.18   -0.19     0.05    0.31  -
0.31
   21    1    -0.02    0.05    0.01    -0.12    0.28    0.04    -0.05    0.12
0.02
   22    1     0.18   -0.11   -0.41    -0.30    0.18    0.68     0.02   -0.01  -
0.04
   23    1     0.12   -0.01    0.17     0.10   -0.01    0.14     0.25   -0.02
0.35
   24    1     0.00    0.00   -0.02     0.00    0.00    0.02     0.00    0.00
0.02
   25    1     0.00    0.00    0.00     0.00    0.00    0.00     0.03    0.02  -
0.02
   26    1     0.00    0.00    0.00     0.00    0.00    0.00     0.00    0.00
0.00
                     70                      71                      72
                     ?A                      ?A                      ?A
 Frequencies --  3313.3793               3316.6623               3335.5170
 Red. masses --     1.0897                  1.0900                  1.0910
 Frc consts  --     7.0486                  7.0648                  7.1514
 IR Inten    --    29.4114                  5.9561                 11.7831
 Raman Activ --    27.8882                259.0625                218.5246
 Depolar     --     0.4082                  0.1235                  0.0884
 Atom AN      X      Y      Z        X      Y      Z        X      Y
Z
    1    6   -0.01    0.00    0.00    -0.02    0.01    0.00     0.01    0.00
0.00
```

2	6	0.00	0.00	0.00	-0.01	0.00	0.01	0.02	0.00	-0.01
3	6	0.00	0.01	0.02	0.00	-0.01	-0.02	0.00	-0.05	-0.06
4	6	-0.01	0.01	-0.03	-0.01	0.02	-0.06	0.00	0.00	0.01
5	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	6	0.00	0.02	-0.02	0.00	-0.02	0.02	0.00	0.01	-0.01
7	6	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
8	6	0.00	0.00	-0.01	0.01	-0.01	-0.03	0.00	0.00	0.00
9	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	6	-0.04	0.00	-0.05	0.01	0.00	0.02	-0.02	0.00	-0.02
11	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	1	0.06	-0.03	0.01	0.19	-0.10	0.04	-0.05	0.03	-0.01
17	1	-0.04	0.00	0.04	0.12	0.00	-0.11	-0.16	0.00	0.14
18	1	0.01	-0.17	-0.20	-0.01	0.17	0.20	-0.03	0.60	0.69
19	1	0.06	-0.15	0.40	0.11	-0.26	0.71	-0.01	0.03	-0.08
20	1	-0.04	-0.26	0.26	0.03	0.18	-0.18	-0.01	-0.09	0.09
21	1	0.02	-0.06	-0.01	-0.05	0.13	0.02	0.01	-0.03	0.00
22	1	-0.04	0.02	0.08	-0.13	0.08	0.29	0.02	-0.01	-0.04
23	1	0.45	-0.03	0.61	-0.15	0.01	-0.20	0.17	-0.02	0.23
24	1	0.00	0.00	0.01	0.01	0.01	0.04	0.00	0.00	-0.01
25	1	0.00	0.00	0.00	0.02	0.02	-0.01	-0.01	-0.01	0.00
26	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

```
 --------------------
 - Thermochemistry -
 --------------------
```

```
Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
Atom  1 has atomic number  6 and mass  12.00000
Atom  2 has atomic number  6 and mass  12.00000
Atom  3 has atomic number  6 and mass  12.00000
Atom  4 has atomic number  6 and mass  12.00000
Atom  5 has atomic number  6 and mass  12.00000
Atom  6 has atomic number  6 and mass  12.00000
Atom  7 has atomic number  6 and mass  12.00000
Atom  8 has atomic number  6 and mass  12.00000
Atom  9 has atomic number  6 and mass  12.00000
Atom 10 has atomic number  6 and mass  12.00000
Atom 11 has atomic number  6 and mass  12.00000
Atom 12 has atomic number  8 and mass  15.99491
Atom 13 has atomic number  6 and mass  12.00000
Atom 14 has atomic number  7 and mass  14.00307
Atom 15 has atomic number  8 and mass  15.99491
Atom 16 has atomic number  1 and mass   1.00783
Atom 17 has atomic number  1 and mass   1.00783
Atom 18 has atomic number  1 and mass   1.00783
Atom 19 has atomic number  1 and mass   1.00783
Atom 20 has atomic number  1 and mass   1.00783
Atom 21 has atomic number  1 and mass   1.00783
Atom 22 has atomic number  1 and mass   1.00783
Atom 23 has atomic number  1 and mass   1.00783
Atom 24 has atomic number  1 and mass   1.00783
Atom 25 has atomic number  1 and mass   1.00783
Atom 26 has atomic number  1 and mass   1.00783
Molecular mass:   201.07898 amu.
Principal axes and moments of inertia in atomic units:
                          1         2         3
    EIGENVALUES --  1774.94378 2292.82308 3062.82353
          X            0.99703   0.07659   0.00756
          Y           -0.07668   0.99698   0.01256
          Z           -0.00658  -0.01311   0.99989
THIS MOLECULE IS AN ASYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER  1.
WARNING-- ASSUMPTION OF CLASSICAL BEHAVIOR FOR ROTATION
          MAY CAUSE SIGNIFICANT ERROR
ROTATIONAL TEMPERATURES (KELVIN)      0.04880     0.03778     0.02828
ROTATIONAL CONSTANTS (GHZ)            1.01679     0.78713     0.58924
   1 IMAGINARY FREQUENCIES IGNORED.
Zero-point vibrational energy     575338.3 (Joules/Mol)
                                  137.50916 (Kcal/Mol)
WARNING-- EXPLICIT CONSIDERATION OF  13 DEGREES OF FREEDOM AS
          VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
VIBRATIONAL TEMPERATURES:    190.31   235.94   265.41   495.14   573.24
         (KELVIN)            645.44   683.09   706.20   769.94   822.85
                             867.60   878.45   891.24   954.30   999.00
                            1070.90  1151.49  1156.50  1187.44  1207.38
                            1260.86  1270.62  1312.96  1331.76  1378.32
                            1413.97  1431.18  1435.27  1454.48  1487.88
                            1499.87  1519.88  1531.68  1559.14  1620.71
                            1670.32  1700.00  1750.71  1775.71  1798.70
                            1816.49  1823.47  1826.15  1871.65  1910.19
```

1954.55	1961.13	1968.38	1993.57	1994.73
2021.27	2028.48	2038.32	2066.02	2084.44
2094.23	2117.26	2145.50	2360.34	3348.46
3693.79	4624.93	4690.97	4708.67	4723.28
4736.27	4742.36	4754.90	4767.19	4771.91
4799.04				

Zero-point correction=	0.219135
(Hartree/Particle)	
Thermal correction to Energy=	0.227554
Thermal correction to Enthalpy=	0.228498
Thermal correction to Gibbs Free Energy=	0.185311
Sum of electronic and zero-point Energies=	-661.037763
Sum of electronic and thermal Energies=	-661.029344
Sum of electronic and thermal Enthalpies=	-661.028400
Sum of electronic and thermal Free Energies=	-661.071587

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	142.792	37.866	90.895
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	41.800
ROTATIONAL	0.889	2.981	30.901
VIBRATIONAL	141.015	31.904	18.194
VIBRATION 1	0.612	1.921	2.913
VIBRATION 2	0.623	1.887	2.503
VIBRATION 3	0.631	1.861	2.283
VIBRATION 4	0.723	1.587	1.193
VIBRATION 5	0.765	1.474	0.968
VIBRATION 6	0.808	1.364	0.800
VIBRATION 7	0.831	1.306	0.724
VIBRATION 8	0.847	1.270	0.681
VIBRATION 9	0.890	1.172	0.576
VIBRATION 10	0.928	1.092	0.501
VIBRATION 11	0.961	1.025	0.445
VIBRATION 12	0.970	1.009	0.432
VIBRATION 13	0.979	0.991	0.417

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.580083D-85	-85.236510	-196.264317
TOTAL V=0	0.361258D+16	15.557817	35.823198
VIB (BOT)	0.409536D-99	-99.387708	-228.848655
VIB (BOT) 1	0.154033D+01	0.187615	0.432000
VIB (BOT) 2	0.123130D+01	0.090363	0.208069
VIB (BOT) 3	0.108711D+01	0.036273	0.083522
VIB (BOT) 4	0.538151D+00	-0.269096	-0.619616
VIB (BOT) 5	0.447870D+00	-0.348848	-0.803252
VIB (BOT) 6	0.382699D+00	-0.417143	-0.960508
VIB (BOT) 7	0.353845D+00	-0.451186	-1.038895
VIB (BOT) 8	0.337558D+00	-0.471651	-1.086017
VIB (BOT) 9	0.297427D+00	-0.526619	-1.212586
VIB (BOT) 10	0.268600D+00	-0.570895	-1.314533
VIB (BOT) 11	0.246854D+00	-0.607559	-1.398957
VIB (BOT) 12	0.241906D+00	-0.616354	-1.419208
VIB (BOT) 13	0.236224D+00	-0.626676	-1.442974

```
VIB (V=0)       0.255046D+02          1.406619          3.238860
VIB (V=0)  1    0.211945D+01          0.326224          0.751158
VIB (V=0)  2    0.182895D+01          0.262201          0.603740
VIB (V=0)  3    0.169658D+01          0.229575          0.528615
VIB (V=0)  4    0.123458D+01          0.091519          0.210730
VIB (V=0)  5    0.117126D+01          0.068653          0.158079
VIB (V=0)  6    0.112965D+01          0.052944          0.121907
VIB (V=0)  7    0.111254D+01          0.046316          0.106647
VIB (V=0)  8    0.110328D+01          0.042685          0.098287
VIB (V=0)  9    0.108178D+01          0.034137          0.078604
VIB (V=0) 10    0.106758D+01          0.028400          0.065393
VIB (V=0) 11    0.105762D+01          0.024329          0.056019
VIB (V=0) 12    0.105544D+01          0.023435          0.053962
VIB (V=0) 13    0.105299D+01          0.022426          0.051637
ELECTRONIC      0.100000D+01          0.000000          0.000000
TRANSLATIONAL   0.112075D+09          8.049510         18.534683
ROTATIONAL      0.126383D+07          6.101688         14.049656
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6           0.000003590   -0.000013460   -0.000005376
   2          6           0.000004562    0.000013856    0.000002851
   3          6           0.000009222    0.000008947   -0.000000097
   4          6           0.000002846    0.000013617    0.000012025
   5          6           0.000008363    0.000078158   -0.000009060
   6          6          -0.000018970    0.000005609   -0.000009654
   7          6           0.000002767   -0.000003771   -0.000010721
   8          6          -0.000001915    0.000009513    0.000000036
   9          6          -0.000012683   -0.000038739    0.000004471
  10          6          -0.000014362    0.000008032    0.000004704
  11          6          -0.000009618   -0.000014509    0.000019826
  12          8          -0.000026536   -0.000057209    0.000007794
  13          6           0.000016257    0.000040668   -0.000023886
  14          7          -0.000000959   -0.000010828    0.000011893
  15          8           0.000022047   -0.000037870    0.000000084
  16          1           0.000001868   -0.000000202    0.000004616
  17          1          -0.000001812   -0.000002323   -0.000004370
  18          1           0.000006828    0.000002256   -0.000002032
  19          1           0.000001550    0.000003365    0.000004816
  20          1           0.000002875    0.000001010    0.000000723
  21          1          -0.000005019   -0.000005275    0.000006437
  22          1          -0.000000959   -0.000011816    0.000003976
  23          1           0.000002638   -0.000016181   -0.000004183
  24          1           0.000009211    0.000003567   -0.000004529
  25          1           0.000000360   -0.000006853   -0.000009923
  26          1          -0.000002151    0.000030437   -0.000000421
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000078158 RMS     0.000016481
-------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------
```

```
  1  C         0.000004(   1)     -0.000013(  27)     -0.000005(  53)
  2  C         0.000005(   2)      0.000014(  28)      0.000003(  54)
  3  C         0.000009(   3)      0.000009(  29)      0.000000(  55)
  4  C         0.000003(   4)      0.000014(  30)      0.000012(  56)
  5  C         0.000008(   5)      0.000078(  31)     -0.000009(  57)
  6  C        -0.000019(   6)      0.000006(  32)     -0.000010(  58)
  7  C         0.000003(   7)     -0.000004(  33)     -0.000011(  59)
  8  C        -0.000002(   8)      0.000010(  34)      0.000000(  60)
  9  C        -0.000013(   9)     -0.000039(  35)      0.000004(  61)
 10  C        -0.000014(  10)      0.000008(  36)      0.000005(  62)
 11  C        -0.000010(  11)     -0.000015(  37)      0.000020(  63)
 12  O        -0.000027(  12)     -0.000057(  38)      0.000008(  64)
 13  C         0.000016(  13)      0.000041(  39)     -0.000024(  65)
 14  N        -0.000001(  14)     -0.000011(  40)      0.000012(  66)
 15  O         0.000022(  15)     -0.000038(  41)      0.000000(  67)
 16  H         0.000002(  16)      0.000000(  42)      0.000005(  68)
 17  H        -0.000002(  17)     -0.000002(  43)     -0.000004(  69)
 18  H         0.000007(  18)      0.000002(  44)     -0.000002(  70)
 19  H         0.000002(  19)      0.000003(  45)      0.000005(  71)
 20  H         0.000003(  20)      0.000001(  46)      0.000001(  72)
 21  H        -0.000005(  21)     -0.000005(  47)      0.000006(  73)
 22  H        -0.000001(  22)     -0.000012(  48)      0.000004(  74)
 23  H         0.000003(  23)     -0.000016(  49)     -0.000004(  75)
 24  H         0.000009(  24)      0.000004(  50)     -0.000005(  76)
 25  H         0.000000(  25)     -0.000007(  51)     -0.000010(  77)
 26  H        -0.000002(  26)      0.000030(  52)      0.000000(  78)
---------------------------------------------------------------------
Internal  Forces:  Max     0.000078158 RMS     0.000016481

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   1 out of a maximum of  88
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
    Eigenvalues ---   -0.18887   0.00452   0.00670   0.00861   0.01250
    Eigenvalues ---    0.02612   0.02897   0.03330   0.04415   0.04604
    Eigenvalues ---    0.04693   0.04721   0.04824   0.05101   0.05184
    Eigenvalues ---    0.05268   0.05334   0.05386   0.05437   0.05662
    Eigenvalues ---    0.05861   0.06097   0.06809   0.07987   0.09121
    Eigenvalues ---    0.10536   0.10866   0.11789   0.13721   0.14334
    Eigenvalues ---    0.14867   0.15867   0.16105   0.18787   0.19827
    Eigenvalues ---    0.19900   0.21668   0.24555   0.24813   0.27919
    Eigenvalues ---    0.32579   0.34737   0.35528   0.37647   0.38395
    Eigenvalues ---    0.39958   0.44614   0.47796   0.49699   0.50292
    Eigenvalues ---    0.51907   0.52712   0.57874   0.59731   0.63804
    Eigenvalues ---    0.64773   0.65586   0.71612   0.72477   0.78508
    Eigenvalues ---    0.87136   0.92417   0.95181   0.95740   0.96952
    Eigenvalues ---    0.98555   0.99760   1.02525   1.05473   1.08199
    Eigenvalues ---    1.10712   3.18485
Eigenvalue   1 out of range, new value =    0.188869 Eigenvector:
                          1
          X1         -0.02278
          Y1         -0.01855
```

Z1	0.00627
X2	-0.01998
Y2	-0.01561
Z2	0.00162
X3	-0.03268
Y3	-0.00599
Z3	0.00085
X4	-0.03220
Y4	-0.01066
Z4	0.00143
X5	0.14396
Y5	-0.14630
Z5	0.00666
X6	-0.00777
Y6	-0.00484
Z6	0.00412
X7	-0.00784
Y7	-0.00540
Z7	-0.00234
X8	-0.01965
Y8	-0.02604
Z8	-0.00269
X9	-0.04445
Y9	-0.00069
Z9	-0.01793
X10	-0.02027
Y10	-0.01445
Z10	0.00240
X11	-0.00488
Y11	-0.01921
Z11	0.00331
X12	0.41770
Y12	0.02626
Z12	-0.03076
X13	-0.02010
Y13	0.05321
Z13	-0.01301
X14	-0.00087
Y14	0.09726
Z14	-0.01591
X15	-0.07737
Y15	-0.11233
Z15	0.07437
X16	-0.02198
Y16	-0.02017
Z16	0.00403
X17	-0.01314
Y17	-0.01453
Z17	0.00548
X18	-0.02469
Y18	0.00433
Z18	-0.00598
X19	-0.02323
Y19	0.00087

Z19	0.00326
X20	0.00006
Y20	-0.00537
Z20	0.00111
X21	0.00688
Y21	0.00200
Z21	-0.00005
X22	-0.01326
Y22	0.00243
Z22	-0.00598
X23	-0.00956
Y23	0.01129
Z23	-0.00336
X24	-0.00065
Y24	-0.01185
Z24	0.00169
X25	-0.00011
Y25	-0.01833
Z25	0.00291
X26	-0.64349
Y26	0.56093
Z26	-0.06161

Angle between quadratic step and forces= 70.48 degrees.
Linear search not attempted -- first point.
TrRot= -0.000002 0.000018 0.000015 0.000008 -0.000001 0.000008

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
X1	-3.95030	0.00000	0.00000	-0.00001	0.00000	-3.95030
Y1	-0.26736	-0.00001	0.00000	0.00006	0.00002	-0.26734
Z1	-0.76810	-0.00001	0.00000	0.00006	0.00007	-0.76803
X2	-3.13671	0.00000	0.00000	-0.00001	-0.00001	-3.13672
Y2	-0.27048	0.00001	0.00000	0.00014	0.00011	-0.27037
Z2	2.05038	0.00000	0.00000	0.00007	0.00009	2.05046
X3	-1.02031	0.00001	0.00000	0.00018	0.00015	-1.02015
Y3	1.75737	0.00001	0.00000	0.00001	0.00001	1.75738
Z3	2.37793	0.00000	0.00000	0.00009	0.00010	2.37804
X4	-1.64404	0.00000	0.00000	0.00006	0.00005	-1.64399
Y4	0.96819	0.00001	0.00000	-0.00001	-0.00002	0.96818
Z4	-2.05848	0.00001	0.00000	0.00011	0.00012	-2.05836
X5	-0.61919	0.00001	0.00000	0.00008	0.00003	-0.61916
Y5	2.97883	0.00008	0.00000	0.00000	0.00001	2.97884
Z5	-0.23239	-0.00001	0.00000	0.00008	0.00009	-0.23230
X6	-1.09955	-0.00002	0.00000	-0.00020	-0.00017	-1.09971
Y6	-2.43612	0.00001	0.00000	0.00002	0.00002	-2.43609
Z6	2.17187	-0.00001	0.00000	0.00000	0.00002	2.17189
X7	-0.98068	0.00000	0.00000	-0.00020	-0.00015	-0.98084
Y7	-3.40084	0.00000	0.00000	-0.00008	-0.00007	-3.40091
Z7	-0.58906	-0.00001	0.00000	0.00007	0.00008	-0.58897
X8	0.40992	0.00000	0.00000	-0.00006	-0.00005	0.40988
Y8	-1.21563	0.00001	0.00000	-0.00016	-0.00014	-1.21577
Z8	-1.93277	0.00000	0.00000	0.00000	0.00002	-1.93275
X9	2.40107	-0.00001	0.00000	0.00001	0.00001	2.40109
Y9	-0.18540	-0.00004	0.00000	-0.00021	-0.00015	-0.18556
Z9	-0.02867	0.00000	0.00000	-0.00010	-0.00008	-0.02875

X10	1.01058	-0.00001	0.00000	-0.00001	-0.00001	1.01057
Y10	-0.39761	0.00001	0.00000	-0.00019	-0.00016	-0.39777
Z10	2.53627	0.00000	0.00000	-0.00004	-0.00003	2.53624
X11	-3.73200	-0.00001	0.00000	-0.00011	-0.00007	-3.73207
Y11	-3.07729	-0.00001	0.00000	0.00006	0.00002	-3.07727
Z11	-1.50778	0.00002	0.00000	-0.00006	-0.00005	-1.50783
X12	-0.47105	-0.00003	0.00000	-0.00027	-0.00036	-0.47141
Y12	5.50462	-0.00006	0.00000	-0.00021	-0.00020	5.50442
Z12	-0.57848	0.00001	0.00000	-0.00015	-0.00013	-0.57861
X13	4.92359	0.00002	0.00000	0.00024	0.00026	4.92385
Y13	-1.20978	0.00004	0.00000	0.00034	0.00043	-1.20935
Z13	-0.20239	-0.00002	0.00000	-0.00014	-0.00012	-0.20251
X14	6.89665	0.00000	0.00000	0.00032	0.00035	6.89701
Y14	-2.06814	-0.00001	0.00000	0.00048	0.00060	-2.06754
Z14	-0.32201	0.00001	0.00000	0.00021	0.00023	-0.32178
X15	2.28506	0.00002	0.00000	0.00007	0.00003	2.28509
Y15	2.51613	-0.00004	0.00000	-0.00008	-0.00003	2.51610
Z15	-0.60002	0.00000	0.00000	0.00006	0.00008	-0.59994
X16	-5.73181	0.00000	0.00000	0.00005	0.00004	-5.73177
Y16	0.65036	0.00000	0.00000	0.00017	0.00010	0.65046
Z16	-1.15322	0.00000	0.00000	0.00009	0.00011	-1.15311
X17	-4.65946	0.00000	0.00000	-0.00006	-0.00006	-4.65951
Y17	-0.30576	0.00000	0.00000	0.00018	0.00013	-0.30563
Z17	3.40355	0.00000	0.00000	0.00001	0.00003	3.40357
X18	-1.11300	0.00001	0.00000	0.00044	0.00039	-1.11261
Y18	3.09862	0.00000	0.00000	0.00001	0.00002	3.09864
Z18	3.90383	0.00000	0.00000	0.00010	0.00011	3.90395
X19	-1.94821	0.00000	0.00000	0.00011	0.00008	-1.94813
Y19	1.67851	0.00000	0.00000	0.00012	0.00011	1.67862
Z19	-3.94378	0.00000	0.00000	0.00016	0.00017	-3.94361
X20	-1.29335	0.00000	0.00000	-0.00020	-0.00014	-1.29349
Y20	-3.87514	0.00000	0.00000	0.00008	0.00007	-3.87506
Z20	3.60137	0.00000	0.00000	0.00006	0.00008	3.60145
X21	-0.14055	-0.00001	0.00000	-0.00036	-0.00028	-0.14083
Y21	-5.24506	-0.00001	0.00000	-0.00018	-0.00017	-5.24522
Z21	-0.83990	0.00001	0.00000	0.00025	0.00026	-0.83964
X22	1.21275	0.00000	0.00000	-0.00020	-0.00017	1.21258
Y22	-1.66554	-0.00001	0.00000	-0.00043	-0.00040	-1.66593
Z22	-3.75297	0.00000	0.00000	0.00001	0.00003	-3.75294
X23	2.22224	0.00000	0.00000	0.00008	0.00008	2.22232
Y23	-0.46740	-0.00002	0.00000	-0.00063	-0.00058	-0.46798
Z23	4.17125	0.00000	0.00000	-0.00013	-0.00011	4.17113
X24	-3.94730	0.00001	0.00000	0.00028	0.00033	-3.94697
Y24	-3.39740	0.00000	0.00000	0.00041	0.00037	-3.39704
Z24	-3.51982	0.00000	0.00000	-0.00018	-0.00016	-3.51998
X25	-5.04559	0.00000	0.00000	-0.00030	-0.00023	-5.04582
Y25	-4.27327	-0.00001	0.00000	-0.00013	-0.00019	-4.27346
Z25	-0.48709	-0.00001	0.00000	-0.00054	-0.00053	-0.48762
X26	2.28122	0.00000	0.00000	-0.00002	-0.00010	2.28113
Y26	4.64978	0.00003	0.00000	0.00002	0.00008	4.64986
Z26	-0.60199	0.00000	0.00000	-0.00049	-0.00047	-0.60247

Item	Value	Threshold	Converged?
Maximum Force	0.000078	0.000450	YES
RMS Force	0.000016	0.000300	YES

```
Maximum Displacement     0.000604     0.001800     YES
RMS     Displacement     0.000200     0.001200     YES
Predicted change in Energy=-4.361354D-08
Optimization completed.
   -- Stationary point found.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

1\1\GINC-PELICAN\Freq\RHF\3-21+G*\C12H11N1O2\SINGH\22-Apr-2002\0\\#N R
HF/3-21+G* FREQ\\Freq calc of output str of mech1str5ts\\0,1\C,-2.0904
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,-0.5399230283,0.9299590849,1.258348\C,-0.8699860283,0.5123460849,-1.0
89299\C,-0.3276610283,1.5763280849,-0.122975\C,-0.5818550283,-1.289136
9151,1.149305\C,-0.5189560283,-1.7996469151,-0.311715\C,0.2169209717,-
0.6432839151,-1.022779\C,1.2705939717,-0.0981119151,-0.015174\C,0.5347
739717,-0.2104049151,1.342136\C,-1.9748880283,-1.6284309151,-0.797885\
O,-0.2492690283,2.9129170849,-0.306116\C,2.6054529717,-0.6401889151,-0
.107102\N,3.6495519717,-1.0944139151,-0.1704\O,1.2092029717,1.33147908
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743750283,-2.7755639151,-0.444455\H,0.6417599717,-0.8813639151,-1.9859
85\H,1.1759579717,-0.2473399151,2.207329\H,-2.0888230283,-1.7978289151
,-1.862608\H,-2.6700100283,-2.2613169151,-0.257757\H,1.2071709717,2.46
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0.00026950,-0.00018148,-0.00001341,0.00033151,-0.00031818,0.00002326,-
0.00006514,-0.00004316,-0.00012444,0.00005309,0.00002483,-0.00870922,0
.00199133,0.01752251\\-0.00000359,0.00001346,0.00000538,-0.00000456,-0
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0.00000561,0.00000965,-0.00000277,0.00000377,0.00001072,0.00000191,-0.
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05721,-0.00000779,-0.00001626,-0.00004067,0.00002389,0.00000096,0.0000
1083,-0.00001189,-0.00002205,0.00003787,-0.00000008,-0.00000187,0.0000

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 226,0.00000203,-0.00000155,-0.00000337,-0.00000482,-0.00000287,-0.0000
 0101,-0.00000072,0.00000502,0.00000527,-0.00000644,0.00000096,0.000011
 82,-0.00000398,-0.00000264,0.00001618,0.00000418,-0.00000921,-0.000003
 57,0.00000453,-0.00000036,0.00000685,0.00000992,0.00000215,-0.00003044
 ,0.00000042\\\@


 HOW IS IT THAT THE SKY FEEDS THE STARS?

                             -- LUCRETIUS
 Job cpu time:  0 days  2 hours 24 minutes 35.2 seconds.
 File lengths (MBytes):  RWF=  252 Int=    0 D2E=    0 Chk=    6 Scr=
1
 Normal termination of Gaussian 98.
```

```
%nproc=2
%chk=mech1s1ts
%nosave

#N RHF/3-21+G* OPT=(TS,NOEIGENTEST,GDIIS) OPTCYC=20

TS search for mech1str1 using input@2.1A from mech1s1S

-1  1

 C                  1.641447    1.304636   -0.269798
 C                  1.198636    0.934717    1.182848
 C                  1.102047   -0.632261    1.254280
 C                  1.227904    0.021379   -1.053404
 C                  1.671445   -1.057255   -0.079347
 C                 -0.367671    1.038449    1.112896
 C                 -0.623151    1.468838   -0.363908
 C                 -0.362322    0.143752   -1.107840
 C                 -0.903176   -0.967919   -0.205344
 C                 -0.478603   -0.513264    1.182819
 C                  0.598082    2.344011   -0.691590
 O                  2.480993   -1.946382   -0.291621
 C                 -2.877132   -0.261870   -0.031270
 N                 -4.014395   -0.034613    0.026285
 O                 -0.924226   -2.175162   -0.555646
 H                  2.685516    1.568954   -0.375716
 H                  1.725715    1.451975    1.971014
 H                  1.518832   -1.153187    2.100197
 H                  1.680656   -0.084592   -2.026982
 H                 -0.882072    1.626161    1.857108
 H                 -1.589871    1.900266   -0.552179
 H                 -0.738711    0.087429   -2.116234
 H                 -1.019809   -0.976344    1.987732
 H                  0.660383    2.607070   -1.742950
 H                  0.640965    3.247634   -0.089917
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