Spring 1972

A NORMAL COORDINATE ANALYSIS OF SEVERAL ACETYL AND TRIFLUOROACETYL HALIDES

ALAN DENNIS CORMIER

INFORMATION TO USERS

This dissertation was produced from a microfilm copy of the original document. While the most advanced technological means to photograph and reproduce this document have been used, the quality is heavily dependent upon the quality of the original submitted.

The following explanation of techniques is provided to help you understand markings or patterns which may appear on this reproduction.

1. The sign or "target" for pages apparently lacking from the document photographed is "Missing Page(s)". If it was possible to obtain the missing page(s) or section, they are spliced into the film along with adjacent pages. This may have necessitated cutting thru an image and duplicating adjacent pages to insure you complete continuity.

2. When an image on the film is obliterated with a large round black mark, it is an indication that the photographer suspected that the copy may have moved during exposure and thus cause a blurred image. You will find a good image of the page in the adjacent frame.

3. When a map, drawing or chart, etc., was part of the material being photographed the photographer followed a definite method in "sectioning" the material. It is customary to begin photoing at the upper left hand corner of a large sheet and to continue photoing from left to right in equal sections with a small overlap. If necessary, sectioning is continued again — beginning below the first row and continuing on until complete.

4. The majority of users indicate that the textual content is of greatest value, however, a somewhat higher quality reproduction could be made from "photographs" if essential to the understanding of the dissertation. Silver prints of "photographs" may be ordered at additional charge by writing the Order Department, giving the catalog number, title, author and specific pages you wish reproduced.

University Microfilms

300 North Zeeb Road
Ann Arbor, Michigan 48106

A Xerox Education Company

A NORMAL COORDINATE ANALYSIS OF SEVERAL ACETYL AND TRIFLUOROACETYL HALIDES

by

ALAN DENNIS CORMIER

B. A., Northeastern University, 1968

A THESIS

Submitted to the University of New Hampshire

In Partial Fulfillment of

The Requirements for the Degree of

Doctor of Philosophy

Graduate School

Department of Chemistry

June, 1972

This thesis has been examined and approved.

Charles V. Berne

Thesis Director, Charles V. Berney, Asst. Prof. of Chemistry

Alexander R. Amell

Alexander R. Amell, Prof. of Chemistry

Colin D. Hubbard

Colin D. Hubbard, Asst. Prof. of Chemistry

Charles W. Owens

Charles W. Owens, Assoc. Prof. of Chemistry

John E. Mulhern Jr.

John E. Mulhern, Jr., Prof. of Physics

May 12, 1972

Date

ACKNOWLEDGEMENTS

I wish to express my gratitude and appreciation to my thesis advisor, Dr. Charles V. Berney, for his invaluable guidance and patience during the course of my graduate education and thesis research. I also wish to extend my appreciation to many of the faculty and graduate students of the chemistry department for their moral support and for numerous stimulating chemical and political discussions.

I wish to thank the entire staff of the computation center for their generous help. In particular I would like to thank Edward Fisher, James Estes, and Stephen Blunden for their invaluable assistance in learning programming methods, and also Howard Stiles and James Shanklin for their help in learning computer operational techniques.

Special thanks and appreciation are due to my wife, Paula, for her continued encouragement in my research and her extensive help in preparation of the manuscript.

I also wish to acknowledge with thanks the support provided by the chemistry department in the form of a National Defense Education Act Fellowship and Teaching Assistantships, and by the Graduate School in the form of Summer Research Fellowships.

TABLE OF CONTENTS

TABLE OF CONTENTS con't

TABLE OF CONTENTS con't

TABLE OF CONTENTS con't

ABSTRACT

A NORMAL COORDINATE ANALYSIS OF SEVERAL
ACETYL AND TRIFLUOROACETYL HALIDES

by

ALAN DENNIS CORMIER

Normal coordinate analyses of the two series of molecules CX_3COZ (X = H, D and Z = H, D, F, Cl, Br) and CF_3COZ (Z = H, D, F, Cl) have been performed. The force fields used have been of the modified Urey-Bradley type with valence interaction force constants added as necessary. Appropriate force constants from the CH_3COZ series were used as a first approximation to the CF_3COZ series of molecules. Similarities between the two series of molecules were used as a chemical constraint on the force field in such a way as to require the force constants to vary only in a chemically reasonable manner.

On a limited scale the relative bonding in the two series is discussed in light of the trends in the respective force fields. The resulting approximate potential energy distributions are given and discussed. The Cartesian displacements are also listed.

Chapter I

THEORY AND ITS APPLICATIONS

A. Introduction

The purpose of this work is to study the potential functions of several molecules containing the acetyl skeleton. The study has many interesting facets to it, not the least of which is an elucidation of the trends in bond characteristics in a series of molecules.

To the chemist, one of the primary goals in any study of molecular structure is an understanding of the bonding between any two component atoms in a molecule.[1] The classical chemical approach succeeds in a qualitative description of bonding in that it easily determines single, double, or triple bonds in a molecule, but does little toward a quantitative assessment of the bond.

There are several alternatives in measuring the degree of bonding. Perhaps the three most prominent are: thermochemical measurements of bond energy, x-ray determinations of equilibrium internuclear separations, and quantum mechanical calculations. In any determination of the energy needed to break a chemical bond, the molecule under study is subject to various rearrangements of its molecular fragments and consequently the resulting energy for each bond is uncertain. The quantum mechanical approach involves a numerical estimation of the valence electron distribution in polyatomic molecules. The bond lengths as

determined by x-ray diffraction methods provide a good criterion of bonding, and in particular their relative values for different bonds between the same pair of atoms are very useful.

Insofar as one is concerned with the normal state of the molecule, one of the best representations of its condition is provided by the potential energy function of the molecule.[1] The potential energy is produced by the forces that arise when atoms are displaced from their equilibrium position. The force field will also contain interaction force constants since as one bond stretches or bends, the electronic distribution shifts, thus altering the remaining bonds in the molecule.

As a byproduct of the force field determination, one obtains the normal coordinates of the molecule. The normal coordinates are a description of the motions of each of the component atoms of a molecule as that molecule undergoes its various modes of vibration. These coordinates provide detailed information for studies concerning the influences of characteristic group frequencies in other molecules. The normal modes are also necessary in absolute intensity calculations.[1]

The uniqueness of this study arises from the fact that force fields have been fitted to two parallel series of closely related molecules, the acetyl compounds (CH_3COZ) and the trifluoroacetyl compounds (CF_3COZ). Many studies have been performed on isolated molecules but relatively

few calculations have appeared on a series of related molecules.

Further along in this chapter, various methods of finding appropriate force fields are discussed. The method adopted here involves use of the Urey-Bradley force field[2] with interaction force constants added. It was found by the author and many others that this method is the only reliable way to obtain a consistent force field in all cases.

Four of the computer programs used in the process are adapted from a series of programs originally written by J. H. Schachtschneider.[3] The two major programs, however, are original. Many of the subroutines used have been written both in Fortran and in Basic Assembly Language; in particular, the diagonalization subroutines NROOT and EIGEN have been written in B.A.L. These are described and listed in Appendix 1B.

B. The Secular Equation

The 3N-6 vibrational frequencies of a nonlinear N-atomic molecule are characteristic of at least two features of the structure of the molecule: first, the spatial geometrical distribution of the component atoms and their corresponding masses, and second, the force field which serves to restore the molecule to its equilibrium configuration following any distortion.[1]

To obtain the force field of the molecule one must

necessarily know the geometrical distribution of the atoms and their appropriate masses. Internal displacement coordinates define displacements of atoms along bonds or angles and completely define the internal configuration of a molecule taking no account of rotations or translations. If 3N-6 internal displacement coordinates, R_i, (i = 1,3N-6), are defined, then the potential energy of the molecule can be expressed in a Taylor series as

$$V = V_e + \sum_i \left(\frac{\partial V}{\partial R_i}\right)_e R_i + \tfrac{1}{2}\sum_i \sum_j \left(\frac{\partial^2 V}{\partial R_i \partial R_j}\right) R_i R_j + (\text{terms of order } R^3 \text{ and higher}). \qquad \text{B1}$$

The term V_e defines the arbitrary zero of the energy scale and can be set equal to zero. The coefficients $\left(\frac{\partial V}{\partial R_i}\right)_e$ are taken at the equilibrium position and are therefore equal to zero. If, in the harmonic oscillator approximation, all of the cubic, quartic, and higher terms are dropped, then the remaining terms are $\left(\frac{\partial^2 V}{\partial R_i \partial R_j}\right)_e$, each of these corresponding to the force constant of a harmonic oscillator F_{ij} as defined in classical physics.

In solving the equations of motion of any system, the expressions for the potential and kinetic energies must first be derived. The equations are:

$$2V = \sum_i \sum_j F_{ij} R_i R_j \qquad \text{B2}$$

$$2T = \sum_i \sum_j M_{ij} \dot{R}_i \dot{R}_j \qquad \text{B3}$$

where $\dot{R}_i$ and $\dot{R}_j$ are the time derivatives of the coordinates used earlier. The coefficients M_{ij} are functions of the spatial geometrical distributions of the atomic masses. Since these are very tedious to calculate, the kinetic energy is most often seen as

$$2T = \sum_i \sum_j G_{ij} P_i P_j \qquad B4$$

where P_i and P_j are the momenta of the vibrations and G_{ij} is related to M_{ij} by:

$$\sum_j G_{ij} M_{jk} = \delta_{ik} \qquad \delta_{ik} = \begin{cases} 1 \text{ for } i = k \\ 0 \text{ for } i \neq k \end{cases} \qquad B5$$

In matrix notation, equations B2 - B5 are given as:

$$2V = \tilde{\mathbf{R}} \mathbf{F} \mathbf{R} \qquad B6$$

$$2T = \tilde{\mathbf{P}} \mathbf{G} \mathbf{P} \qquad B7$$

$$2T = \tilde{\dot{\mathbf{R}}} \mathbf{M} \dot{\mathbf{R}} \qquad B8$$

$$\mathbf{GM} = \mathbf{I} \text{ , or } \mathbf{M} = \mathbf{G}^{-1} \qquad B9$$

where $\mathbf{R}$, $\dot{\mathbf{R}}$, and $\mathbf{P}$ are column matrices and $\tilde{\mathbf{R}}$, $\tilde{\dot{\mathbf{R}}}$, and $\tilde{\mathbf{P}}$ indicate the transposes of $\mathbf{R}$, $\dot{\mathbf{R}}$, and $\mathbf{P}$. $\mathbf{G}$, $\mathbf{M}$, and $\mathbf{F}$ are square matrices of order n x n, and $\mathbf{I}$ is the identity matrix.

Since the F_{ij} define the force field and the M_{ij} or G_{ij} define the kinetic properties of the system, they together control the frequencies and the modes of the normal vibrations.

As was mentioned earlier, normal coordinates are

those coordinates describing the normal modes of vibration, and thus are made up of appropriate changes in bond lengths and/or bond angles. The coordinates R_i used above are those coordinates describing all the possible deformations of the bonds and bond angles as earlier implied, and the relationship between the normal coordinates Q_j and the displacement coordinates R_i is given as:*

$$\sum_{i=1}^{3n-6} R_i = \sum_{i=1}^{3n-6} \sum_{j=1}^{3n-6} L_{ij} Q_j \qquad \text{B10}$$

where R_i and Q_j are column matrices and L_{ij} are the constant transformation coefficients. It can be shown that the L_{ij} can always be chosen in such a way that the energies in terms of normal coordinates have the following diagonal forms:

$$2V = \tilde{\mathbf{Q}}\tilde{\mathbf{L}}\mathbf{F}\mathbf{L}\mathbf{Q} = \tilde{\mathbf{Q}}\boldsymbol{\Lambda}\mathbf{Q} \qquad \text{B11}$$

$$2T = \dot{\tilde{\mathbf{Q}}}\tilde{\mathbf{L}}\mathbf{G}^{-1}\mathbf{L}\dot{\mathbf{Q}} = \dot{\tilde{\mathbf{Q}}}\mathbf{I}\dot{\mathbf{Q}} \qquad \text{B12}$$

Here $\boldsymbol{\Lambda}$ is a diagonal matrix whose nonzero elements are $\lambda_k = 4\pi^2\nu_k^2$, where the ν_k are the vibrational frequencies. Therefore it is easily seen that:

$$\tilde{\mathbf{L}}\mathbf{G}^{-1}\mathbf{L} = \mathbf{I} \qquad \text{B13}$$

---

*The following discussion was taken in part from reference 4.

and

$$\tilde{\mathbf{L}}\,\mathbf{F}\,\mathbf{L} = \mathbf{\Lambda} \qquad \text{B14}$$

Solving equation (B13) for $\tilde{\mathbf{L}}$ and substituting into equation (B14), one obtains:

$$\mathbf{L}^{-1}\,\mathbf{G}\,\mathbf{F}\,\mathbf{L} = \mathbf{\Lambda} \qquad \text{B15}$$

This matrix equation represents a set of simultaneous equations whose solution defines the L matrix and yields a set of calculated vibrational frequency parameters λ_k.

Writing equation (B15) in long form one gets

$$\sum_j \left[(GF)_{ij} - \delta_{ij}\lambda_k\right]L_{jk} = 0 \qquad k = 1,2,\ldots,n \qquad \text{B16}$$

This, then, leads to one form of the secular equation, namely:

$$\left|\mathbf{G}\mathbf{F} - \mathbf{I}\lambda_k\right| = 0 \qquad \text{B17}$$

For the purpose of this thesis, equation B15 is the important equation, for if the elements of both the $\mathbf{G}$ and $\mathbf{F}$ matrices were known then the diagonalization of their product would result in both the frequencies of vibration and the transformation from the internal displacement coordinates to the desired normal coordinates.

C. The Wilson $\mathbf{G}\,\mathbf{F}$ Method

In the preceding section it was established that diagonalization of the product of the potential energy

matrix **F** and the inverse kinetic energy matrix **G** gave the vibrational frequencies associated with the potential field.[4] Since the frequencies are known experimentally and the potential force field is what is being sought, then to solve the problem the elements of the inverse kinetic energy matrix must be known. Calculation of the individual elements is straightforward since they depend only on the atomic masses and the equilibrium molecular geometry. A simple method to do this using matrix notation was introduced by Wilson[5] and Decius[6].

Wilson's method is to construct the inverse kinetic energy matrix **G** in terms of internal displacement coordinates according to a series of algorithms which Decius derived. The potential energy force field is also set up in terms of the same coordinate system and arranged in matrix form lending itself readily to modification using any symmetry of the molecule. This method is particularly suitable for adaptation to computers since the diagonalization procedure for the product matrix is of an iterative type.

D. Construction of the G Matrix

1. Internal Coordinate Space

Before the actual computation of the G matrix can be accomplished, the coordinate space in which it is set must be defined. The Wilson treatment is carried out in internal coordinate space and to best describe and exemplify this

space the simple, yet not trivial, molecule formaldehyde is appropriate. The following three diagrams completely demonstrate the space for formaldehyde:

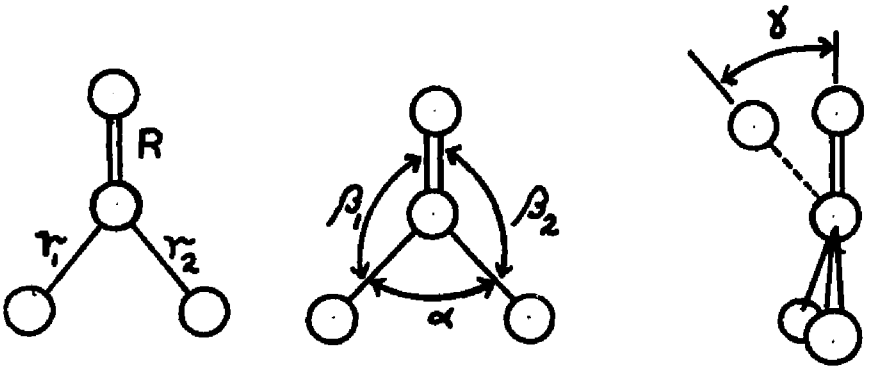


Fig. 1-1

It is important to note that the symbols R, r, α, β, and γ do <u>not</u> represent the bond lengths and angles as it appears, but infinitesimal changes in those bond lengths and angles. Thus the coordinates are most descriptively named internal displacement coordinates.

Two sets of coordinates are of particular note: the β's and γ. If both β_1 and β_2 are increased simultaneously then there must be an accompanying decrease in the α coordinate. Thus the angle deformations have been overdefined and consequently they are related by the redundancy condition $\alpha + \beta_1 + \beta_2 = 0$. The γ coordinate defines the motion of the oxygen atom bending out of the plane of the carbon and two hydrogens. The coordinates r_1, r_2 and β_1, β_2 are labeled as such since they represent symmetrically equivalent bonds and angles respectively.

There is only one type of internal coordinate which does not occur in formaldehyde and this is a torsion (τ) about a bond, of one group of atoms relative to another group of atoms. An example of this is the torsion of one methyl group relative to the other methyl group in ethane.

2. Sample Algorithms

In the G matrix there are two basic types of elements: the diagonal elements and the cross terms or off-diagonal elements. In the case of formaldehyde the G matrix will have the dimensions 7 x 7 since there are seven separate internal coordinates. The rows and columns of r_1 and r_2 will be the same as will β_1 and β_2 since again they are symetrically equivalent.

A complete set of equations for various G matrix elements is listed in Decius's paper[6]. Below are a few associated with formaldehyde. The elements are doubly subscripted to eliminate ambiguities.

Diagonal Terms

$G_{RR} = \mu_O + \mu_C$ (μ_i is the reciprocal of the i^{th} mass.)

$$G_{\beta_1 \beta_1} = \rho_{HC}^2 \mu_H + \rho_{CO}^2 \mu_O + (\rho_{HC}^2 + \rho_{CO}^2 - 2 \rho_{HC} \rho_{CO} \cos(\angle HCO)) \mu_C$$

where ρ_{HC} is the interatomic distance between H and C.

Cross Terms

$$G_{Rr_1} = \mu_C \cos(\measuredangle HCO)$$

$$G_{R\beta_1} = -\rho_{CH}\mu_C \sin(\measuredangle HCO)$$

$$G_{\beta_1\alpha} = (\rho_{H_1C}{}^2 \cos(\psi_{314}))\mu_{H_1} + ((\rho_{H_1C} - \rho_{CO}\cos(\measuredangle HCO) - \rho_{CH_2}\cos(\measuredangle HCH)) - \rho_{H_1C}\cos(\psi_{314}) + (\sin(\measuredangle HCO)\sin(\measuredangle HCH)\sin^2(\psi_{314}) + \cos(\measuredangle HCO)\cos(\psi_{314}))\rho_{CO}\rho_{CH})\mu_C$$

where $\cos(\psi_{314}) = \dfrac{\cos(\measuredangle OCH) - \cos(\measuredangle HCO)\cos(\measuredangle HCH)}{\sin(\measuredangle HCO)\sin(\measuredangle HCH)}$

$$G_R = -(\rho_{CH_1}\sin(\measuredangle OCH_1)\cos(\psi_{314}) + \rho_{CH_2}\sin(\measuredangle OCH_2)\cos(\psi_{314}))\mu_C$$

The above-listed elements cover all of the different types of diagonal and off-diagonal terms in the G matrix for formaldehyde.

It is obvious that for any system larger than four atoms the calculation becomes extremely time comsuming. However, Schachtschneider has written a series of computer programs for the 7094 computer in Fortran level G. His program for calculating the G matrix elements is divided up into two major parts: one, the main deck which reads in the input data comprising the atom numbers for the internal coordinates, the Cartesian coordinates, and the atomic

masses; two, the subroutines which calculate the elements before they have been multiplied by the appropriate inverse atomic masses. The main deck handles the multiplication with the inverse masses.

The program as I have adapted it to the IBM/360 model 50 computer, has all of the subroutines intact, but the main deck has been completely rewritten to suit the facilities at this university as well as the particular problem of this thesis. The listing of the program is in Appendix 1A along with a description of the order and form of the input data.

E. Calculation of Cartesian Coordinates

As was mentioned in the previous section, in order to calculate the G matrix elements, the Cartesian coordinates are necessary since they are used in determining various interatomic distances.

The Cartesian coordinates are also useful in another sense. Once an arbitrary set of Cartesian coordinates is determined for a molecule, the inertial tensor can be formed and diagonalized in such a way that the products of inertia become zero. The transformation obtained in this diagonalization is then subsequently used to transform the arbitrary coordinates to the principal Cartesian coordinates which are the natural coordinates of the molecule. The axes of this coordinate system are referred to as the principal axes, and are those axes about which the molecule

rotates in its quantized rotational states. Band shapes[7] and intensities[8] in an infrared spectrum must be discussed in terms of these axes and consequently they are necessary in the process of making vibrational assignments.

The molecules of this study have been investigated either by x-ray, microwave, or electron diffraction techniques and consequently their structures have been determined in terms of bond lengths and bond angles. To define an arbitrary set of Cartesian coordinates, it is necessary and sufficient to have values for bond angles and bond lengths as well as appropriate dihedral angles. A dihedral angle is the angle between the two planes defined by four atoms.

The computer program to calculate the principal Cartesian coordinates of a molecule was originally part of the Schachtschneider package[3] of programs. The algorithms used in the calculation have been retained; however, the remaining portion of the program was written as part of this work. The program is listed and explained in Appendix 1A.

F. Use of Molecular Symmetry in the Secular Equation

The molecules in this investigation possess a plane of symmetry. Larger molecules with no formal symmetry often have an approximate element of symmetry or at least isolated groups on them that possess some local symmetry. These elements of symmetry either of the molecule as a

whole or for local groups can be exploited by the use of group theory as applied to the molecular vibrations.[8,9]

This use of group theory can enormously reduce the work involved in calculating the normal modes of vibration. Perhaps a quotation from chapter five in Wilson et. al.[4] can best sum up the uses of molecular symmetry:

> ...without any other information whatsoever, the symmetry and geometry of a molecular model can be used to determine the number of fundamental frequencies, their degeneracies, the selection rules for the infrared and Raman spectra, the degrees of the factors of the secular equation, the number of independent constants in the quadratic part of the potential energy function, the splitting of overtone levels, the possibility of perturbations due to resonance, the nature of the rotational structure of the infrared bands, the polarization properties of the Raman lines, and other useful information.

For this work the most important feature of those listed above is the utilization of symmetry properties in factoring the secular equation. This process is thoroughly described in many books currently available and perhaps most coherently by Cotton[8] and by Wilson et. al.[4]

To illustrate the overall process on a simple level, the molecule formaldehyde, whose internal coordinates were defined earlier, will be carried through to the point of factoring its secular equation. It is easily seen that formaldehyde has a two fold rotation axis C_2 and also two mutually-perpendicular mirror planes whose junction is the C_2 axis. The symmetry group to which this belongs is C_{2v},

where the 2 is the highest rotational axis and the v indicates there are two planes of symmetry not normal to the rotational axis. The character table for this symmetry group is:[8]

C_{2v}	E	C_2	σ_{xz}	σ_{yz}	Translations Rotations	
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

Table 1-1

The E above is the identity element. Each of the symmetry species A_1, A_2, B_1, and B_2 is an irreducible representation of the symmetry group C_{2v}. The terms z, R_z, etc. are the classical translations in the x, y, and z directions and rotations R about the x, y, and z axes. The elements x^2, y^2, z^2, xy, xz, and yz are elements of the polarizability tensor and indicate that a vibration belonging to a particular symmetry species is Raman active. Those symmetry species containing the translations x, y, and z are the infrared active species. Thus we see that fundamental vibrations belonging to the A_2 symmetry species are not observed in the infrared but are observed in the Raman.

The next step is to determine how many fundamental vibrations belong to each symmetry species. The calculation makes use of the number of unshifted atoms

on the application of each symmetry element, and also the character χ per unshifted atom for each of these symmetry elements. The first calculation determines the total number of motions in each symmetry species Γ_k including the translational and rotational motions. The formula is:

$$\Gamma_{cart} = \sum n_k \Gamma_k$$

$$n_k = (n_{USA})(\chi_{USA})(\chi_k)/n_g$$

where k indicates the symmetry species and n_g is the total number of elements of the point group. A complete table and sample calculation for formaldehyde follow:

C_{2v}	E	C_2	σ_{xz}	σ_{yz}	Trans. Rot.	Polar Tensor	Γ_{cart}	Γ_{vib}
A_1	1	1	1	1	z	x^2, y^2, z^2	4	3
A_2	1	1	-1	-1	R_z	xy	1	0
B_1	1	-1	1	-1	x, R_y	xz	3	1
B_2	1	-1	-1	1	y, R_x	yz	4	2
χ_{USA}	3	-1	1	1				
USA	4	2	2	4				

Table 1-2

$$\Gamma^{A_1}_{cart} = \frac{(4)(3)(1)+(2)(-1)(1)+(2)(1)(1)+(4)(1)(1)}{4} = 4$$

$$\Gamma^{A_2}_{cart} = \frac{(4)(3)(1)+(2)(-1)(1)+(2)(1)(-1)+(4)(1)(-1)}{4} = 1$$

$$\Gamma^{B_1}_{cart} = \frac{(4)(3)(1)+(2)(-1)(-1)+(2)(1)(1)+(4)(1)(-1)}{4} = 3$$

$$\Gamma^{B_2}_{cart} = \frac{(4)(3)(1)+(2)(-1)(-1)+(2)(1)(-1)+(4)(1)(1)}{4} = 4$$

Γ_{vib} is the representation of the molecular point group formed by the vibrational modes, expressed as a linear combination of the irreducible representations (symmetry species) in which the coefficient of each species is the number of fundamental modes possessing the indicated symmetry. It is found by subtracting from the appropriate element in Γ_{cart} the rotational and translational degrees of freedom. The result is $\Gamma_{vib} = 3A_1 + B_1 + 2B_2$, a total of 6 vibrations which agrees with the previously determined number (3N-6) = 6, where N is the number of atoms.

What is left to determine is the approximate form of each of the vibrations in the three symmetry species. This is easily done in terms of symmetry coordinates. The symmetry coordinates are linear combinations of the internal displacement coordinates. When the internal coordinates are operated on by specific symmetry operators belonging to the symmetry group of the molecule, they transform either into themselves or into other internal coordinates. If they transform into themselves but the displacement vector is in the opposite direction then they are referred to as transforming into minus themselves. After the transformation by a particular symmetry element is performed the result is multiplied by the appropriate character element for the symmetry species being considered. This is done for each symmetry element in a given symmetry species and

the normalized sum is the appropriate symmetry coordinate for that symmetry species. For example, if the internal coordinate r_1 for formaldehyde is operated on by the C_2 symmetry element the, result is r_2 since a 180° rotation about the C_2 axis brings r_1 into r_2. Likewise reflection through the xz plane transforms r_1 into r_2, while reflection in the yz plane transforms r_1 into itself, as does the identity operator E. The combinations when multiplied by the characters of symmetry species yield:

	E	C_2	xz	yz	sum	result
A_1	r_1	r_2	r_2	r_1	$N(2r_1+2r_2)$	$\frac{1}{\sqrt{2}}(r_1+r_2)$
A_2	r_1	r_2	$-r_2$	$-r_1$	0	0
B_1	r_1	$-r_2$	r_2	$-r_1$	0	0
B_2	r_1	$-r_2$	$-r_2$	r_1	$N(2r_1-2r_2)$	$\frac{1}{\sqrt{2}}(r_1-r_2)$

Table 1-3

Thus, one of the two carbon-hydrogen bond stretches belongs to the A_1 symmetry species and is referred to as the "totally symmetric C-H stretch" while the other belongs to the B_2 species and is called the "antisymmetric C-H stretch". Below are listed the symmetry coordinates S_i for formaldehyde.

Species	Coordinates
A_1	$S_R = R$
	$S_{r_1} = N(r_1 + r_2)$
	$S_{\beta_1} = N(\beta_1 + \beta_2 - 2\alpha)$
B_1	$S = \gamma$
B_2	$S_{r_1} = N(r_1 - r_2)$
	$S_{\beta_1} = N(\beta_1 - \beta_2)$

Table 1-4

This approximate description is in reality a new coordinate space which is termed symmetry space. Defining the symmetry space is an attempt to guess as closely as possible the form of the normal modes of vibration of the molecule.

The above combinations of internal coordinates serve to factor the secular equation. Below is a diagram demonstrating the initial and final starting forms of the product FG matrix when the internal coordinates are appropriately combined.

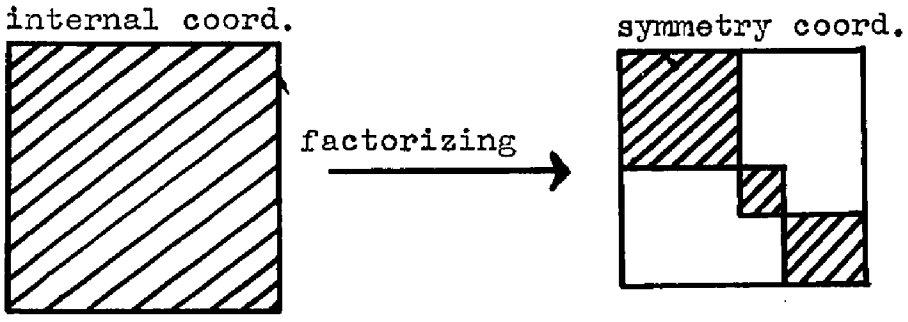


Fig. 1-2

Obviously the problem has been tremendously simplified. What was once a matrix containing 28 independent

elements ($\frac{1}{2}N(N + 1)$) has been converted into a series of 3 independent matrices containing 10 unique elements. The next section goes into more detail about the factorization.

G. Transformation from Internal to Symmetry Coordinate Space

1. General Format

In practice the product (FG) matrix is not symmetrized but the individual G and F matrices are. Since G and F are arrayed in matrix format the procedure is to construct a transformation matrix, capable of transforming internal coordinate space into symmetry coordinate space. To accomplish this it is best to observe the transformation in schematic form. For example if the G matrix is in internal coordinate space then its rows and columns would both be labeled with the internal coordinates in a given order. In matrix notation, the general form for the symmetrization of a matrix in internal coordinate space is

$$\mathbf{U M \tilde{U}} = \mathbf{M'}$$

The transformation matrix U above is a matrix whose rows are labeled with the symmetry coordinates and whose columns are labeled with the internal coordinates.

2. Elimination of the Redundant Coordinate

Looking back at the molecule formaldehyde as an example, note that there are seven internal coordinates but the system can be uniquely defined with only six internal coordinates. The extra coordinate arises from the fact

that the coordinates β_1, β_2, and α are not all independent, since the sum ($\beta_1 + \beta_2 + \alpha$) will always equal zero. It is easily determined that the redundancy condition belongs to the A_1 symmetry species. If it is included in the U matrix and the G or F matrices are symmetrized, then the row and column associated with the redundant symmetry coordinate will have zeros as their elements, and therefore that row and column can be deleted from the matrix. This, of course, happens only if the redundancy condition is known a priori which is not always the case, e.g. in puckered ring molecules. When the redundancy condition is not known there is an explicit mathematical procedure for determining it.[10]

3. Combined Symmetry Coordinates

Again referring to the molecule formaldehyde, and looking strictly at the symmetry operations of the symmetry group C_{2v} we see that there is no symmetry operation which will transform either β coordinate into the α coordinate. Strictly speaking according to the symmetry rules the totally symmetric O=C-H deformation should be $\beta_1 + \beta_2$ with no α coordinate subtracted. From a physical standpoint, however, that is not realistic since the H-C-H angle must decrease when both of the O=C-H angles open up; consequently, the force field must include the contributions from each of the β's and the α coordinate in making up the potential energy. This carries over into

many different configurations in different molecules and in each, one's chemical and geometric knowledge must override the strict formalism in writing those symmetry coordinates which best approximate the normal coordinates. Thus it often arises that internal coordinates which are not symmetrically related are still incorporated into a specific symmetry coordinate.

H. The Potential Energy Matrix F

1. Construction in Internal Coordinate Space

It was stated earlier that the Wilson GF method is based entirely on the harmonic oscillator approximation to molecular vibrations. The classical harmonic oscillator follows Hooke's law which is

$$\frac{\partial V}{\partial x} = F = -kx$$

where V is the potential energy, F is the force, x is the displacement of the oscillator from its equilibrium position, and k is a constant characteristic of the oscillator called its force constant. The stiffer the spring, the greater is its force constant.

The F matrix is an array of these force constants which in the harmonic oscillator approximation completely describe the potential field of a molecule. If the ordered labels of the F matrix rows and columns are the internal coordinates, then the diagonal elements of the F matrix are the force constants associated with each individual

internal coordinate, while any off-diagonal element is an interaction force constant describing the effect the state of one oscillator has on the force constant of the other oscillator.

2. Transformation to Symmetry Space

This transformation is identical to that performed on the G matrix. The total effect now is that each symmetry force constant is made up of linear combinations of the internal force constants. The same holds true for any interaction force constants, i.e. they are now interactions between symmetry oscillators (combined groups of oscillators).

3. The Urey-Bradley Force Field

The force fields discussed above are simple force fields and do not include any contributions from non-bonded interactions such as van der Waals forces or electrostatic forces. In many of the molecules treated in this fashion to date, the simple internal valence force field has not been as useful as the Urey-Bradley force field,[2,11] which takes into account the non-bonded interaction forces. The Urey-Bradley approach is to determine that portion of a valence force constant which is due to non-bonded interactions and which is due to the bond itself. What makes this so desirable is that the portion of the force constant which is associated with the bond has been found in very many cases to be transferable between related mole-

cules. Another outcome of this procedure (which is of convenience in some cases and not in others) is the fact that the total number of force-field variables has been considerably reduced, since the method uses only the diagonal valence force constants and the non-bonded interaction force constants, but not the valence interaction force constants.

The potential functions and the appropriate relationships for determining the non-bonded interactions are quite involved and are given in the original paper by Urey and Bradley[2]. A comprehensive discussion is also given by Shimanouchi[11], who proposed modifications in the original procedure.

4. Urey-Bradley and Valence Interaction Force Constants

It is often the case that the Urey-Bradley force field alone will not reproduce the observed frequencies to within the desired limits. There are various reasons for this, perhaps most important of which is the lack of consideration of the valence interaction force constants. These interaction force constants are the characteristic constants for the bend-bend, bend-stretch, and stretch-stretch interactions, and are a measure of the electronic rearrangements which take place in a bond when a neighboring bond is bent or stretched. In most cases where the frequency data cannot be reproduced with a Urey-Bradley force field, it becomes necessary to add the appropriate valence

interaction force constants to the Urey-Bradley force field in order to better describe, on an accurate level, the harmonic force field of the molecule.

From a chemical standpoint we expect that the interaction force constants would all be nonzero, though many would be very small.

I. The Urey-Bradley Z Matrix

1. General Format

In the previous section the nature of the Urey-Bradley force field was explained. In practice, the force field must be displayed in matrix form in symmetry coordinate space. To form the valence force field from the Urey-Bradley force field, the Urey-Bradley Z matrix is calculated and used as a transformation matrix such that

$$F_{ij} = \sum_k Z_{ijk} \Phi_k$$

where F_{ij} is the i^{th} row and j^{th} column element of the F matrix, Φ_k is the k^{th} Urey-Bradley force constant, and Z_{ijk} is the element of the three-dimensional transformation matrix Z.

The elements of the Z matrix are the factors by which the Urey-Bradley force constants must be multiplied in order to obtain the proper weighting of that force constant for the valence force constants.

It is a simple matter at this point to add the valence interaction force constants directly into the list of the

Φ_k and give the corresponding Z matrix element the value of 1.000. The appropriate Z matrix element is the one defined by the i^{th} row and j^{th} column of the internal (valence) force field.

As implied above, the resulting force field is in internal coordinate space and consequently must be transformed into symmetry coordinate space. The Z matrix, however, can itself be transformed in such a way that the resulting force field will be in symmetry coordinate space upon transformation. The transformation of the Z matrix into this form follows:

$$\sum_k U Z_k \tilde{U} = \sum_k Z'_k = Z'$$

where U is the internal-coordinate to symmetry-coordinate transformation already defined, and Z' is the symmetrized Z matrix.

2. Molecular Configurations

In the Schachtschneider package UBZM is a program to calculate the Z matrix elements, as defined by Urey and Bradley and modified by Shimanouchi. The calculation is broken down into the three different configurations shown below:

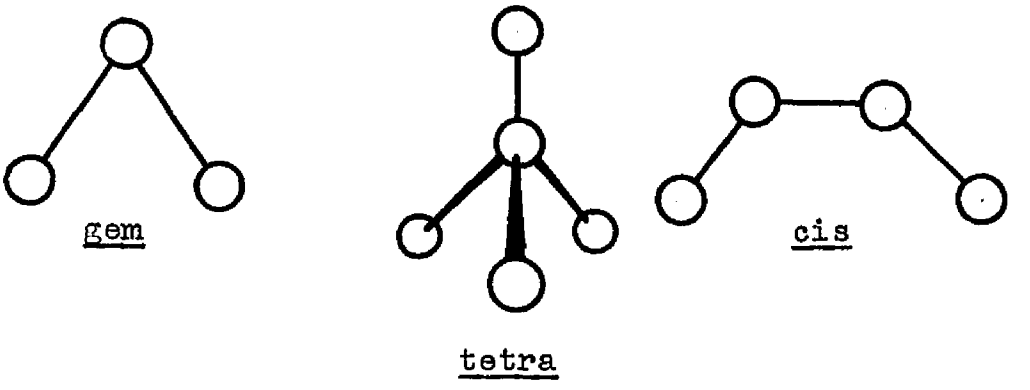


Fig. 1-3

The gem and tetra configurations were worked out by Urey and Bradley while the cis configuration was added by Shimanouchi. The contributions to the Z matrix from each of the configurations are listed by Schachtschneider[3].

J. Methods of Determining the Force Field

1. General Discussion

There are several approaches for determining the force field of a molecule. All of the methods involve mathematically reproducing some experimentally obtained data which depend on the force field. The earliest works on the simplest molecules relied totally on the assigned vibrational frequencies. Other data, such as Coriolis coupling coefficients, centrifugal distortion constants, and mean square amplitudes of vibration have been used in more recent studies. Unfortunately these last forms of experimental data are rarely available.

Since there are in general many more force constants to be determined than experimental data available, other methods for determining the correct force field must be

used. Recently Redington and Aljibury[12] have shown a possible method in noting that the correct force fields of small molecules for which ample experimental data were available were obtained when the diagonal valence force constants were given their maximum values consistent with reproduction of the vibrational frequencies. Unfortunately the difficulty of this parameterization of the force field increases rapidly with the size of the molecule. Bruns and Person[13] and also Levin and coworkers[14] have exploited intensity data using CNDO/2 methods to calculate predicted infrared intensities for a given force field and compare them with the experimental results. Again this method is difficult for all but the simplest molecules.

A more chemical approach was undertaken by Schachtschneider on the paraffins[15] where the potential functions of a series of closely related molecules were studied and the chemical similarity of the molecules used as an additional constraint on the force field. This approach is of interest to the chemist in that the resulting set of force fields can not only be readily transferred to other similar molecules but, more important, they can easily be used for a chemical interpretation of the molecules and their bonding effects.

Implicit in the above discussion is the fact that there is an infinite number of possible force fields which will reproduce the frequency data, and that the real problem is to select the one which best represents the force

field of the molecule.

In practice once one force field has been found which will reproduce the frequency data, then many of the others are readily found by perturbing one of the force constants and adjusting all others to refit the frequencies. Finding the first force field however may (and usually does) turn out to be quite difficult. There are several reasons for this difficulty, but two major areas can be outlined. First of all from a mathematical standpoint, in working either with a general valence force field or with a Urey-Bradley force field the tendency is to keep the number of variables small. In line with this tendency is the practice of arbitrarily setting all or most all valence interaction force constants to zero, with the reasoning that they are most likely to be small in absolute value anyway. The underlying assumption is that if the interaction force constant is small then its influence on the calculated vibrational frequencies will be small also. This assumption is frequently invalid, as was found in the course of the current study. Indeed, it will be seen that very small values and changes in values of interaction force constants often have a profound effect on the calculated frequencies, as well as on the potential energy distribution. If the interaction force constants are required to be zero then in many cases a satisfactory reproduction of the vibrational frequencies cannot be achieved, since for some interaction force constants the set of all possible values

for frequency reproduction may not include the value of zero. Thus it may be necessary to undertake a complete study of the interaction force constants of a particular molecule in order to find even one force field which will satisfactorily reproduce the experimental data.

The second area of difficulty can be subdivided into two sections. The first section is the consideration of anharmonicity in the potential function. If a particular vibration is not closely approximated by a harmonic function then the observed frequency may be quite different from the theoretically predicted frequency using the best harmonic force constants. The extent of this difference has been shown in the past to be on the order to 2 to 3 per cent of the observed frequency. This display of anharmonic behavior is greatest for large amplitude vibrations, such as those involving motion of light atoms like hydrogen. The percentage difference can be even greater for vibrations of loosely-bound light atoms such as aldehydic hydrogens. The second section is the case where a molecule exhibits nonrigid behavior. A nonrigid vibration is one in which a normal mode of vibration involves motion described by symmetry coordinates from two different symmetry species. Since the method used in most normal coordinate treatments does not allow for interactions between symmetry species then any normal mode involving nonrigid motion may be difficult to reproduce.

The problem at hand then is to determine at least one

force field of the molecule in question which will reproduce the vibrational frequency data while keeping the above mentioned problems in mind.

2. The Iterative Process

The iterative process is a technique, used in many fields of science, which employs successive approximations to a final answer, where each consecutive approximation is based on the results of the previous approximation. Figure 1-4 is a schematic diagram of the iterative process as applied to determining a force field of a molecule. It is easily seen that the entire system hinges on formation and use of the J (Jacobian) matrix. Before describing the iterative loop in detail it is beneficial to derive the formulation of the procedure and thus define the nature of the J matrix.* Let n be the number of experimental fundamentals υ^{o}. The i^{th} member of this set is labeled υ_i^{o}. Furthermore the problem involves a set of m independent force constants ($m \leq n$) whose j^{th} member is termed f_j^{k} where the superscript k indicates the stage of approximation and may therefore take on the values 1, 2, 3, ... The fundamentals calculated from the k^{th} set of force constants are labeled υ_i^{k}. The differences between the $(k+1)^{th}$ and $(k)^{th}$ set of calculated frequencies is given by

*The following discussion was taken in part from reference 16.

$$\Delta \upsilon_i^k = \upsilon_i^{k+1} - \upsilon_i^k \qquad J1$$

A similar expression holds for the change in force constants,

$$\Delta f_j^k = f_j^{k+1} - f_j^k \qquad J2$$

The assumption governing these two expressions is that the adjustments to be made are in the nature of refinements, so the magnitudes of the Δf_j are small, leading to small changes in the calculated frequencies. If this assumption does not hold, then a better guess at the force constants must be made.

A variance S is defined by:

$$S^k = \sum_{i=1}^{n} W_i (\upsilon_i^k + \Delta \upsilon_i^k - \upsilon_i^o)^2 \qquad J3$$

where the W_i are appropriately chosen weighting factors. In matrix notation equation J3 becomes

$$S^k = \left[V^k + \Delta V^k - V^o\right]' W \left[V^k + \Delta V^k - V^o\right] \qquad J4$$

where the quantity $\left[V^k + \Delta V^k - V^o\right]$ is a column matrix, and its primed counterpart is the transpose and thus a row matrix, and W is a diagonal matrix. A relationship between ΔV^k and Δf^k is

$$\Delta V^k = \left(\frac{\partial V_i^k}{\partial f_j^k}\right) \left[\Delta f^k\right] \qquad J5$$

If

$$J_{ij}^{k} \equiv \frac{\partial v_i^k}{\partial f_j^k} \qquad J6$$

then J^k is a Jacobian matrix of dimension n x m. Substituting J6 into J5 and the result into J4 we obtain

$$S^k = \left[V^k - V^o\right]' W \left[V^k - V^o\right] + 2\left[V^k - V^o\right]' WJ^k \left[\Delta f^k\right] + \left[\Delta f^k\right]' J'^k W J^k \left[\Delta f^k\right] \qquad J7$$

Taking the partial of S^k with respect to Δf^k,

$$\frac{\partial S^k}{\partial \left[\Delta f^k\right]} = 2\left[V^k - V^o\right]' WJ^k + 2\left[\Delta f^k\right]' J'^k W J^k \qquad J8$$

Then upon setting

$$\frac{\partial S^k}{\partial \left[\Delta f^k\right]} = 0, \quad \text{and} \quad \left[V^k - V^o\right] = X^k, \qquad J9$$

it follows that

$$\left[\Delta f^k\right] = (J'^k W J^k)^{-1} J'^k W \left[X^k\right]. \qquad J10$$

If in equation J3 the term W_i were dropped and the derivation similarly carried out, the resulting equation would take on the form

$$\left[\Delta f^k\right] = (J'^k J^k)^{-1} J'^k \left[X^k\right] \qquad J11$$

similar to equation J10. This would be used if a weighting matrix was not desired.

It is evident from equation J6 that ideally the elements of the J matrix would be the infinitesimal changes in the calculated frequencies for a corresponding infinitesimal

change in a particular force constant. Since these elements are not known, the following equation is used as an approximation,

$$J_{ij}^{k} \cong \frac{\Delta V_i^k}{\Delta f_j^k} \qquad \text{J12}$$

where Δf_j^k is quite small and in the case of the vibrational problem is taken as 0.01 millidynes/A.

Equation J10 or J11 is the key equation in the iterative loop, and to utilize this equation the J matrix must be computed and the X matrix formed from the differences between the calculated and observed frequencies.

There is one major assumption concerning the use of the J matrix in the iterative loop and this is that the elements of the J matrix change in a linear fashion over a relatively large range of changes in the force constants. For some force constants this assumption will hold, while for others it may be quite incorrect. In order to make the changes more nearly linear, the following alterations can be made:

$$J_{ij}^{k} = \frac{\partial \log(V_i^k)}{\partial f_j^k} = \frac{\Delta \log(V_i^k)}{\Delta f_j^k} \qquad \text{J13}$$

$$X^k = \log(V_i^k) - \log(V^o). \qquad \text{J14}$$

These two new definitions tend to damp out much of the nonlinearity inherent in the calculations.

With the J matrix defined, the iterative loop can be elucidated. As stated in the schematic, the symmetrized F

matrix is first constructed using the Urey-Bradley force field and the appropriate transformation matrix Z, then the eigenvalues and eigenvectors of the product FG are formed. The loop is then entered, the J matrix computed and the matrix $(JJ)^{-1}J$ is formed by simple matrix transposition, multiplication, and inversion. The difference matrix X is formed and the absolute value of its elements compared to a set of maximum-difference values previously selected. If the absolute value of each element of the X matrix is less than its corresponding maximum-difference value, then the iterative looping is discontinued and the best-fit force field has been found; otherwise the looping is continued. At this point the new changes in the Urey-Bradley force constants $\Delta\Phi$ are formed as shown and then damped in such a way that the decimal point is moved one place to the left in a stepwise procedure for all elements of the $\Delta\Phi$ matrix until all elements are less than 0.1 millidynes/Å. A new set of Urey-Bradley force constants is formed by adding each element of the $\Delta\Phi$ matrix to the corresponding element in Φ. Then a new symmetry force field is constructed and the eigenvalues and eigenvectors are developed. The loop is started again after a check to see if the number of passes through the loop has exceeded the maximum number of passes previously set.

When the loop is terminated either by homing in on the best-fit force field or by exceeding the maximum number of cycles through the loop, then the best set of force con-

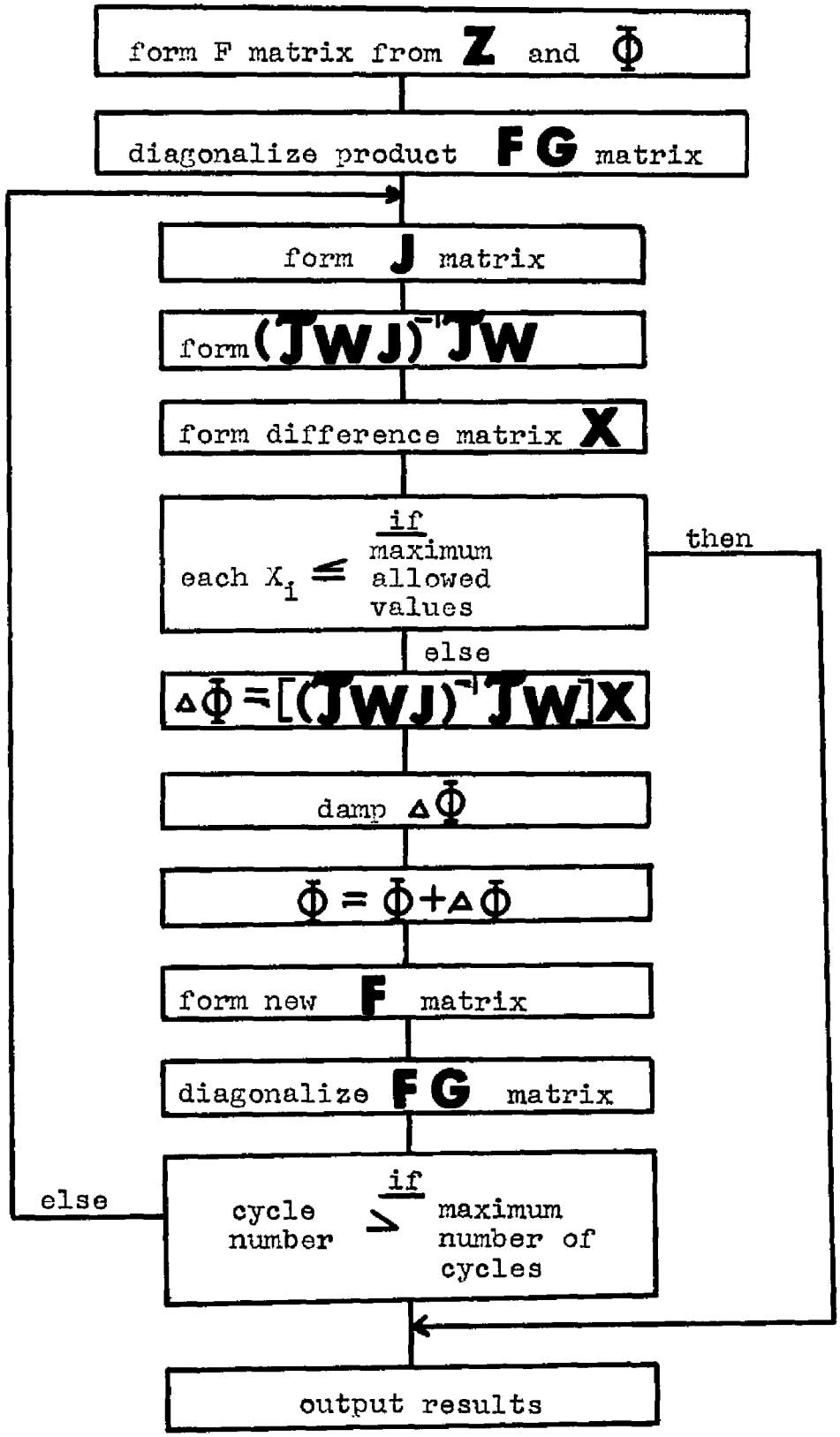

form F matrix from Z and Φ
diagonalize product FG matrix
form J matrix
form (JWJ)⁻¹JW
form difference matrix X
each $X_i \leq$ maximum allowed values if
then
else
ΔΦ = [(JWJ)⁻¹JW]X
damp ΔΦ
Φ = Φ + ΔΦ
form new F matrix
diagonalize FG matrix
cycle number > maximum number of cycles if
else
output results

Fig. 1-4

stants and their associated calculated frequencies are printed, along with the L matrix and potential energy distribution.

There are several limitations associated with the iterative procedure, the three most prominent of which will be discussed below. Perhaps the single most important problem arises from the nonlinearity of the changes making up the J matrix. This is the reason for an iterative solution in the first place, since if all of the changes were completely linear then the final value of the force constants could be solved for directly. If the elements of the J matrix are sufficiently nonlinear, oscillations about the solution will occur. It may turn out that there is no real set of force constants which reproduce the frequencies. To alleviate this problem, interaction force constants must be added to the Urey-Bradley force field. This leads to the second major limitation, which is the fact that in virtually all but the most simple molecules, there will be more force constants than frequencies and consequently one must decide which subset of the force constants to use in the Jacobian. Through multiple regression techniques[15] the most important force constants can be found; however, that does not eliminate the problem since the simultaneous adjustment of more force constants than one has frequencies may be required. The last of the major limitations is concerned with the vibrational assignment of the molecule. Assuming the vibrational assignment is firmly

made with all of the necessary experimental evidence, then the resulting potential energy distribution should, to a reasonable degree, reflect that assignment through the proper weighting of the appropriate symmetry coordinates. If, however, for the initial calculation of the vibrational frequencies the initial force field has transposed two or more of the ordered set of calculated frequencies as compared to the assigned experimental frequencies, then the resulting iterative attempt at solving for a final force field will be invalid.

The combination of the three of these limitations has led to the following aid in homing in on the final force field.

3. The Significance Matrix

This matrix is very similar to the J matrix except for two points. First, the elements are the changes in wave numbers of the calculated frequencies for a change of 0.01 millidynes/Å in the force constants, and not the change in the log of the frequencies. Second, this matrix is over all of the Urey-Bradley force constants as well as all added non-Urey-Bradley valence-interaction force constants.

The purpose in constructing this matrix is to allow the overall visual inspection by the researcher of the effects on all frequencies from changes in all of the force constants. This proves to be particularly useful when relatively large changes in some few individual frequencies appear to be necessary. If one frequency must be either

decreased or increased by a large amount while all other frequencies are held more or less constant, then the appropriate combination of force constants to do the task can be selected by inspection of the significance matrix. In the present work the significance matrix has proved to be indispensable.

4. The Potential Energy Distribution (P.E.D.)*

The potential energy in matrix notation is

$$2V = \tilde{\mathbf{R}}\mathbf{F}\mathbf{R} \qquad \text{J15}$$

where $\mathbf{R}$ and $\tilde{\mathbf{R}}$ are column and row vectors of internal coordinates. This can be rewritten as

$$2V = \tilde{\mathbf{Q}}\tilde{\mathbf{L}}\mathbf{F}\mathbf{L}\mathbf{Q} \qquad \text{J16}$$

since

$$\mathbf{R} = \mathbf{L}\,\mathbf{Q} \qquad \text{J17}$$

where $\mathbf{L}$ is the normal coordinate to internal coordinate transformation and $\mathbf{Q}$ is the normal coordinate vector.

The potential function can be written in an alternate manner as

$$2V = \tilde{\mathbf{Q}}\Lambda\mathbf{Q} \qquad \text{J18}$$

---

*The following discussion was taken in part from reference 17.

where Λ is a diagonal matrix of vibrational frequency parameters. Appropriate combination of equations J18 and J16 leads to

$$\Lambda = \tilde{L} F L \qquad \text{J19}$$

If this is written for one normal vibration whose frequency parameter is λ_n, we have

$$\lambda_n = \sum_{ij} l_{ni} F_{ij} l_{jn} = \sum_{ij} F_{ij} l_{in} l_{jn} \qquad \text{J20}$$

Then the potential energy due to this vibration is expressed by

$$V(Q) = \tfrac{1}{2} Q_n^2 \sum_{ij} F_{ij} l_{in} l_{jn} \qquad \text{J21}$$

The value of $F_{ij} l_{in} l_{jn}$ is usually large when $i = j$. Therefore, the $F_{ii} l_{in}^2$ are most important in determining the distribution of the potential energy. Thus the terms $F_{ii} l_{in}^2$ provide a measure of the relative contribution of each internal coordinate (or symmetry coordinate) to a particular normal coordinate. If any $F_{ii} l_{in}^2$ is large compared with the others, the vibration is assigned to the mode associated with R_i. If $F_{ii} l_{in}^2$ and $F_{jj} l_{jn}^2$ are both large compared to the others then the vibration is assigned to a mode associated with both R_i and R_j and is thus best described as a coupled vibration.

To obtain the final form of the potential energy distribution matrix, each column of the L matrix is divided by the appropriate eigenvalue of the product FG matrix. The

P.E.D. matrix then is computed according to the following equation:

$$PED_{ij} = F_{ii} l_{ij}^2 / \lambda_j \qquad J22$$

The P.E.D. is necessary in the overall process of the force field determination, as described in earlier sections.

K. Transformation From Normal Coordinates to Cartesian Displacement Coordinates[18,19]

When the secular equation is solved for its eigenvalues and eigenvectors a complete description of the normal coordinates in terms of symmetry coordinates is obtained. However, when significant portions of a normal coordinate are made up of two or more complex symmetry coordinates then the corresponding motions of the atoms in the molecule may not be immediately obvious. A clearer description is obtained if the normal modes are transformed to a coordinate system which shows the displacement of each atom in Cartesian coordinates. These new sets of coordinates, termed Cartesian displacement coordinates, can now be plotted in such a way as to give two-dimensional projections of the molecule experiencing its various normal modes of vibration.

The transformation from Cartesian displacement coordinates X to internal coordinates R is readily written as

$$\mathbf{R = B X} \qquad K1$$

where $\mathbf{B}$ is the transformation matrix (this matrix has no inverse since it is not square). In the construction of the Wilson G matrix described in an earlier section, the simplest process is first to construct the transformation from Cartesian space to internal-coordinate space, namely the matrix $\mathbf{B}$ above, and then apply it in the following fashion:

$$\tilde{\mathbf{B}}\,\mathbf{M}^{-1}\,\mathbf{B} = \mathbf{G} \qquad \text{K2}$$

where $\mathbf{M}^{-1}$ is a diagonal matrix of the inverse masses of each atom (taken once for each of the three Cartesian coordinates per atom). The $\mathbf{B}$ matrix is in fact first formed in the programs used to calculate the G matrix.

A transformation matrix from internal-coordinate space to Cartesian-coordinate space can be written, e.g.

$$\mathbf{X} = \mathbf{A}\,\mathbf{R} \qquad \text{K3}$$

where the matrix $\mathbf{A}$ is the transformation matrix. The relationship between the two transformation matrices $\mathbf{A}$ and $\mathbf{B}$ is easily shown to be

$$\mathbf{B}\,\mathbf{A} = \mathbf{I}_{3N-6} \qquad \text{K4}$$

where I is the identity matrix. If in equation K2 the G matrix on the right side of the equation is transposed to the left the following equation is obtained,

$$\tilde{\mathbf{B}}\,\mathbf{M}^{-1}\mathbf{B}\,\mathbf{G}^{-1} = \mathbf{I}_{3N-6} \qquad \text{K5}$$

Combining equations K4 and K5, the desired relationship between **A** and **B** is obtained:

$$\mathbf{A} = \mathbf{M}^{-1}\mathbf{B}\mathbf{G}^{-1} \qquad \text{K6}$$

Since in a previous section it was shown that

$$\mathbf{R} = \mathbf{U}\mathbf{L}\mathbf{Q} \qquad \text{K7}$$

then it is easily seen that

$$\mathbf{X} = \mathbf{A}\mathbf{U}\mathbf{L}\mathbf{Q} = [\mathbf{M}^{-1}\mathbf{B}\mathbf{G}^{-1}\mathbf{U}\mathbf{L}]\mathbf{Q} \qquad \text{K8}$$

where the resulting matrix in brackets is the final desired transformation matrix.

L. The Chemical Significance of the Resulting Force Field

A good approximation to the potential energy for diatomic molecules is the Morse potential[1],

$$V = D_e\left[1 - e^{-a(r - r_e)}\right]^2 \qquad \text{L1}$$

where D_e is the dissociation energy, and a is a constant characteristic of the bond. Under the assumption of small vibrational displacement it can be shown that

$$a = \sqrt{\frac{k}{2D_e}} \qquad \text{L2}$$

and

$$k = 2D_e a^2 \qquad \text{L3}$$

Thus if the constant (a) does not change much over a series

similar bonds then the force constant will be nearly proportional to the dissociation energy, i.e. the bond becomes stronger as the force constant becomes larger. It should be noted, however, that a general theoretical relationship between the dissociation energy and the force constant is difficult to derive even for a diatomic molecule, since the quantum-mechanical expression for the potential function involves a Coulomb integral, an exchange integral, and an overlap integral, and thus calculation of k from the second derivative of the potential evaluated at the equilibrium separation is not simple.[17]

The force constant is a measure of the curvature of the potential well near the equilibrium position, whereas the dissociation energy is given by the depth of the potential energy curve. Thus a large force constant means a sharp curvature of the potential well near the bottom but does not necessarily indicate a deep potential well. Usually, however, a larger force constant is an indication of a stronger bond in a series of molecules belonging to the same type.

Keeping the above approximations in mind, the Urey-Bradley force constants are easily interpretable in the two series of molecules studied in this work as are the van der Waals nonbonded force constants. The interaction force constants are to be interpreted from two aspects: magnitude and sign. The magnitude of the interaction force constants, when compared both with other interaction force

constants and with the valence force constant, will elucidate the extent to which the electrons in one bond interact with other adjacent bonds when these bonds bend or stretch. While the magnitude indicates the quantitative nature of the interaction the sign determines the qualitative nature of the interaction. For instance, as one bond stretches (or bends), near-by bonds will either lose electron density to the bond in question (a negative sign for the interaction) or will gain electron density (a positive sign). In conclusion then it is seen that these interaction force constants can be of tremendous use in determining the effect one bond has on its neighbors.

Chapter II

SYSTEMS USED IN THIS STUDY

A. General Parameters for the Series CX_3COZ

1. Internal Valence Coordinate Definitions

Internal valence coordinates were defined in the first chapter in terms of changes in bond lengths and angles. Since all of the molecules of this work have the same skeletal structure, only one general set of internal coordinates need be described. Figure 2-1 schematically shows all of the internal coordinates of the CX_3COZ structure with the exception of the oxygen out-of-plane wag and the CX_3 torsion.

Diagram 2-1A shows the bond stretching coordinates. In the diagram the coordinate of the planar C-X bond is distinguished from the two out-of-plane C-X bonds by a prime. The reason for this is that the molecules are best treated as having only a plane of symmetry and not as having a threefold rotational axis on one end while the other end has a plane of symmetry. The lack of a local threefold rotational axis for the CX_3COZ structure was first assumed by Schachtschneider[20] in his work on acetaldehyde and further substantiated by a complete microwave analysis of acetyl fluoride,[21] where the in-plane H-C-C angle was found to be significantly different from the two out-of-plane angles.

Diagrams 2-1B and 2-1C define the angle-bending co-

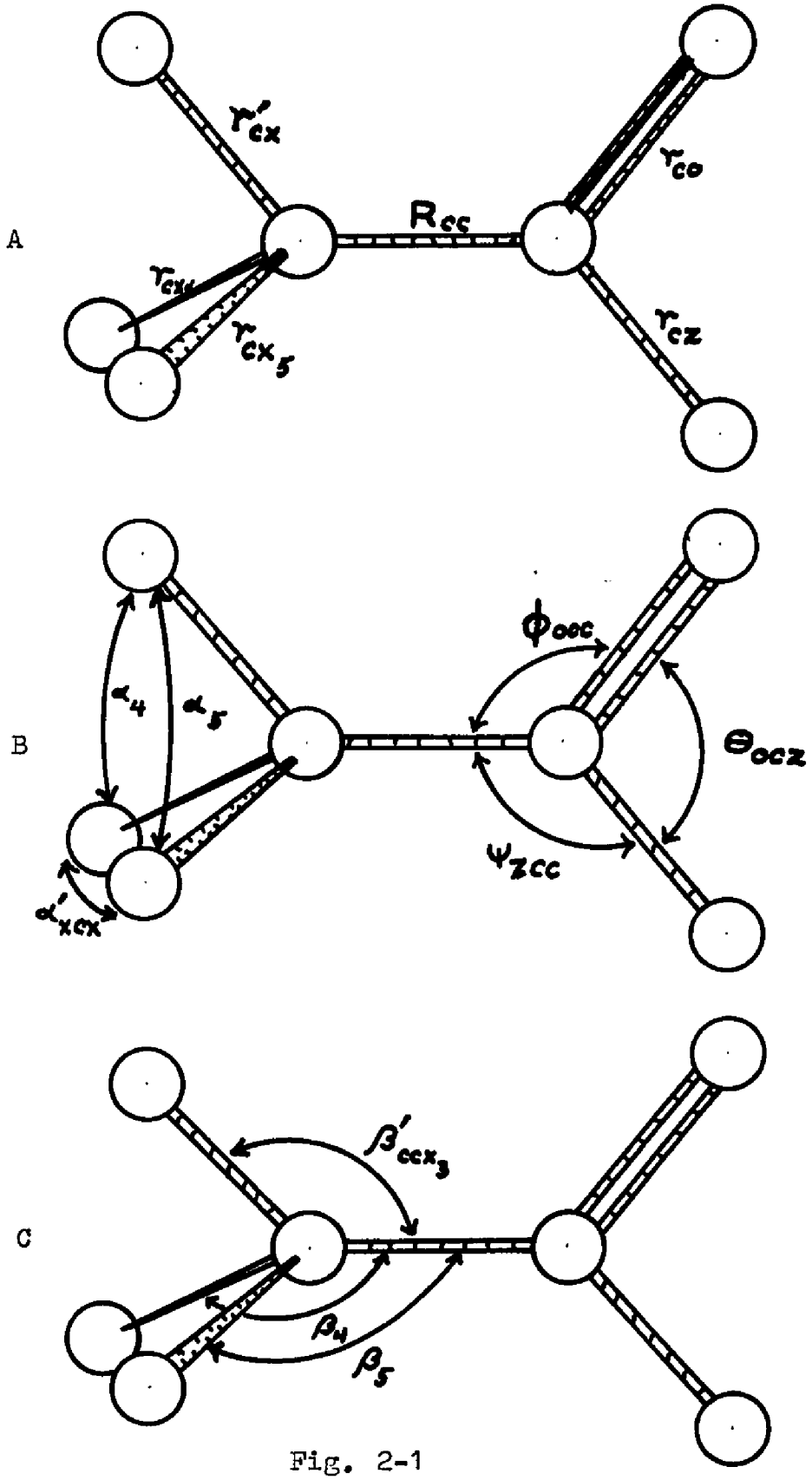

A
r'_{cx}
r_{co}
R_{cc}
r_{cx_4}
r_{cx_5}
r_{cz}
B
ϕ_{occ}
α_4
α_5
θ_{ocz}
ψ_{zcc}
α'_{xcx}
C
β'_{ccx_3}
β_4
β_5

Fig. 2-1

ordinates. The in-plane angle-bending coordinates are distinguished from the out-of-plane coordinates for the same reasons as in the case of the bond stretches.

Table 2-1 is a listing of all of the internal coordinates and a brief description of each. The list contains the torsion and the out-of-plane wag coordinates. This last coordinate requires a further explanation. There are two possible ways of defining the out-of-plane wag coordinate: the oxygen atom lifting out of the plane of the molecule, or the Z atom lifting out. The lighter of the two atoms will be the one to experience the greater part of the motion making up the normal vibration. Consequently when Z is a hydrogen or deuterium atom the wag is defined in terms of the H atom bending out of the plane, whereas when Z represents either F, Cl, or Br, it is defined in terms of the oxygen atom bending out of the plane.

2. Atomic Masses of the Atoms in the CX_3COZ Series

Table 2-2 lists the masses[22] for all atoms pertinent to this study. The masses used are those of the most stable isotopes with the exception of chlorine and bromine, which have significant contributions from two stable isotopes. In these cases the average atomic weight was used.

	Internal Coordinate	Description
1	R_{CC}	Δr for C-C bond
2	r_{CO}	Δr for C=O bond
3	r_{CZZ}	Δr for C-Z bond
4	r'_{CX}	Δr for in-plane C-X bond
5	r_{CX_4}	Δr for out-of-plane CX bond
6	r_{CX_5}	Δr for out-of-plane CX bond
7	α'_{XCX}	$\Delta\alpha$ for unique XCX angle
8	α_{XCX_4}	$\Delta\alpha$ for out-of-plane XCX angle
9	α_{XCX_5}	$\Delta\alpha$ for out-of-plane XCX angle
10	β'_{CCX}	$\Delta\beta$ for unique CCX angle
11	β_{CCX_4}	$\Delta\beta$ for out-of-plane CCX angle
12	β_{CCX_5}	$\Delta\beta$ for out-of-plane CCX angle
13	Θ_{OCZ}	$\Delta\Theta$ for OCZ angle
14	Φ_{OCC}	$\Delta\phi$ for OCC angle
15	Ψ_{ZCC}	$\Delta\psi$ for ZCC angle
16	γ	wag
17	τ	torsion

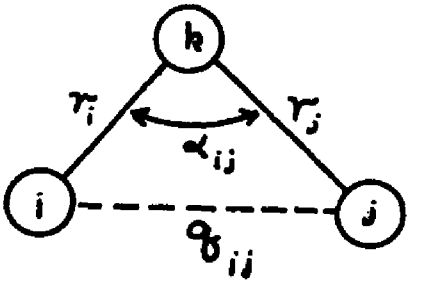
Table 2-1

Element	Mass
Hydrogen	1.00797
Deuterium	2.01410
Carbon	12.000
Oxygen	15.9949
Fluorine	18.9994
Chlorine	35.453
Bromine	79.907

Table 2-2

3. Urey-Bradley Configurations of CX_3COZ

There are three types of subconfigurations that the Urey-Bradley process utilizes in calculating the contribution each non-bonded interaction force constant makes to the potential function. To best understand the origin of the elements of the Urey-Bradley transformation matrix Z, the simplest of the three subconfigurations is considered.* The following diagram shows the labeled configuration,



where r_i, r_j, and α_{ij} are the three internal coordinates and q_{ij} is the distance between atoms i and j. The potential energy in the Urey-Bradley approximation is

*The following discussion was taken in part from reference 3.

$$2V = \sum_i \left[2k_i' r_x(\Delta r_i) + k_i(\Delta r_i)^2\right] +$$

$$2H_{ij}' r_x(r_x \Delta\alpha_{ij}) + H_{ij}(r_x \Delta\alpha_{ij})^2 +$$

$$2F_{ij}' q_{ij}(\Delta q_{ij}) + F_{ij}(\Delta q_{ij})^2 \qquad \text{A1}$$

The linear terms are included since Δr_i, Δr_j, $\Delta\alpha_{ij}$, and Δq_{ij} are not independent. The scaling parameter r_x is taken to be 1.0; it and the q_{ij} are inserted into the potential function to make all of the force constants dimensionally similar. The terms Δq_{ij} and Δq_{ij}^2 are removed by expanding Δq_{ij} in a Taylor series about Δr_i, Δr_j, and $\Delta\alpha_{ij}$. Using the relation

$$q_{ij}^2 = r_i^2 + r_j^2 - 2r_i r_j \cos\alpha_{ij}$$

we obtain

$$q_{ij} = S_{ij}\Delta r_i + S_{ji}\Delta r_j + (t_{ij}t_{ji})^{1/2} r_{ij}(\Delta\alpha_{ij}) +$$

$$\left[t_{ij}^2(\Delta r_i)^2 + t_{ji}^2(\Delta r_j)^2 - S_{ij}S_{ji}r_{ij}^2(\Delta\alpha_{ij})^2 -\right.$$

$$2t_{ij}t_{ji}(\Delta r_i)(\Delta r_j) + 2t_{ij}S_{ji}r_j(\Delta r_i)(\Delta\alpha_{ij}) +$$

$$\left.2t_{ji}S_{ij}r_i(\Delta r_i)(\Delta\alpha_{ij})\right] 2q_{ij} \qquad \text{A2}$$

where

$$r_{ij} = (r_i r_j)^{1/2}$$

$$S_{ij} = (r_i - r_j\cos\alpha_{ij})/q_{ij}$$

$$S_{ji} = (r_j - r_i\cos\alpha_{ij})/q_{ij}$$

$$t_{ij} = r_j \sin \alpha_{ij} / q_{ij}$$

$$t_{ji} = r_i \sin \alpha_{ij} / q_{ij}$$

Equation A2 is then substituted into equation A1 to give the contribution of the force constants F_{ij} and F'_{ij}. It is important to note that the terms Δr_i, Δr_j, and $\Delta \alpha_{ij}$ in equation A1 are independent and can be set equal to zero (which corresponds to setting the potential energy equal to zero in the equilibrium configuration). Table 2-3 lists the contributions to the Z matrix from the gem subconfiguration.

Valence Force Term	F_{ij}	F'_{ij}
$(\Delta r_i)^2$	S_{ij}^2	t_{ij}^2
$(\Delta r_i)(\Delta r_j)$	$S_{ij}S_{ji}$	$-t_{ij}t_{ji}$
$(\Delta r_i)(\Delta \alpha_{ij})$	$S_{ij}(t_{ij}t_{ji}r_i r_j)^{\frac{1}{2}}/r_x$	$t_{ij}S_{ji}r_j/r_x$
$(\Delta r_j)^2$	S_{ji}^2	t_{ji}^2
$\Delta r_j(\Delta \alpha_{ij})$	$S_{ji}(t_{ij}t_{ji}r_i r_j)^{\frac{1}{2}}/r_x$	$t_{ji}S_{ij}r_i/r_x$
$(\Delta \alpha_{ij})^2$	$t_{ij}t_{ji}r_j r_i/r_x$	$-S_{ij}S_{ji}r_j r_i/r_x^2$

Table 2-3

The contributions to the Z matrix from the remaining two subconfigurations are listed in references 3, 16, and 18. The two repulsive force constants F_{ij} and F'_{ij} arise from the quadratic and linear terms, respectively, in the potential function. It was noted by Shimanouchi[16,23,24] that

$$F' = -F/(n + 1) \qquad n = 9, 10, \text{ or } 12 \qquad A3$$

This relationship means that F' is far smaller than F and that the approximation

$$F' \cong -0.1F \qquad A4$$

will not lead to serious errors in the calculation of the force constants. Approximation A4 has subsequently been widely adopted in normal coordinate analyses, and is used in the present work.

The subconfiguration tetra is used for the $C\text{-}CX_3$ group in the CX_3COZ molecules. Unique to a tetrahedral structure is a four branch-point redundancy condition arising from the interdependency of all of the bond-length and bond-angle changes. This redundancy condition gives rise to a force constant which is most often described as the molecular tension of the tetrahedral group.

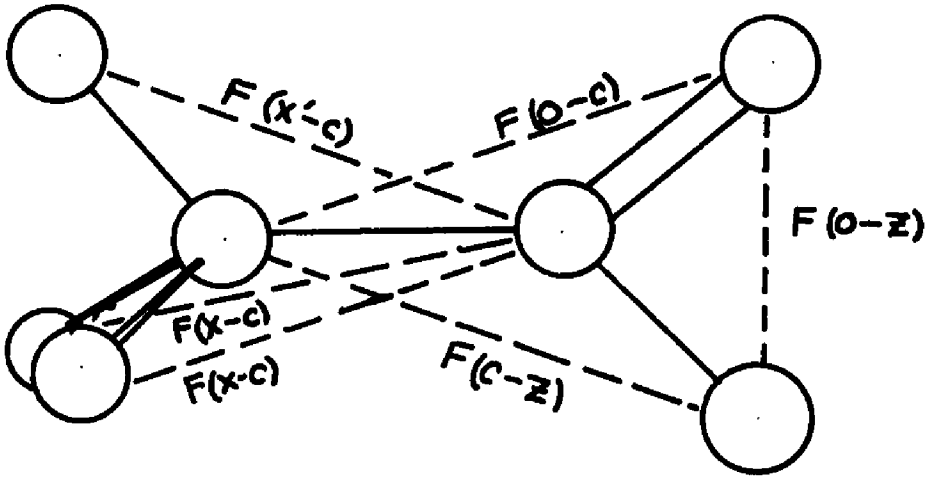
Table 2-4 is a list of all of the repulsive force constants of the CX_3COZ structure, while Figure 2-2 gives a graphic description.

	Force Constant	Description
1	F(X)	X--X
2	F(X')	2(X--X')
3	F(XC)	3(X--C)
4	F(OC)	O--C
5	F(CZ)	C--Z
6	F(OZ)	O--Z
7	C(X'O)	X'---O
8	C(XZ)	2(X---Z)
9	$\varkappa$	Molecular tension

Table 2-4

4. Valence Interaction Force Constants

An effort was made in this study to consider all significant interaction force constants in order to observe their effect on both the calculated frequencies and the potential energy distribution; however, not all of the interaction force constants were allowed to vary from a value of zero. Figure 2-3 is a matrix whose rows and columns are labeled with the internal coordinates. The diagonal elements are the simple valence force constants, whereas the off-diagonal elements are the valence interaction force constants. The numbers in each of the blocks correspond to the force constant numbers of the Urey-Bradley Z matrix. Any two blocks having the same numbers are symmetrically equivalent and any blocks which are not numbered are force constants which were not considered in



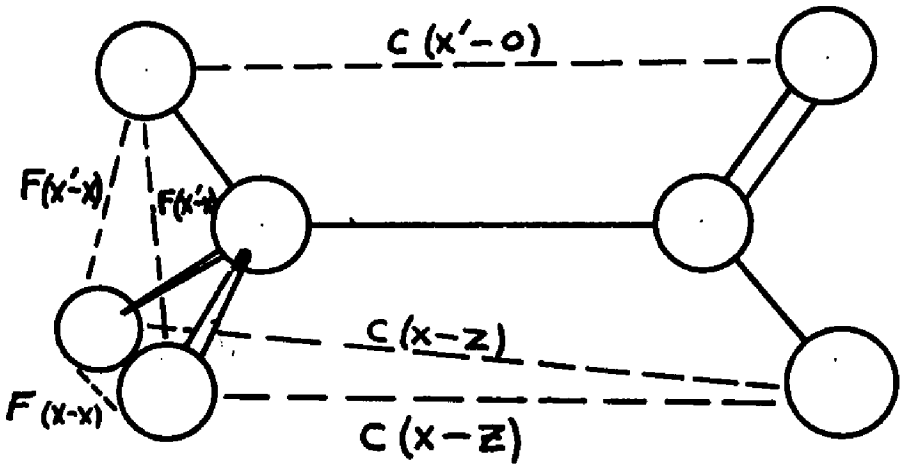


Fig. 2-2

this study. Certain force constants were ignored because it was considered unlikely they would exert any significant effect on the calculated frequencies.

In Figure 2-3, force constants 70 and 71 take on special importance. They are the force constants for the interaction between the nonplanar coordinates α and β and the out-of-plane wag. In chapter I it was noted that the weighting of an interaction force constant in the Z matrix is 1.000. If for force constant 71, both the interaction between α_{FCF_4} and the wag and between α_{FCF_5} and the wag are given a value of 1.000, then upon symmetrization, an interaction between symmetry species results rather than the intended interaction between the antisymmetric methyl rock and the wag. To overcome this problem, a value of -1.000 is given for the α_{FCF_4} and β_{CCF_4} coordinates and a +1.000 for the others. In this case the interaction between symmetry species is canceled out and the intended interaction is formed. From a physical standpoint, the necessity of making one value negative is evident, since as the oxygen atom bends out of the plane of symmetry it will affect the C-X bond on one side of the plane in an opposite fashion from the C-X bond on the opposite side of the plane.

5. Symmetry Space of the CX_3COZ Structure

All of the molecules of this study will be treated as having only a plane of symmetry. The point group for these

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1 r_{CC}	1	24	25	25	26	27	28	29	29	30	31	31	32	33	34		
2 r'_{CF}		2	35	35			36	37	37	38	39	39					
3 r_{CF_4}			3	40			41	42	43	44	45	46					
4 r_{CF_5}				3			41	43	42	46	46	44					
5 r_{CO}					4	47							48	49	50		
6 r_{CZ}						5							51	52	53		
7 α'_{FCF}							6	54	54	55	56	55					
8 α_{FCF_5}								7	57	58	59	60				71	
9 α_{FCF_4}									7	60	59	58				71	
10 β_{CCF_5}			symmetric							8	61	62					
11 β'_{CCF}											9	61	63	64	65	70	
12 β_{CCF_4}												9				70	
13 θ_{OCZ}													10	66	67		
14 ϕ_{OCC}														11	68		
15 ψ_{ZCC}															12		
16 Wag																13	69
17 τ																	14

Fig. 2-3

molecules is C_s, which has only two symmetry species, a' and a". Table 2-5 is the character table for the point group C_s.

C_s	E		Translations Rotations		Γ_{cart}	Γ_{vib}
a'	1	1	x, y, R_z	x^2, y^2, z^2, xy	13	10
a"	1	-1	z, R_x, R_y	yz, xz	8	5

Table 2-5

The number of normal modes of vibration for this seven-atomic system is fifteen, and using the procedures outlines in chapter I, it is seen that there are ten vibrations in the a' species and five in the a" species. The symmetry coordinates are the same for each of the molecules, but the order depends on the assignment of the infrared frequencies to the approximate normal modes. Table 2-6 is a list of the symmetry coordinates for the CX_3COZ structure.

B. Structures of CX_3COZ Molecules

1. The Acetyl Halides

All of the structural parameters for the acetyl halides included in this study were obtained from microwave studies. The bond angles and bond lengths supplied by the microwave studies were used to calculate the principal Cartesian coordinates of the molecules, which in turn were needed for the calculation of the G matrix and the Urey-Bradley Z matrix.

Symmetry Coordinate	Description
Symmetry Species a'	
$S_1 = r_{CO}$	C=O Str.
$S_2 = N(r'_{CX} + r_{CX_4} + r_{CX_5})$	Sym. CX_3 Str.
$S_3 = N(2r_{CX} - r_{CX_4} - r_{CX_5})$	Asym. XCX_2 Str.
$S_4 = r_{CC}$	C-C Str.
$S_5 = r_{CZ}$	C-Z Str.
$S_6 = N(\alpha' + \alpha_4 + \alpha_5 - \beta' - \beta_4 - \beta_5)$	Umbrella Bend
$S_7 = N(2\alpha' - \alpha_4 - \alpha_5)$	Asym. XCX_2 Def.
$S_8 = N(2\beta' - \beta_4 - \beta_5)$	XCX_2 Rock
$S_9 = N(2\theta_{OCZ} - \phi_{OCC} - \psi_{ZCC})$	Scissors Bend
$S_{10} = N(\phi_{OCC} - \psi_{ZCC})$	OCZ Rock
$S_{16} = N(\alpha' + \alpha_4 + \alpha_5 + \beta' + \beta_4 + \beta_5)$	Redundant
$S_{17} = N(\theta_{OCZ} + \phi_{OCC} + \psi_{ZCC})$	Redundant
Symmetry Species a"	
$S_{11} = N(r_{CX_4} - r_{CX_5})$	XCX_2 Str.
$S_{12} = N(\alpha_{XCX_4} - \alpha_{XCX_5})$	XCX_2 Def.
$S_{13} = N(\beta_{CCX_4} - \beta_{CCX_5})$	XCX_2 Wag
$S_{14} = \gamma$	Wag
$S_{15} = \tau$	Torsion

Table 2-6

The input data for the program used to calculate the principal Cartesian coordinates (Appendix 2A) requires the input parameters listed in Table 2-7.

Bond Lengths	Bond Angles	Dihedral Angles
C-X' (in plane)	X'-C-C	O=C-C-X' (0°)
C-X	X-C-C	Z-C-C-X' (180°)
C-X	X-C-C	X'_4>C-C (120°)
C-C	C-C=O	X'_5>C-C (-120°)
C=O	C-C-Z	
C-Z		

Table 2-7

Note in Table 2-7 that for a CX_3COZ molecule all of the dihedral angles are fixed and easily determined.

Table 2-8 lists the structural parameters for the acetyl halides.

Bond Length Å	Aldehyde[25]	Fluoride[21]	Chloride[26]	Bromide[27]
C-H (in plane)	1.086	1.082	1.083	1.083
C-H	1.086	1.096	1.083	1.083
C-H	1.086	1.096	1.083	1.083
C-C	1.5005	1.502	1.499	1.499
C=O	1.2155	1.185	1.192	1.192
C-Z	1.114	1.343	1.789	1.960

Bond Angle	Aldehyde	Fluoride	Chloride	Bromide
C-C-H (in plane)	110.335°	110.400°	110.350°	110.350°
C-C-H	110.335°	108.800°	110.350°	110.350°
C-C-H	110.335°	108.800°	110.350°	110.350°
C-C=O	123.918°	127.900°	127.080°	127.080°
C-C-Z	117.474°	110.735°	112.650°	112.650°

Table 2-8

2. The Trifluoroacetyl Halides

The structure of trifluoroacetaldehyde was obtained from a microwave study by Woods[28] and an electron diffraction study by Schwendeman[29]. The structures of trifluoroacetyl fluoride and chloride were determined by Boulet[30] using electron diffraction methods. Table 2-9 lists the structural parameters.

Bond Length Å	Aldehyde	Fluoride	Chloride
C-F (in plane)	1.332	1.315	1.340
C-F	1.332	1.315	1.340
C-F	1.332	1.315	1.340
C-C	1.54	1.544	1.52
C=O	1.204	1.171	1.17
C-Z	1.09	1.330	1.79

Bond Angle	Aldehyde	Fluoride	Chloride
C-C-F (in plane)	109.8°	108.48°	111.38°
C-C-F	109.8°	108.48°	111.38°
C-C-F	109.8°	108.48°	111.38°
C-C=O	121.8°	131.0°	128.0°
C-C-Z	118.2°	108.0°	109.0°

Table 2-9

The principal Cartesian coordinates along with a two-dimensional plot of the coordinates for both the acetyl halides and the trifluoroacetyl halides appear in Appendix 2A.

C. Vibrational Assignments of the CX_3COZ Molecules

The fundamental vibrations of the molecules of this study have been thoroughly studied and assigned by several authors. Tables 2-10, 2-11, and 2-12 list the assigned fundamentals of the acetyl halides, deuterated acetyl halides, and the trifluoroacetyl halides respectively.

Certain torsional frequencies are too weak to be observed in the infrared spectra. In these cases the torsional frequencies were calculated from the barrier to internal rotation given in the microwave studies. The calculated torsional frequencies are in parentheses in Tables 2-10 and 2-11.

Symmetry Species	Symmetry* Coordinate	Z = H^{20}	D^{20}	F^{32}	Cl^{33}	Br^{34}
A'	Sym. CH_3 Str.	2967	2970	2953	2934	2945
	Asym. HCH_2 Str.	3010	3014	3043	3029	3026
	C=O Str.	1743	1743	1870	1822	1821
	C-C Str.	919	1109	826	958	942
	C-Z Str.	2822	2071	1187	608	570
	Umbrella Bend	1400	1353	1378	1370	1362
	Asym. HCH_2 Def.	1441	1442	1437	1432	1425
	HCH_2 Rock	1113	1043	1000	1109	1092
	Scissors Bend	1352	849	598	436	347
	OCZ Rock	509	500	420	348	304
A''	XCX_2 Str.	3010	3014	3004	3029	3025
	XCX_2 Bend	1420	1420	1440	1432	1438
	XCX_2 Wag	867	802	1053	1029	1021
	O or Z Wag	763	668	567	514	492
	Torsion	150	145	(112)	(137)	(137)

$\underline{CH_3COZ}$

Table 2-10

*See Table 2-6 for a complete description.

Symmetry Species	Symmetry Coordinate	Z H^{35}	D^{20}	F^{32}	Cl^{33}	Br^{34}
A'	Sym. CD_3 Str.	2117	2130	2144	2104	2105
	Asym. DCD_2 Str.	2254	2265	2274	2280	2275
	C=O Str.	1753	1737	1869	1820	1825
	C-C Str.	1131	1151	778	962	808
	C-Z Str.	2812	2060	1204	563	525
	Umbrella Bend	960	1028	1149	1040	1010
	Asym. DCD_2 Def.	1038	1045	1030	1132	1122
	DCD_2 Rock	774	747	839	818	951
	Scissors Bend	1390	938	577	437	345
	OCZ Rock	443	436	378	317	275
A"	DCD_2 Str.	2223	2225	2243	2280	2275
	DCD_2 Bend	1028	1028	1057	1040	1043
	DCD_2 Wag	626	573	915	877	855
	O or Z Wag	761	676	491	498	440
	Torsion	122	116	(93)	(102)	(101)

$\underline{CD_3COZ}$

Table 2-11

Z

Symmetry Species	Symmetry Coordinate	H^{36}	D^{36}	F^{37}	Cl^{38}
A'	Sym. CF_3 Str.	1310	1302	1340	1284
	Asym. FCF_2 Str.	1202	1244	1254	1240
	C=O Str.	1788	1770	1899	1811
	C-C Str.	840	811	806	937
	C-Z Str.	2864	2150	1099	750
	Umbrella Bend	706	693	692	583
	Asym. FCF_2 Def.	580	580	595	703
	FCF_2 Rock	256	253	228	198
	Scissors Bend	1384	1033	761	511
	OCZ Rock	431	428	390	334
A"	FCF_2 Str.	1183	1177	1214	1202
	FCF_2 Bend	531	521	519	517
	FCF_2 Wag	322	318	242	234
	O or Z Wag	958	842	427	390
	Torsion	55	52	50	45

$\underline{CF_3COZ}$

Table 2-12

Chapter III

RESULTS AND DISCUSSION

A. The Frequency Fit

For each normal coordinate Appendix 2D1 contains the observed and calculated frequency, its difference, and percent difference. In each case it is easily seen that the percent difference is quite small with respect to the range of 3 to 4 percent allowable for anharmonicity. The only notably large percent difference occurs for υ_{12} of the molecule CF_3COH. This motion is a mixture of the out-of-plane hydrogen wag and the out-of-plane trifluoromethyl wag. It was not possible to reduce the percentage difference of the out-of-plane wag without seriously altering the frequency fit for the CF_3 wag as well as for the corresponding vibrations in the deuterated analogs. The source of this problem is the limitation of the harmonic oscillator approximation as pointed out by C.V. Berney[36] and C.B. Moore and G.C. Pimentel[39].

The most difficult frequencies to fit were those vibrations belonging to the a" symmetry species involving largely the out-of-plane motions. The only other set of frequencies that gave trouble were the a' vibrations described by the scissors and OCZ rock symmetry coordinates. The corresponding modes are mixtures of both of these symmetry coordinates.

There is some question concerning the choice of how

the symmetry coordinate is constructed for the OCZ rock. The scissors bend symmetry coordinate involves all three of the angle-bending internal coordinates around the carbonyl carbon and consequently all three force constants associated with these internal coordinates enter into the construction of the normal coordinate. The OCZ rock on the other hand involves only two of the three internal coordinates. The normal mode associated primarily with the OCZ rock is likely to be a complex combination of motions of all three bends and therefore cannot be adequately described by the rock symmetry coordinate alone. The effect of this problem is to make the simultaneous fit of both the rock and scissors vibrations difficult. A way to alleviate this is to include all three internal coordinates into both the rock and the scissors. However, more serious problems are created doing this than are solved. If all three internal coordinates are used to make up the rock then one is left with the problem of how each internal coordinate is to be weighted in the symmetry coordinate. Due to the redundancy condition involving all three internal coordinates, there are definite restrictions governing the makeup of the rock symmetry coordinate, i.e. if two of the angles open up by a unit amount then the remaining angle must close down by two units. The actual weighting of each internal coordinate will be different for each molecule (different even for isotopically substituted molecules). In the present study it was felt that it was

better to use the same symmetry coordinate makeup for purposes of comparison between molecules.

B. The Force Fields

Appendix 2D2 contains the tables of the force constants for both the acetyl halides and the trifluoroacetyl halides. It is felt that the force constants are close to the true harmonic force constants since both series of molecules show remarkable consistency in trends, magnitudes, and signs of the force constants. The primary goal of this study has been to find force fields which vary only in a reasonable way from molecule to molecule.

The valence force constants are perhaps the most interesting to look at since they are the easiest to interpret from a chemical standpoint. In Chapter I it was noted that force constants can usually be thought of as being proportional to bond strengths for a given series of molecules. With this in mind some interesting correlations of certain force constants can be made. In both the acetyl and trifluoroacetyl halide series the C=O stretching force constant is largest when the Z atom is fluorine and is consistently larger for the trifluoro- series. The C-C stretching force constant is very much greater for the acetyl series, which is clear evidence for a weakening of the carbon-carbon bond due to the electron-withdrawal property of the CF_3 group. In both series the carbon-halogen stretching force constant decreases as Z changes

from H to Br. This agrees very well with the bond dissociation energies[40] for acetaldehyde, acetyl chloride, and acetyl bromide. The energies are 86.0, 83.2, and 67.8 kcal/mole respectively. The C-F bond for the CX_3 group seems to be stronger than the C-H bond, which is evidenced not only by the CF_3 group having the larger stretching force constants but also by the larger XCX and XCC bending force constants. In addition, the molecular tension force constant is an order of magnitude larger for the CF_3 series. This is consistent with the CF_3 group being a tightly bound unit.

The Urey-Bradley non-bonded repulsive force constants are large for the CF_3 group, and when compared to the CH_3 group indicate strong repulsion among the fluorines and also between the fluorines and the carbonyl carbon.

The CF_3- series required many more interaction force constants than did the CH_3- series to obtain consistent force fields. Indeed, several interaction force constants were needed to obtain even one force field which reproduced the assigned frequencies. There are some interactions which deserve particular note. The interaction between the C-C stretch and the C-Z stretch is small and negative but necessary for a satisfactory frequency fit. The negative sign indicates that as the C-Z bond stretches, electron density flows into the C-Z bond and similarly as the C-C bond stretches electron density flows into it. The interactions between the C-C bond stretch and the C-F bond

stretches, FCF angle bends, and FCC angle bends were very important for the trifluoro- series, as were the interactions among the C-F bond stretches and angle bends. The magnitudes of the interactions between the out-of-plane wag and the methyl rock, methyl deformation, and torsion may be relatively small but are perhaps the most significant in terms of the extent to which they effect the a" frequencies.

C. The Potential Energy Distribution

Appendix 2D5 contains the various potential energy distribution matrices for all of the molecules and their isotopically substituted analogs.

There are several normal coordinates in the trifluoro- series which are made up of two or more symmetry coordinates. In some cases the mixing is extensive. In all cases the a' C-F stretches mix as do the scissors and OCZ rock. With the exception of the aldehyde, the C-C and C-Z stretches are perhaps best thought of as an in-phase and out-of-phase combination stretch. The a" trifluoromethyl wag and the out-of-plane oxygen wag are extensively mixed. The oxygen wag is also mixed with the torsion. Similar mixing takes place in the acetyl series. The mixing often shifts markedly on going to the deuterated counterparts in the acetyl series.

In many cases where the mixing is extensive, a clearer picture of a given normal mode can be gained by examining the Cartesian displacements of all the atoms. These dis-

placements can be found in Appendix 2D6.

D. Comparison of Results to Past Work

There have been only two past studies done on any of the molecules. Acetaldehyde was worked on by Cossee and J.H. Schachtschneider in 1965 and a paper on acetyl chloride was published by J. Overend et al. in 1961.

In the case of acetaldehyde, there are very few differences between the force field previously published and the present work. The major difference concerns the out-of-plane wag and the torsion. The value of both force constants is considerably larger in the present study. This is a result of the introduction of the wag-torsion interaction force constant. Though the magnitude of this interaction is small the calculated wag and torsion frequencies are extremely sensitive to it. Consequently the wag and torsion valence force constants are correspondingly sensitive to its size.

Overend's work on acetyl chloride was limited to transferring Urey-Bradley force constants from the molecules $COCl_2$ and $(CH_3)_2CO$ and calculating the frequencies. His resulting frequency fit was fairly good with a few exceptions. The force field obtained in this study is very similar to Overend's. The chief differences are in the C=O and C-Cl stretching force constants, which for this study are considerably larger, leading to a much better frequency fit.

E. Conclusion

It was found in the course of this study that it is necessary to include many non-Urey-Bradley valence interaction force constants in any study where chemical similarity between a series of molecules is used as a constraint on the force field. It is felt by the author that such a force field constraint provides an excellent method for finding force fields which are chemically useful and likely to be transferable to much larger molecules. This last point is particularly important in light of the great deal of work being done on biologically-active molecules. Recently several papers[41-48] have been published where structures and strain energies of biologically-active molecules were determined by transferring appropriate Urey-Bradley force constants to them, substituting them into the potential function of the molecule and minimizing the resulting potential energy by systematically varying the structure. In several cases the biological role the molecule plays was explained in terms of the calculated structure[49].

Chapter IV

APPENDICES

1. Computer Programs

The programs listed in this appendix are all of the necessary programs used in a normal coordinate analysis. The first four main programs are modifications of programs listed and explained in reference 3. For these programs the explanation of the input data will be limited to the incorporated modifications.

A. Fortran -- Main Programs

1. PREIGEN

This program calculates the principal Cartesian coordinates of a molecule given its bond lengths, bond angles, and dihedral angles. All input data follow exactly the form described by J. H. Schachtschneider[3], with the exception of the control card. Columns 73 and 76 are control indicator positions. If a 1 is placed in column 73 the Cartesian coordinates are written onto intermediate tape or disk storage for use in later programs. A 1 in column 76 will instruct the computer to plot three two-dimensional projections of the molecule. The plotting subroutine is listed after the main program.

```
      DIMENSION DQ(50,5C)
      DIMENSION NAME(16),COR(500,3),W(500),VBA(3),VCA(3),TRANS(3,3),
     1PRC(3),RJA(3),X(100),Y(100),Z(100),A(3,3),S(3,3),CMC(1,3),
     2PCC(1,3),P(3,3),Q(3,3),U(3,3),B(100),C(100),D(100),T(3,3) ,
     3 B8(500,3),NR(15C0),NCC(1500),CAT(1500)
C WRITE PERTINANT DATA IN CCLS. 1-64 + THE = OF ATCMS IN COLS. 69,70
  100 READ(5,60C) NAME,NOAT,IN,IPLOT
  600 FORMAT(16A4,I6,2I3)
      IF (NOAT) 500,5C0,601
  601 WRITE(6,602) NAME,NOAT
  602 FORMAT('1',1oA4,I6)
      CON=.174532925E-01
  101 READ(5,111) NO,NA,NB,NC,R,TE,PH,WT
  111 FORMAT (4I3,4F12.6)
   55 WRITE (6,119) NC,NA,NB,NC,R,TE,PH,WT
  119 FORMAT (2H  4I4,4F12.6)
      W(NO)=WT
      CCR(NO,1)=0.0
      CCR(NO,2)=0.0
      CCR(NO,3)=0.0
      N1=NO
  110 READ(5,111)NC,NA,NB,NC,R,TE,PH,WT
      WRITE(6,119)NO,NA,NB,NC,R,TE,PH,WT
      CCR(NO,1)=R
      CCR(NO,2)=0.0
      CCR(NO,3)=0.0
      W(NO)=WT
  11o READ(5,111)NO,NA,NB,NC,R,TE,PH,WT
      WRITE(6,119)NO,NA,NB,NC,R,TE,PH,WT
      W(NO)=WT
      IF(TE)120,118,120
  11d CS=-0.33333333
      SS=0.94280907
      GO TO 121
  120 CS=COS(CON*TE)
      SS=SIN(CON*TE)
  121 IF(NA-N1)128,122,128
  122 CCR(NO,1)=COR(NA,1)+R*CS
      GO TO 129
  12d CCR(NO,1)=COR(NA,1)-R*CS
  129 CCR(NO,2)=R*SS
      CCR(NO,3)=0.0
      IF(NOAT-3)500,161,130
  130 DO 160 I=4,NOAT
      READ(5,111)NO,NA,NB,NC,R,TE,PH,WT
      WRITE(6,119)NO,NA,NB,NC,R,TE,PH,WT
      W(NO)=WT
      IF(TE)133,132,133
  132 CS=-0.33333333
      SS=0.94280907
      GO TO 135
  133 CS=COS(CON*TE)
      SS=SIN(CON*TE)
```

```
 135 DSQ=0
     DO 138 M=1,3
     VBA(M)=COR(NB,M)-COR(NA,M)
     VCA(M)=COR(NC,M)-COR(NA,M)
 138 DSQ=DSQ+VBA(M)**2
     RAB=SQRT(DSQ)
     SCALE=0.0
     DO 142 M=1,3
     TRANS(M,1)=VBA(M)/RAB
 142 SCALE=SCALE+TRANS(M,1)*VCA(M)
     DSQ=0.0
     DO 146 M=1,3
     RJA(M)=VCA(M)-SCALE*TRANS(M,1)
 146 DSQ=DSQ+RJA(M)**2
     RAJ=SQRT(DSQ)
     DO 148 M=1,3
 148 TRANS(M,2)=RJA(M)/RAJ
     TRANS(1,3)=TRANS(2,1)*TRANS(3,2)-TRANS(3,1)*TRANS(2,2)
     TRANS(2,3)=TRANS(3,1)*TRANS(1,2)-TRANS(1,1)*TRANS(3,2)
     TRANS(3,3)=TRANS(1,1)*TRANS(2,2)-TRANS(2,1)*TRANS(1,2)
     PRC(1)=R*CS
     PRC(2)=R*SS*COS(CON*PH)
     PRC(3)=R*SS*SIN(CON*PH)
     DO 160 M=1,3
     COR(NO,M)=COR(NA,M)
     DO 160 K=1,3
 160 COR(NO,M)=COR(NO,M)+TRANS(M,K)*PRC(K)
 161 WRITE(6,60)
  60 FORMAT(55HO ATOM NO.        X             Y             Z          MASS)
     DO 164 I=1,NOAT
 164 WRITE(6,62)I,(COR(I,M),M=1,3),W(I)
  62 FORMAT(4X,I3,3X,3F12.6,F13.6)
     DO 63 I=1,NOAT
     X(I)=COR(I,1)
     Y(I)=COR(I,2)
  63 Z(I)=COR(I,3)
     DO 1730 I=1,NOAT
     BB(I,1)=X(I)
     BB(I,2)=Y(I)
1730 BB(I,3)=Z(I)
     NX=0
     DO 1715 I=1,NOAT
     DO 1715 M=1,3
     IF(0.000005-ABS(BB(I,M))) 1705,1705,1710
1705 NX=NX+1
     NR(NX)=M
     NCO(NX)=I
     DAT(NX)=BB(I,M)
     GO TO 1715
1710 BB(I,M)=0.0
1715 CONTINUE
     NX=NX+1
     NR(NX)=-1
```

```
      NCO(NX)=0.0
      DAT(NX)=0.0
      IF(IN) 15,171,170
  170 NX1=-3
      NX2=0
  174 NX1=NX1+4
      NX2=NX2+4
      WRITE(11)  (NR(I),NCC(I),DAT(I),I=NX1,NX2)
      DO 173 I=NX1,NX2
      IF(NR(I).LT.0)  GO TO 171
  173 CONTINUE
      GO TO 174
  171 WRITE(7,720)  (NR(I),NCO(I),DAT(I),I=1,NX)
   15 SUMW=0
   16 SUMWX=0
   17 SUMWY=0
   18 SUMWZ=0
   19 DO 23 I= 1,NOAT
   20 SUMW= SUMW + W(I)
   21 SUMWX= SUMWX + W(I)*X(I)
   22 SUMWY= SUMWY + W(I)*Y(I)
   23 SUMWZ= SUMWZ + W(I)*Z(I)
   24 XO= SUMWX/SUMW
   25 YO= SUMWY/SUMW
   26 ZO= SUMWZ/SUMW
   27 WRITE (6,28)
   28 FORMAT('OCENTER OF MASS IN THE ORIGINAL COORD. SYSTEM IS',1X)
   29 WRITE (6,30)
   30 FORMAT ('0',25X,'XO          YO          ZO',1X)
      WRITE (6,43) XO,YO,ZO
   43 FORMAT (22X,3F10.7)
   31 DO 34 I=1,NOAT
   32 X(I)= X(I)-XO
   33 Y(I)= Y(I)-YO
   34 Z(I)= Z(I)-ZO
      WRITE (6,35)
   35 FORMAT('OATOMIC COORDINATES REFERRED TO THE CENTER OF MASS',1X)
      WRITE (6,36)
   36 FORMAT('C',19X,'I       M          XO(I)      YO(I)      ZO(I)',1X)
   37 DO 39 I=1,NOAT
   39 WRITE(6,12) I,W(I),X(I),Y(I),Z(I)
   12 FORMAT(16X,I4,4X,4F10.5)
   40 AIXX= 0
      AIYY= 0
      AIZZ= 0
   42 CYZ=0
      CXZ=0
      CXY=0
   45 DO 51 I=1,NOAT
   46 AIXX= AIXX +W(I)*(Y(I)**2 + Z(I)**2)
   47 AIYY= AIYY + W(I)*(X(I)**2 + Z(I)**2)
   48 AIZZ= AIZZ + W(I)*(X(I)**2 + Y(I)**2)
   49 CYZ= CYZ + W(I)*Y(I)*Z(I)
```

```
   50 CXZ= CXZ + W(I)*X(I)*Z(I)
   51 CXY = CXY + W(I)*X(I)*Y(I)
      WRITE (6,52)
   52 FORMAT('0THE UNTRANSFORMED MOMENTS + PRODUCTS OF INERTIA ARE',1X)
      WRITE (6,53)
   53 FORMAT('0',5X,'IXX        IYY        IZZ             CYZ        CXZ
     1    CXY',1X)
      WRITE (6,54) AIXX,AIYY,AIZZ,CYZ,CXZ,CXY
   54 FORMAT (3F10.4,4X,3F10.4)
  150 CRIT= ABS(CYZ)+ABS(CXZ)+ABS(CXY)
  151 IF (.01-CRIT) 200,154,154
  200 A(1,1)=AIXX
      A(2,2)= AIYY
      A(3,3)=AIZZ
      A(2,1)=-CXY
      A(3,1)=-CXZ
      A(3,2)=-CYZ
      A(1,2)=A(2,1)
      A(1,3)=A(3,1)
      A(2,3)=A(3,2)
      CALL ARRAY(2,3,3,3,3,A,A)
      CALL MSTR(A,P,3,0,1)
      CALL EIGEN(P,Q,3,0)
      CALL MSTR(Q,S,3,0,0)
      CALL MSTR(P,U,3,1,0)
      CALL ARRAY(1,3,3,3,3,S,S)
      CALL ARRAY(1,3,3,3,3,U,U)
      WRITE (6,202)
  202 FORMAT('0THE PRINCIPAL MOMENTS ARE',1X)
      WRITE(6,205)U(1,1),U(2,2),U(3,3),U(1,2),U(1,3),U(2,3)
  205 FORMAT(18X,3F15.6)
      WRITE(6,206)
  206 FORMAT('0THE TRANSFORMATION MATRIX IS',1X)
  207 WRITE(6,205) S(1,1),S(1,2),S(1,3)
      WRITE(6,205) S(2,1),S(2,2),S(2,3)
      WRITE(6,205) S(3,1),S(3,2),S(3,3)
  154 BX=16.8575/U(1,1)
      BY=16.8575/U(2,2)
      BZ=16.8575/U(3,3)
      WRITE(6,155)
  155 FORMAT('0ROTATIONAL CONSTANTS ARE     BX         BY         BZ:,1X)
      WRITE(6,157) BX,BY,BZ
  157 FORMAT (30X,3F10.7)
      CALL ARRAY(2,3,3,3,3,S,S)
      CALL GMTRA(S,T,3,3)
      DO 700 I=1,NOAT
      CMC(1,1)=X(I)
      CMC(1,2)=Y(I)
      CMC(1,3)=Z(I)
      CALL ARRAY(2,3,1,3,1,CMC,CMC)
      CALL GMPRD(T,CMC,PCC,3,3,1)
      CALL ARRAY(1,3,1,3,1,PCC,PCC)
      B(I)=PCC(1,1)
```

```
      C(I)=PCC(1,2)
  703 D(I)=PCC(1,3)
      WRITE(6,701)
  701 FORMAT('1 THE PRINCIPLE CART. COORD. ARE',1X)
      DO 304 I=1,NOAT
  304 WRITE(6,303) I,B(I),C(I),D(I)
  303 FORMAT(5X,I4,5X,F10.5,5X,F10.5,5X,F10.5)
      DO 730 I=1,NOAT
      BB(I,1)=B(I)
      BB(I,2)=C(I)
  730 BB(I,3)=D(I)
      NX=0
      DO 715 I=1,NOAT
      DO 715 M=1,3
      IF(0.000005-ABS(BB(I,M))) 705,705,710
  705 NX=NX+1
      NR(NX)=M
      NCC(NX)=I
      DAT(NX)=BB(I,M)
      GO TO 715
  710 BB(I,M)=0.0
  715 CONTINUE
      NX=NX+1
      NR(NX)=-1
      NCC(NX)=0.0
      DAT(NX)=0.0
      WRITE(7,720) (NR(I),NCC(I),DAT(I),I=1,NX)
  720 FORMAT (2I3,F12.6,2I3,F12.6,2I3,F12.6,2I3,F12.6)
      DO 743 I=1,NCAT
      DO 743 J=1,NOAT
  743 DC(I,J)=SQRT((B(I)-B(J))**2+(C(I)-C(J))**2+(D(I)-D(J))**2)
      DO 744 I=1,NOAT
      WRITE(6,745)  I
  745 FORMAT(//,'  THE DISTANCE FROM ATOM',I3,'  TO THE ATOM LISTED BELO
     1W IS',/)
  744 WRITE(6,746) (J,DC(I,J),J=1,NCAT)
  746 FORMAT(3(I5,' =',F8.4))
      IF(IPLOT.EQ.0)  GO TO 56
      CALL PLOTER(BB,NOAT)
   56 GO TO 100
  500 CALL EXIT
      END
```

```
      SUBROUTINE PLOTER(Y,NOAT)
      INTEGER *2M,A,B
      DIMENSION Y(500,3),IY(20,3),NCO(20),IZ1(3),I1(20),I2(20),IZ2(3),
     1  M(11),A(121)
      DATA M/'0','1','2','3','4','5','6','7','8','9',' '/,A/121*' '/
      DO 5 J=1,3
      DO 5 I=1,NOAT
      ITEMP =IFIX(Y(I,J)*100)
      IY(I,J) = ITEMP/10
      ITEMP = MOD(ITEMP,10)
      IF(ITEMP.GT.4) IY(I,J) = IY(I,J) + 1
      IF(ITEMP.LT.-4) IY(I,J) = IY(I,J) - 1
    5 CONTINUE
      WRITE(6,616)
  616 FORMAT('0')
      DO 6 I=1,NOAT
    6 WRITE(6,607) (IY(I,J),J=1,3)
  607 FORMAT(10X,3I5)
      IZ2(1) = 2
      IZ2(2) = 3
      IZ2(3) = 3
      IZ1(1) = 1
      IZ1(2) = 1
      IZ1(3) = 2
      DO 10 I=1,NOAT
   10 NCO(I) = 0
      DO 210 IJK = 1,3
      IQ1 = IZ1(IJK)
      IQ2 = IZ2(IJK)
      DO 15 I=1,NOAT
      I1(I) = IY(I,IQ1) + 31
      I2(I) = IY(I,IQ2)
   15 NCO(I) = I
      DO 20 I=1,NOAT
      IT2=I2(I)
      IN=I
      DO 21 J=I,NOAT
      IF(IT2.GE.I2(J))  GO TO 21
      IT2=I2(J)
      IN=J
   21 CONTINUE
      I2(IN)=I2(I)
      IT1=I1(IN)
      IN1=NCO(IN)
      I1(IN)=I1(I)
      NCO(IN)=NCO(I)
      I2(I)=IT2
      I1(I)=IT1
      NCO(I)=IN1
   20 CONTINUE
   78 DO 16 I=1,NOAT
      IF(I2(I).GT.31)  GO TO 17
   16 CONTINUE
```

```
      GO TO 18
   17 WRITE(6,611)
  611 FORMAT('-',10X,' THE VALUE OF THE ORDINATE WAS GREATER THAN 31, TH
     1E PROGRAM WILL SKIP THIS PROJECTION'/)
      GO TO 210
   18 II = 1
      WRITE(6,600)
  600 FORMAT('1')
      IJQ = 31
      IF(I2(1).EQ.31) I2(1) = 30
      DO 25 I=1,30
      WRITE(6,617)
  617 FORMAT(' ')
      IJQ = IJQ - 1
      IFLAG=0
      IF(I2(II).EQ.IJQ)  GO TO 30
  601 FORMAT('+',65X,'I')
      GO TO 24
   30 K = NCO(II)/10 + 1
      IF(K.EQ.1) K=11
      KK = MOD(NCO(II),10) + 1
      JI = 2*(I1(II) - 1) -1
      IF(JI.EQ.59)  IFLAG=1
      WRITE(6,606) (A(M1),M1=1,JI),M(K),M(KK)
  205 CONTINUE
      IG = 1
      IP = II
      II = II + 1
      IF(I2(IP).EQ.I2(II))  GO TO 30
      IF(IFLAG.NE.1)  GO TO 24
      GO TO 25
   24 WRITE(6,601)
   25 CONTINUE
      WRITE(6,604)
      IF(I2(II).EQ.0)  GO TO 35
  604 FORMAT(6X,60('-'),'+',60('-'))
      GO TO 80
   35 K = NCO(II)/10 + 1
      IF(K.EQ.1) K=11
      KK = MOD(NCO(II),10) + 1
      JI = 2*(I1(II)-1) -1
      WRITE(6,606) (A(M1),M1=1,JI),M(K),M(KK)
  606 FORMAT('+',5X,121A1)
   45 CONTINUE
      IP = II
      IG1 = IG
      II = II + 1
      IF(I2(II).EQ.I2(IP))  IG = IG + 1
      IF(IG1.EQ.IG)  GO TO 80
      GO TO 35
   80 DO 50 I=1,29
      WRITE(6,617)
      IF(II.GT.NOAT)  GO TO 49
```

```
      IFLAG=0
      IF(IABS(I2(II)).EQ.I)  GO TO 55
      GO TO 49
   55 K = NCO(II)/10 + 1
      IF(K.EQ.1) K=11
      KK = MOD(NCO(II),10) + 1
      JI=(I1(II) - 1)*2 -1
      IF(JI.EQ.59)  IFLAG=1
      WRITE(6,606) (A(M1),M1=1,JI),M(K),M(KK)
   65 CONTINUE
      IP = II
      II=II+1
      IF(II.GT.NOAT)  GO TO 48
      IF(I2(II).EQ.I2(IP))  GO TO 55
   48 IF(IFLAG.NE.1)  GO TO 49
      GO TO 50
   49 WRITE(6,601)
   50 CONTINUE
  210 CONTINUE
      RETURN
      END
```

2. GMATRIX

There are several changes on the control card for this program. A sample control card in the new format follows. A value of 1 activates a given option, while a value of 0 bypasses it.

Card Column Field	Values	Options
1-3	-09	problem indicator
4-9	NOP	problem number
10-13	NOAT	number of atoms
14-17	NINT	number of internal coordinates
18-21	1	pass data on disk to program UBZM
22-25	1	isotopic molecules will follow
26-29	1	punch B matrix
30-33	1	punch unsymmetrized G matrix
34-37	1	punch symmetrized G matrix
38-41	0	read U matrix from cards
	1	read U matrix from previous molecule
42-45	1	write symmetrized G matrix on disk
46-49	1	read Cartesian coordinates from disk
	0	read Cartesian coordinates from cards

```
      DIMENSION  GMAT(50,50)
      DIMENSION NR(875),NC(875)
      DIMENSION B(875),NRG(950)
      DIMENSION NCG(950),DG(950)
      DIMENSION NRU(625),NCU(625)
      DIMENSION DU(625),X(3,50)
      DIMENSION WT(50),W(150)
      DIMENSION BB(150),G(150)
      DIMENSION GU(150),NRS(250)
      DIMENSION NCS(250),GS(250)
      DIMENSION NROW(4),NCOL(4)
      DIMENSION DAT(4),NE(4)
      DIMENSION NCOD(4),NI(4)
      DIMENSION NJ(4),NK(4)
      DIMENSION NL(4),NX(4)
      DIMENSION NY(4),RECORD(40)
      DIMENSION REC(14),NB(20)
      DIMENSION U(150),UG(150)
      DIMENSION DA(150)
      DIMENSION DIV(200)
      DIMENSION NSBW1(10)
      COMMON NRG,NRU,NCG,NCU,DG,DU,IND,NOPROB,NOAT,NQ,INTC,NISO
      COMMON IFB,NOINT,NU2,N1,N2,N3,N4,N5,N6,MX,JOKER,NOB,NA
      EQUIVALENCE (X(1),NRG(1)),(NCG(1),WT(1)),(NRG(701),NR(1)),(NCG(
     1701),NC(1)),(DG(701),B(1)),(G(1),DA(1),U(1),UG(1)),(GU(1),BB(
     11))
      REWIND 8
      REWIND 11
   90 READ(5,10)IND
   10 FORMAT (I3)
   91 IF (9+IND)90,92,900
   92 READ(5,12) IND,NOPROB,NOAT,NC,INTC,NISO,IFB,IND1,IND2,IND3,NSBW,
     1 IND4
   12 FORMAT(I3,I6,10I4)
   13 READ(5,14)(RECORD(I),I=1,40)
   14 FORMAT(20A4)
      NA=3*NOAT
      WRITE(6,50) NOPROB,NOAT,NC,(RECORD(I),I=1,40)
   50 FORMAT (19H1  G MATRIX PROBLEM17,7H. NOAT=I4,I6,22H INTERNAL COORD
     1INATES./(1X,20A4))
      JOKER=0
      DO 102 I=1,3
      DO 102 J=1,NOAT
  102 X(I,J)=0.0
      IF(IND4.GT.0)  GO TO 106
  104 READ(5,16)(NROW(L),NCOL(L),DAT(L),L=1,4)
   16 FORMAT (4(2I3,F12.6))
      IF(INTC.EQ.0)  GO TO 107
      WRITE(11)  (NROW(L),NCOL(L),DAT(L),L=1,4)
      GO TO 107
  106 READ(11) (NROW(L),NCOL(L),DAT(L),L=1,4)
  107 DO 110 L=1,4
      IF (NROW(L))112,110,105
```

```
  105 I=NROW(L)
      J=NCOL(L)
      X(I,J)=DAT(L)
  110 CONTINUE
      IF(IND4.GT.0)  GO TO 106
      GO TO 104
  112 IF (1+NROW(L))600,115,600
  115 NOB=0
      WRITE(6,1271)
 1271 FORMAT(//,'     THE CARTESIAN COORDINATES ARE     X          Y
     1      Z',/)
      DO 1272 J=1,NOAT
 1272 WRITE(6,1273) (X(I,J),I=1,3)
 1273 FORMAT(37X,F8.5,3X,F8.5,3X,F8.5)
      NOINT=0
      WRITE(6,51)
   51 FORMAT (34HO  INTERNAL COORDINATE DEFINITIONS/41HO  NO.  CODE   I
     1   J    K    L   IX   JX)
  116 READ(5,18)(NE(L),NCOD(L),NI(L),NJ(L),NK(L),NL(L),NX(L),NY(L),L=1,
     13)
   18 FORMAT (24I3)
  120 DO 180 L=1,3
      IF (NE(L))182,122,124
  122 IF(NCOD(L))180,180,9001
 9001 DIV(NOINT)=DIV(NCINT)+1.0
      GO TO 125
  124 NOINT=NCINT+1
      DIV(NOINT)=1.0
  125 IF (6-NCOD(L))605,126,126
  126 MX=NCOD(L)
      N1=NI(L)
      N2=NJ(L)
      N3=NK(L)
      N4=NL(L)
      N5=NX(L)
      N6=NY(L)
      WRITE(6,53)NOINT,MX,N1,N2,N3,N4,N5,N6
   53 FORMAT (2I5,I6,5I5)
      GO TO (130,140,150,160,170,172),MX
  130 CALL BOST
      GO TO 174
  140 CALL BEND
      GO TO 174
  150 CALL OPLA
      GO TO 174
  160 CALL TORS
      GO TO 174
  170 NC2=NOINT+1
      CALL LIBE
      NOINT=NOINT+1
      GO TO 174
  172 CALL LIBE
  174 IF (JOKER)180,180,605
```

```
 180 CONTINUE
     GO TO 118
 182 NIB=NOB+1
     NR(NIB)=-5
     NC(NIB)=0
     B(NIB)=0.0
9005 NT=1
     DO 9006 K=1,NA
9006 BB(K)=0.0
     NOB=0
     DO 9040 K=1,NIB
9008 IF(NR(K)-NT) 9009,9036,9009
9009 DO 9020 JX=1,NA
     IF(ABS(BB(JX))-0.00005) 9020,9020,9010
9010 NCB=NOB+1
     NR(NOB)=NT
     NC(NOB)=JX
     B(NOB)=BB(JX)/DIV(NT)
9020 CONTINUE
     IF(NR(K)) 9042,9042,9022
9022 NT=NT+1
     DO 9034 I=1,NA
9034 BB(I)=0.0
     GO TO 9008
9036 JX=NC(K)
9040 BB(JX)=BB(JX)+B(K)
9042 NIB=NOB+1
     NR(NIB)=-5
     NC(NIB)=0
     B(NIB)=0.0
     IF (IFB)200,195,190
 190 WRITE(6,54)IND,NCB,(RECORD(I),I=1,15)
  54 FORMAT(2H  ,I3,5H NOB=I4,15A4)
 192 WRITE(7,56)(NR(K),NC(K),B(K),K=1,NIB)
  56 FORMAT (4(2I3,F12.6))
     GO TO 196
 195 WRITE(6,55)NCB,(RECORD(I),I=1,15)
  55 FORMAT(6H0 NOB=I4,15A4)
 196 WRITE(6,57)(NR(K),NC(K),B(K),K=1,NCB)
  57 FORMAT (4(2I4,F11.6))
 200 IF(NISO)210,210,202
 202 REWIND 8
     NK4 = 1
     NK8 = 4
 208 WRITE(8)  (NR(K),NC(K),B(K),K=NK4,NK8)
     DO 209 I=NK4,NK8
     IF(NR(I).LT.0)  GO TO 210
 209 CONTINUE
     NK4 = NK4 + 4
     NK8 = NK8 + 4
     GO TO 208
 210 READ(5,10)IND
     IF (IND+6)91,212,91
```

```
212 READ(5,20) IND,IFU,NSB,NS,(REC(I),I=1,14)
 20 FORMAT(4I3,14A4)
    READ(5,22)(WT(L),L=1,NOAT)
 22 FORMAT (6F12.6)
    WRITE(6,67)(REC(I),I=1,14),(WT(J),J=1,NOAT)
 67 FORMAT (17H1 UNSYMMETRIZED G,14A4/11H FOR MASSES/(6F12.6))
    NG=0
    NT=1
    NUB=1
    DO 216 L=1,NOAT
    DO 216 M=1,3
    K=3*(L-1)+M
    W(K)=1.0/WT(L)
216 BB(K)=0.0
    DO 218 I=1,NQ
218 G(I)=0.0
    IF(NISO)220,220,219
219 REWIND 8
    NK4 = 1
    NK8 = 4
223 READ(8) (NR(K),NC(K),B(K),K=NK4,NK8)
    DO 224 I=NK4,NK8
    IF(NR(I).LT.0)  GO TO 220
224 CONTINUE
    NK4 = NK4 + 4
    NK8 = NK8 + 4
    GO TO 223
220 DO 250 K=1,NIB
221 IF (NR(K)-NT)222,240,222
222 DO 226 L=NUB,NOB
    I=NR(L)
    J=NC(L)
226 G(I)=G(I)+BB(J)*W(J)*B(L)
    DO 232 I=NT,NQ
    IF (ABS(G(I))-0.00005)232,232,229
229 NG=NG+1
    NRG(NG)=NT
    NCG(NG)=I
    DG(NG)=G(I)
232 CONTINUE
    IF (NR(K))252,252,234
234 NT=NT+1
    NUB=K
    DO 238 I=NT,NQ
238 G(I)=0.0
    DO 239 I=1,NA
239 BB(I)=0.0
    GO TO 221
240 JX=NC(K)
250 BB(JX)=BB(JX)+B(K)
252 NOG=NG+1
    NRG(NOG)=-1
    NCG(NOG)=0
```

```
      DC(NOG)=0.0
      IF(IND1.GT.0) GO TO 256
      IF(IFU)253,256,253
  253 IF(IFB) 260,258,256
  256 WRITE(7,56) (NRG(L),NCG(L),DG(L),L=1,NOG)
  258 WRITE(6,59)NG,(REC(I),I=1,14)
   59 FORMAT(6HO NOG=I4,14A4)
      WRITE(6,57)(NRG(L),NCG(L),DG(L),L=1,NG)
  260 IF (IFU)261,210,263
  261 REWIND 9
      NK4 = 1
      NK8 = 4
  262 READ(9)  (NRU(K),NCU(K),DU(K),K=NK4,NK8)
      DO 269 I=NK4,NK8
      IF(NRU(I).LT.0)  GO TO 282
  269 CONTINUE
      NK4 = NK4 + 4
      NK8 = NK8 + 4
      GO TO 262
  263 NOU=0
      JX=1
      DSQ=0.0
      WRITE(6,1264)
 1264 FORMAT(//,'    THE INPUT U-MATRIX  NOT NORMALIZED IS    ROW     CO
     1L     ELEMENT',/)
  264 IF(IND3.GT.0)  GO TO 5264
      READ(5,16)  (NROW(L),NCOL(L),DAT(L),L=1,4)
      GO TO 5266
 5264 READ(8) (NROW(L),NCOL(L),DAT(L),L=1,4)
      GO TO 5267
 5266 WRITE(8) (NROW(L),NCOL(L),DAT(L),L=1,4)
 5267 WRITE(16)  (NROW(L),NCOL(L),DAT(L),L=1,4)
      DO 1265 L=1,4
 1265 WRITE(6,1266) NROW(L),NCOL(L),DAT(L)
 1266 FORMAT(45X,I2,6X,I2,7X,F4.1)
      DO 274 L=1,4
      IF (NROW(L))276,274,266
  266 IF (NS-NROW(L))615,267,267
  267 IF (NROW(L)-JX)615,270,268
  268 DA(JX)=1.0/SQRT(DSQ)
      JX=JX+1
      DSQ=0.0
      GO TO 267
  270 DSQ=DSQ+DAT(L)**2
      NCU=NOU+1
      NRU(NOU)=NROW(L)
      NCU(NOU)=NCOL(L)
      DU(NOU)=DAT(L)
  274 CONTINUE
      GO TO 264
  276 IF (3+NROW(L))615,277,615
  277 DA(JX)=1.0/SQRT(DSQ)
      IF (NS-JX)615,278,615
```

```
278 DO 279 I=1,NOU
    J=NRU(I)
279 DU(I)=DA(J)*DU(I)
    NCU=NOU+1
    NRU(NOU)=-3
    NCU(NOU)=0
    DU(NOU)=0.0
    REWIND 8
    IF(NISO)282,282,280
280 REWIND 9
    NK4 = 1
    NK8 = 4
283 WRITE(9) (NRU(K),NCU(K),DU(K),K=NK4,NK8)
    DO 284 I=NK4,NK8
    IF(NRU(I).LT.0) GO TO 282
284 CONTINUE
    NK4 = NK4 + 4
    NK8 = NK8 + 4
    GO TO 283
282 READ(5,18)(NB(I),I=1,NSB)
    IF(NSBW.EQ.0)  GO TO 291
    READ(5,18)  (NSBW1(I),I=1,NSB)
291 CONTINUE
    NU=NOU-1
    JL=1
    JX=2
    NUT=1
    NUB=1
    IX=1
    IQ1=1
    IJQ=1
290 WRITE(6,60)IND,JL,(REC(I),I=1,14)
 60 FORMAT(2HW0,I3,12H SYM.G.BLOCK[3,14A4)
    NP=NB(JL)
    NT=NB(JX)
    NEL=0
300 DO 302 I=1,NQ
    GU(I)=0.0
302 U(I)=0.0
303 DO 320 K=NUB,NOU
    IF (NRU(K)-IX)306,315,306
306 DO 312 L=1,NG
    I=NRG(L)
    J=NCG(L)
309 GU(I)=GU(I)+U(J)*DG(L)
    IF (I-J)310,312,310
310 GU(J)=GU(J)+U(I)*DG(L)
312 CONTINUE
    GO TO 322
315 JU=NCU(K)
    U(JU)=DU(K)
320 CONTINUE
322 NUB=K
```

```
      DO 324 I=IX,NS
  324 UG(I)=0.0
      ASSIGN 330 TO JAK
      DO 335 L=NUT,NU
      GO TO JAK,(330,332)
  330 IF (NRU(L)-IX)331,332,331
  331 ASSIGN 332 TO JAK
      NWY=L
  332 I=NRU(L)
      J=NCU(L)
      UG(I)=UG(I)+DU(L)*GU(J)
  335 CONTINUE
      NUT=NWY
      DO 350 J=IX,NS
      IF (0.00005-ABS(UG(J)))342,350,350
  342 IF (NT-J)343,343,344
  343 WRITE(6,72)IX,J
   72 FORMAT (40H0 ERROR,ERROR,ERROR- G NOT FACTORING.ROW I4,7H COLUMN I4)
  344 NEL=NEL+1
      IF (101-NEL)345,345,347
  345 WRITE(6,56)(NRS(I),NCS(I),GS(I),I=1,100)
      NEL=1
  347 NRS(NEL)=IX-NP+1
      NCS(NEL)=J-NP+1
      GS(NEL)=UG(J)
  350 CONTINUE
      IX=IX+1
      IF (NT-IX)354,354,300
  354 NEL=NEL+1
      NRS(NEL)=-1
      NCS(NEL)=0
      GS(NEL)=0.0
  356 WRITE(6,56)(NRS(I),NCS(I),GS(I),I=1,NEL)
      DO 1115 I=1,NQ
      DO 1115J=1,NQ
 1115 GMAT(I,J)=0.0
      NEL1=NEL-1
      DO 1111 I=1,NEL1
      GMAT(NCS(I),NRS(I))=GS(I)
 1111 GMAT(NRS(I),NCS(I))=GS(I)
      NN=NT-NP
      WRITE(6,1114)
 1114 FORMAT (//,'    THE G SYMMETRY BLOCK IS',/)
      DO 1112 I=1,NN
 1112 WRITE(6,1113) (GMAT(I,J),J=1,NN)
 1113 FORMAT (14F9.5)
      IF(NSBW.EQ.0)  GO TO 1132
      IF(IQ1.EQ.NSBW1(IJQ))  GO TO 1131
      GO TO  1132
 1131 WRITE(10)        ((GMAT(I,J),J=1,NN),I=1,NN)
 1132 IF(IND2.GT.0)  GO TO 1124
      GO TO 1125
 1124 WRITE(7,1123) ((GMAT(I,J),J=1,NN),I=1,NN)
```

```
1123 FORMAT(8F10.7)
1125 JL=JL+1
     JX=JX+1
     IQ1=IQ1+1
     IJQ=IJQ+1
 300 IF (NSB-JX)210,290,290
 600 WRITE(6,80)NOPROB,L,NROW(L),NCOL(L),DAT(L)
  80 FORMAT (24HO X MATRIX ERROR PROBLEMI7,6H FIELDI3,6H READS2I4,F12.6
    1)
     GO TO 90
 605 WRITE(6,82)L,NE(L),NCOD(L),NI(L),NJ(L),NK(L),NL(L),NX(L),NY(L),
    1JOKER
  82 FORMAT (33HO INTERNAL COORDINATE ERROR.FIELDI3,6H READS8I4,8H JOKE
    1R =I3)
     GO TO 90
 615 WRITE(6,84)NOPROB,L,NROW(L),NCOL(L),DAT(L)
  84 FORMAT (24HO U MATRIX ERROR PROBLEMI7,6H FIELDI3,6H READS2I4,F12.6
    1)
     GO TO 90
 900 CALL EXIT
     END
```

```
      SUBROUTINE BOST
      DIMENSION NR(875),NC(875)
      DIMENSION B(875),NRG(950)
      DIMENSION NCG(950),DG(950)
      DIMENSION NRU(625),NCU(625)
      DIMENSION DU(625),X(3,50)
      DIMENSION WT(50),RIJ(3)
      COMMON NRG,NRU,NCG,NCU,DG,DU,IND,NOPROB,NOAT,NQ,INTC,NISO
      COMMON IFB,NOINT,NO2,N1,N2,N3,N4,N5,N6,MX,JOKER,NOB,NA
      EQUIVALENCE (NRG(1),X(1)),(NCG(1),WT(1)),(NR(1),NRG(701)),(NCG(
     1701),NC(1)),(B(1),DG(701))
  100 IF (N6)130,101,130
  101 IF (N5)130,102,130
  102 IF (N4)130,103,130
  103 IF (N3)130,104,130
  104 IF (NOAT-N2)130,105,105
  105 IF (NOAT-N1)130,106,106
  106 I=N1
      J=N2
      DIJSQ=0.0
  109 DO 112 M=1,3
      RIJ(M)=X(M,J)-X(M,I)
  112 DIJSQ=DIJSQ+RIJ(M)*RIJ(M)
  114 DO 120 M=1,3
      IF (ABS(RIJ(M))-0.00005)120,120,115
  115 NOB=NOB+1
      NR(NOB)=NCINT
      NC(NOB)=3*(I-1)+M
      B(NOB)=-RIJ(M)/SQRT(DIJSQ)
      NOB=NOB+1
      NR(NOB)=NCINT
      NC(NOB)=3*(J-1)+M
      B(NOB)=RIJ(M)/SQRT(DIJSQ)
  120 CONTINUE
      GO TO 132
  130 JOKER=1
  132 RETURN
      END
      SUBROUTINE BEND
      DIMENSION NR(875),NC(875)
      DIMENSION B(875),NRG(950)
      DIMENSION NCG(950),DG(950)
      DIMENSION NRU(625),NCU(625)
      DIMENSION DU(625),X(3,50)
      DIMENSION RJI(3),RJK(3)
      DIMENSION RIXJX(3),EJI(3)
      DIMENSION EJK(3),WT(50)
      COMMON NRG,NRU,NCG,NCU,DG,DU,IND,NOPROB,NOAT,NQ,INTC,NISO
      COMMON IFB,NOINT,NO2,N1,N2,N3,N4,N5,N6,MX,JOKER,NOB,NA
      EQUIVALENCE (NRG(1),X(1)),(NCG(1),WT(1)),(NR(1),NRG(701)),(NCG(
     1701),NC(1)),(B(1),DG(701))
  100 IF (NOAT-N6)150,101,101
  101 IF (NOAT-N5)150,102,102
```

```
102 IF (N4)150,103,150
103 IF (NOAT-N3)150,104,104
104 IF (NOAT-N2)150,105,105
105 IF (NOAT-N1)150,106,106
106 I=N1
107 J=N2
    K=N3
    IX=N5
    JX=N6
    IF (IX)110,110,112
110 IX=1
    JX=1
112 DJISQ=0.0
    DJKSQ=0.0
    DXSQ=0.0
115 DO 122 M=1,3
    RJI(M)=X(M,I)-X(M,J)
    RJK(M)=X(M,K)-X(M,J)
    RIXJX(M)=X(M,JX)-X(M,IX)
    DJISQ=DJISQ+RJI(M)*RJI(M)
    DJKSQ=DJKSQ+RJK(M)*RJK(M)
122 DXSQ=DXSQ+RIXJX(M)*RIXJX(M)
123 DJI=SQRT(DJISQ)
    DJK=SQRT(DJKSQ)
    DX=SQRT(DXSQ)
    IF (DX)128,127,128
127 DX=1.0
128 DOTJ=0.0
129 DO 132 M=1,3
    EJI(M)=RJI(M)/DJI
    EJK(M)=RJK(M)/DJK
132 DOTJ=DOTJ+EJI(M)*EJK(M)
    IF (1.0-ABS(DOTJ))152,152,134
134 SINJ=SQRT(1.0-DOTJ*DOTJ)
136 DO 144 M=1,3
    SMI=(DX*(DOTJ*EJI(M)-EJK(M)))/(DJI*SINJ)
    IF (ABS(SMI)-0.00005)138,138,137
137 NCB=NOB+1
    NR(NOB)=NOINT
    NC(NOB)=3*(I-1)+M
    B(NOB)=SMI
138 SMK=(DX*(DOTJ*EJK(M)-EJI(M)))/(DJK*SINJ)
    IF (ABS(SMK)-0.00005)140,140,139
139 NCB=NOB+1
    NR(NOB)=NOINT
    NC(NOB)=3*(K-1)+M
    B(NOB)=SMK
140 SUM=SMI+SMK
    IF (ABS(SUM)-0.00005)144,144,142
142 NCB=NOB+1
    NR(NOB)=NOINT
    NC(NOB)=3*(J-1)+M
    B(NOB)=-SUM
```

```
144 CONTINUE
    GO TO 154
150 JOKER=1
    GO TO 154
152 JOKER=2
154 RETURN
    END
    SUBROUTINE OPLA
    DIMENSION NR(875),NC(875)
    DIMENSION B(875),NRG(950)
    DIMENSION NCG(950),DG(950)
    DIMENSION NRU(625),NCU(625)
    DIMENSION DU(625),X(3,50)
    DIMENSION EJK(3),WT(50)
    DIMENSION RJI(3),RJK(3)
    DIMENSION RIXJX(3),EJI(3)
    DIMENSION EJL(3),C1(3)
    DIMENSION C2(3),C3(3)
    DIMENSION RJL(3)
    COMMON NRG,NRU,NCG,NCU,DG,DU,IND,NOPROB,NOAT,NQ,INTC,NISO
    COMMON IFB,NOINT,NO2,N1,N2,N3,N4,N5,N6,MX,JOKER,NOB
    EQUIVALENCE (NRG(1),X(1)),(NCG(1),WT(1)),(NR(1),NRG(701)),(NCG(
   1701),NC(1)),(B(1),DG(701))
100 IF (NOAT-N6)170,101,101
101 IF (NOAT-N5)170,102,102
102 IF (NOAT-N4)170,103,103
103 IF (NOAT-N3)170,104,104
104 IF (NOAT-N2)170,105,105
105 IF (NOAT-N1)170,106,106
106 I=N1
    J=N2
    K=N3
    L=N4
    IX=N5
    JX=N6
    IF (IX)110,110,112
110 IX=1
    JX=1
112 DJISQ=0.0
    DJKSQ=0.0
    DJLSQ=0.0
115 DXSQ=0.0
116 DO 124 M=1,3
    RJI(M)=X(M,I)-X(M,J)
    DJISQ=DJISQ+RJI(M)*RJI(M)
    RJK(M)=X(M,K)-X(M,J)
    DJKSQ=DJKSQ+RJK(M)*RJK(M)
    RJL(M)=X(M,L)-X(M,J)
    DJLSQ=DJLSQ+RJL(M)*RJL(M)
    RIXJX(M)=X(M,JX)-X(M,IX)
124 DXSQ=DXSQ+RIXJX(M)*RIXJX(M)
126 DJI=SQRT(DJISQ)
    DJK=SQRT(DJKSQ)
```

```
      DJL=SQRT(DJLSQ)
      DX=SQRT(DXSQ)
  130 IF (DX)132,131,132
  131 DX=1.0
  132 DO 136 M=1,3
      EJI(M)=RJI(M)/DJI
      EJK(M)=RJK(M)/DJK
  136 EJL(M)=RJL(M)/DJL
  137 C1(1)=EJK(2)*EJL(3)-EJK(3)*EJL(2)
      C1(2)=EJK(3)*EJL(1)-EJK(1)*EJL(3)
      C1(3)=EJK(1)*EJL(2)-EJK(2)*EJL(1)
      C2(1)=EJL(2)*EJI(3)-EJL(3)*EJI(2)
      C2(2)=EJL(3)*EJI(1)-EJL(1)*EJI(3)
      C2(3)=EJL(1)*EJI(2)-EJL(2)*EJI(1)
      C3(1)=EJI(2)*EJK(3)-EJI(3)*EJK(2)
      C3(2)=EJI(3)*EJK(1)-EJI(1)*EJK(3)
  139 C3(3)=EJI(1)*EJK(2)-EJI(2)*EJK(1)
  140 DET=EJI(1)*C1(1)+EJI(2)*C1(2)+EJI(3)*C1(3)
      DOTI=0.0
  142 DO 143 M=1,3
  143 DOTI=DOTI+EJK(M)*EJL(M)
  144 IF (1.0-ABS(DOTI))172,172,146
  146 SINI=SQRT(1.0-DOTI*DOTI)
  147 SINT=DET/SINI
  148 IF (1.0-ABS(SINT))174,174,149
  149 COST=SQRT(1.0-SINT*SINT)
  150 TANT=SINT/COST
  155 DO 168 M=1,3
  157 SMI=((C1(M)/(COST*SINI))-(TANT*EJI(M)))/DJI
      IF (ABS(SMI)-0.00005)160,160,158
  158 NOB=NOB+1
      NR(NOB)=NOINT
      NC(NOB)=3*(I-1)+M
      B(NOB)=DX*SMI
  160 SMK=((C2(M)/(COST*SINI))-((TANT*(EJK(M)-DOTI*EJL(M)))/(SINI*SINI))
     *1)/DJK
      IF (ABS(SMK)-0.00005)163,163,161
  161 NOB=NOB+1
      NR(NOB)=NCINT
      NC(NOB)=3*(K-1)+M
      B(NOB)=DX*SMK
  163 SML=((C3(M)/(COST*SINI))-((TANT*(EJL(M)-DOTI*EJK(M)))/(SINI*SINI))
     1)/DJL
      IF (ABS(SML)-0.00005)166,166,164
  164 NOB=NOB+1
      NR(NOB)=NOINT
      NC(NOB)=3*(L-1)+M
      B(NOB)=DX*SML
  166 SUM=SMI+SMK+SML
      IF (ABS(SUM)-0.00005)168,168,167
  167 NOB=NOB+1
      NR(NOB)=NOINT
      NC(NOB)=3*(J-1)+M
```

```
      B(NOB)=-DX*SUM
  100 CONTINUE
      GO TO 178
  170 JOKER=1
      GO TO 178
  172 JOKER=2
      GO TO 178
  174 JOKER=3
  178 RETURN
      END
      SUBROUTINE TORS
      DIMENSION NR(875),NC(875)
      DIMENSION B(875),NRG(950)
      DIMENSION NCG(950),DG(950)
      DIMENSION NRU(625),NCU(625)
      DIMENSION DU(625),X(3,50)
      DIMENSION EJK(3),WT(50)
      DIMENSION RIJ(3),RJK(3)
      DIMENSION RKL(3),RIXJX(3)
      DIMENSION EKL(3),CR1(3)
      DIMENSION CR2(3),EIJ(3)
      COMMON NRG,NRU,NCG,NCU,DG,DU,IND,NOPROB,NOAT,NQ,INTC,NISO
      COMMON IFB,NOINT,NO2,N1,N2,N3,N4,N5,N6,MX,JOKER,NOB,NA
      EQUIVALENCE (NRG(1),X(1)),(NCG(1),WT(1)),(NR(1),NRG(701)),(NCG(
     1701),NC(1)),(B(1),DG(701))
  100 IF (NOAT-N6)180,101,101
  101 IF (NOAT-N6)180,102,102
  102 IF (NOAT-N4)180,103,103
  103 IF (NOAT-N3)180,104,104
  104 IF (NOAT-N2)180,105,105
  105 IF (NOAT-N1)180,106,106
  106 I=N1
      J=N2
      K=N3
      L=N4
      IX=N5
      JX=N6
      IF (IX)110,110,112
  110 IX=1
      JX=1
  112 DIJSQ=0.0
      DJKSQ=0.0
      DKLSQ=0.0
  115 DXSQ=0.0
  116 DO 124 M=1,3
      RIJ(M)=X(M,J)-X(M,I)
      DIJSQ=DIJSQ+RIJ(M)*RIJ(M)
      RJK(M)=X(M,K)-X(M,J)
      DJKSQ=DJKSQ+RJK(M)*RJK(M)
      RKL(M)=X(M,L)-X(M,K)
      DKLSQ=DKLSQ+RKL(M)*RKL(M)
      RIXJX(M)=X(M,JX)-X(M,IX)
  124 DXSQ=DXSQ+RIXJX(M)*RIXJX(M)
```

```
      DIJ=SQRT(DIJSQ)
      DJK=SQRT(DJKSQ)
      DKL=SQRT(DKLSQ)
      DX=SQRT(DXSQ)
  130 IF (DX)132,131,132
  131 DX=1.0
  132 DO 136 M=1,3
      EIJ(M)=RIJ(M)/DIJ
      EJK(M)=RJK(M)/DJK
  136 EKL(M)=RKL(M)/DKL
  138 CR1(1)=EIJ(2)*EJK(3)-EIJ(3)*EJK(2)
      CR1(2)=EIJ(3)*EJK(1)-EIJ(1)*EJK(3)
      CR1(3)=EIJ(1)*EJK(2)-EIJ(2)*EJK(1)
      CR2(1)=EJK(2)*EKL(3)-EJK(3)*EKL(2)
      CR2(2)=EJK(3)*EKL(1)-EJK(1)*EKL(3)
  142 CR2(3)=EJK(1)*EKL(2)-EJK(2)*EKL(1)
  143 DOTPJ=0.0
      DOTPK=0.0
  145 DO 147 M=1,3
      DOTPJ=DOTPJ-EIJ(M)*EJK(M)
  147 DOTPK=DOTPK-EJK(M)*EKL(M)
  148 IF (1.0-ABS(DOTPJ))182,182,149
  149 IF (1.0-ABS(DOTPK))182,182,150
  150 SINPJ=SQRT(1.0-DOTPJ*DOTPJ)
      SINPK=SQRT(1.0-DOTPK*DOTPK)
  152 DO 164 M=1,3
      SMI=-CR1(M)/(DIJ*SINPJ*SINPJ)
      IF (ABS(SMI)-0.00005)156,156,154
  154 NOB=NOB+1
      NR(NOB)=NOINT
      NC(NOB)=3*(I-1)+M
      B(NOB)=DX*SMI
  156 F1=(CR1(M)*(DJK-DIJ*DOTPJ))/(DJK*DIJ*SINPJ*SINPJ)
      F2=(DOTPK*CR2(M))/(DJK*SINPK*SINPK)
      SMJ=F1-F2
      IF (ABS(SMJ)-0.00005)158,158,157
  157 NOB=NOB+1
      NR(NOB)=NOINT
      NC(NOB)=3*(J-1)+M
      B(NOB)=DX*SMJ
  158 SML=CR2(M)/(DKL*SINPK*SINPK)
      IF (ABS(SML)-0.00005)160,160,159
  159 NOB=NOB+1
      NR(NOB)=NOINT
      NC(NOB)=3*(L-1)+M
      B(NOB)=DX*SML
  160 SUM=SMI+SMJ+SML
      IF (ABS(SUM)-0.00005)164,164,162
  162 NOB=NOB+1
      NR(NOB)=NOINT
      NC(NOB)=3*(K-1)+M
      B(NOB)=-DX*SUM
  164 CONTINUE
```

```
      GO TO 186
  180 JOKER=1
      GO TO 186
  182 JOKER=2
  186 RETURN
      END
      SUBROUTINE LIBE
      DIMENSION NR(875),NC(875)
      DIMENSION B(875),NRG(950)
      DIMENSION NCG(950),DG(950)
      DIMENSION NRU(625),NCU(625)
      DIMENSION DU(625),X(3,50)
      DIMENSION EJK(3),WT(50)
      DIMENSION RJI(3),RJK(3)
      DIMENSION A(3),RIXJX(3)
      DIMENSION UN(3),UNIT(3)
      DIMENSION UP(3),EJI(3)
      COMMON NRG,NRU,NCG,NCU,DG,DU,INC,NOPROB,NOAT,NQ,INTC,NISO
      COMMON IFB,NOINT,NC2,N1,N2,N3,N4,N5,N6,MX,JOKER,NOB,NA
      EQUIVALENCE (NRG(1),X(1)),(NCG(1),WT(1)),(NR(1),NRG(701)),(NCG(
     1701),NC(1)),(B(1),DG(701))
      JSTOP=0
  100 IF (NOAT-N6)160,101,101
  101 IF (NOAT-N5)160,102,102
  102 IF (NOAT-N4)160,103,103
  103 IF (NOAT-N3)160,104,104
  104 IF (NOAT-N2)160,105,105
  105 READ(5,24) (A(I),I=1,3)
   24 FORMAT (3F12.6)
      IF (N4)160,109,108
  108 I=N2
      J=N3
      K=N4
      JSTOP=1
      GO TO 110
  109 I=N1
      J=N2
      K=N3
  110 IX=N5
      JX=N6
      IF (IX)111,111,112
  111 IX=1
      JX=1
  112 DJISQ=0.0
      DJKSQ=0.0
      DXSQ=0.0
  116 DAJSQ=0.0
  117 DO 124 M=1,3
      RJI(M)=X(M,I)-X(M,J)
      DJISQ=DJISQ+RJI(M)*RJI(M)
      RJK(M)=X(M,K)-X(M,J)
      DJKSQ=DJKSQ+RJK(M)*RJK(M)
      RIXJX(M)=X(M,JX)-X(M,IX)
```

```
      DXSQ=DXSQ+RIXJX(M)*RIXJX(M)
      UN(M)=A(M)-X(M,J)
  124 DAJSQ=DAJSQ+UN(M)*UN(M)
  126 DJI=SQRT(DJISQ)
      DJK=SQRT(DJKSQ)
      DX=SQRT(DXSQ)
      DAJ=SQRT(DAJSQ)
  130 IF (DX)132,131,132
  131 DX=1.0
  132 DOTJ=0.0
      DOTP=0.0
  134 DO 140 M=1,3
      EJI(M)=RJI(M)/DJI
      EJK(M)=RJK(M)/DJK
      UNIT(M)=UN(M)/DAJ
      DOTJ=DOTJ+EJI(M)*EJK(M)
  140 DOTP=DOTP+EJI(M)*UNIT(M)
      TEST=(ABS(DOTJ)-1.0)
      IF (0.0001-ABS(TEST))162,142,142
  142 IF (0.00005-ABS(DOTP))162,143,143
  143 UP(1)=EJK(2)*UNIT(3)-EJK(3)*UNIT(2)
      UP(2)=EJK(3)*UNIT(1)-EJK(1)*UNIT(3)
      UP(3)=EJK(1)*UNIT(2)-EJK(2)*UNIT(1)
  146 DO 149 M=1,3
      IF (ABS(UNIT(M))-0.00005)149,149,147
  147 NOB=NOB+1
      NR(NOB)=NOINT
      NC(NOB)=3*(I-1)+M
      B(NOB)=-DX*UNIT(M)/DJI
      NOB=NOB+1
      NR(NOB)=NOINT
      NC(NOB)=3*(K-1)+M
      B(NOB)=-DX*UNIT(M)/DJK
      NOB=NOB+1
      NR(NOB)=NCINT
      NC(NOB)=3*(J-1)+M
      B(NOB)=DX*(1.0/DJI+1.0/DJK)*UNIT(M)
  149 CONTINUE
      IF (JSTOP)164,164,150
  150 DO 158 M=1,3
      IF (ABS(UP(M))-0.00005)158,158,151
  151 NOB=NOB+1
      NR(NOB)=NO2
      NC(NOB)=3*(I-1)+M
      B(NOB)=-DX*UP(M)/DJI
      NOB=NOB+1
      NR(NOB)=NO2
      NC(NOB)=3*(K-1)+M
      B(NOB)=-DX*UP(M)/DJK
      NOB=NOB+1
      NR(NOB)=NO2
      NC(NOB)=3*(J-1)+M
      B(NOB)=DX*(1.0/DJI+1.0/DJK)*UP(M)
```

```
158 CONTINUE
    GO TO 164
160 JOKER=1
    GO TO 164
162 JOKER=2
164 RETURN
    END
```

3. UBZM

The modified control card is explained below.

Card Column Field	Values	Options
1-3	-09	problem indicator
4-9	NOP	problem number
10-12	NOAT	number of atoms
13-15	NINT	number of internal coordinates
16-18	NF	number of Urey-Bradley force constants
19-23	NOF	number of non-Urey-Bradley force constants
24-25	1	print gem, tetra, and cis matrices
26-27	NP	number of punched copies of Z matrix
28-29	1	read Cartesian coordinates from disk
	0	read Cartesian coordinates from cards
30-31	1	write Z matrix on disk

In addition, immediately following the literal data card are two sets of cards containing labels, in 8 column fields, for the Urey-Bradley force constants and the internal coordinates respectively.

```
      DIMENSION NC1(2000),NC2(3000)
      DIMENSION NFO(2000),DATINZ(2000)
      DIMENSION NA(5),K000FX(10)
      DIMENSION NFOR(400),NINT(200),R(3)
      DIMENSION N1(400),N2(400)
      DIMENSION NROWX(4),NCOLX(4)
      DIMENSION DATINX(4),RECORD(40)
      DIMENSION D(100,100),X(3,100)
      DIMENSION  UBFCON(100,2),INTCOR(100,2)
      COMMON D,IND,NOPROB,NOAT,NCOR,NF,NOPT,NCOD,NA,K000FX,NFOR
      COMMON NZ,JOKE,INFRA,X
      EQUIVALENCE (D(1),NC1(1)),(D(3001),NC2(1)),(NFO(1),D(6002)),(
     1D(9003),DATINZ(1))
      REWIND 11
   90 READ(5,2)IND
    2 FORMAT (I3)
   91 IF(IND.EQ.-9) GO TO 92
      GO TO 90
   92 READ(5,4)IND,NOPROB,NCAT,NCOR,NF,IFF,NOFF,INFRA,IFTC,INDX,INDZ
    4 FORMAT (I3,I6,3I3,I2,I3,4I2)
   94 IF(IND.EQ.0)  CALL EXIT
  100 READ(5,6) (RECORD(I),I=1,40)
    6 FORMAT(20A4)
  102 WRITE(6,50) NOPROB,(RECORD(I),I=1,40)
   50 FORMAT(22H1 Z MATRIX PROBLEM NO.I8/(12X,20A4))
      READ(5,146) ((UBFCON(I,J),J=1,2),I=1,NF)
      READ(5,146)  ((INTCOR(I,J),J=1,2),I=1,NF)
  146 FORMAT(10(2A4))
  105 DO 107 I=1,3
      DO 107 J=1,NOAT
  107 X(I,J)=0.0
      IF(INDX.EQ.0)  GO TO 110
  111 READ(11) (NROWX(L),NCOLX(L),DATINX(L),L=1,4)
      GO TO 112
  110 READ(5,8)(NROWX(L),NCOLX(L),DATINX(L),L=1,4)
    8 FORMAT (4(2I3,F12.6))
  112 DO 118 L=1,4
      IF (NROWX(L))120,118,114
  114 IF (3-NROWX(L))605,115,115
  115 IF (NOAT-NCOLX(L))605,116,116
  116 I=NROWX(L)
      J=NCOLX(L)
      X(I,J)=DATINX(L)
  118 CONTINUE
      IF(INDX.GT.0)  GO TO 111
      GO TO 110
  120 IF (1+NROWX(L))605,130,605
  130 READ(5,10)(NINT(J),NFOR(J),J=1,NCOR)
   10 FORMAT (24I3)
  132 NZ=0
      WRITE(6,144)
  144 FORMAT(///,'     THE CARTESIAN COORDINATES ARE',/26X,'X',12X,'Y',1
     112X,'Z',//)
```

```
      DO 141 J=1,NOAT
  141 WRITE(6,196)    (X(I,J),I=1,3)
  196 FORMAT(20X,3F12.6)
  140 DO 145 K=1,NCOR
      IF (NCOR-NINT(K))610,142,142
  142 IF (NF-NFOR(K))610,143,143
  143 NZ=NZ+1
      NC1(NZ)=NINT(K)
      NC2(NZ)=NINT(K)
      NFO(NZ)=NFOR(K)
  145 DATINZ(NZ)=1.0
  150 IF (NOFF)170,170,152
  152 READ(5,10)(N1(I),N2(I),NFOR(I),I=1,NOFF)
  160 DO 168 K=1,NOFF
      IF (NCOR-N2(K))610,162,162
  162 IF (N2(K)-N1(K))610,163,163
  163 IF (NF-NFOR(K))610,164,164
  164 NZ=NZ+1
      NC1(NZ)=N1(K)
      NC2(NZ)=N2(K)
      NFO(NZ)=NFOR(K)
  168 DATINZ(NZ)=1.0
  170 JOKE=0
      WRITE(6,147)
  147 FORMAT(///,'  THE UREY-BRADLEY FORCE CONSTANTS AND INTERNAL COORDI
     1NATES ARE'//20X,'U-B FORCE CONSTANTS',20X,'INTERNAL COORDINATES',/
     2)
      DO 148 KK=1,NF
  148 WRITE(6,149) KK,(UBFCON(KK,J),J=1,2),KK,(INTCOR(KK,J),J=1,2)
  149 FORMAT(20X,I2,' ------- ',2A4,20X,I2,' -------- ',2A4)
  172 READ(5,10)NOPT,NCOD,(NA(I),I=1,5),(KOOOFX(J),J=1,10),(NFOR(K),K=1
     1,13)
      WRITE(6,80)NCOD,NOPT,(NA(I),I=1,5)
   80 FORMAT (24H0  SUBCONFIGURATION CODE14,8H, OPTION13/14H  ATOM NUMBE
     1RS/1H 5I4)
      WRITE(6,81)(KOOOFX(J),J=1,10)
   81 FORMAT (29H  INTERNAL COORDINATE NUMBERS/1H 10I4)
      WRITE(6,82)(NFOR(K),K=1,13)
   82 FORMAT (25H  FORCE CONSTANT NUMBERS /1H 13I4)
  174 IF (NOPT)410,410,180
  180 IF (NCOD)615,615,181
  181 IF (4-NCOD)615,182,182
  182 DO 184 I=1,5
      IF (NA(I))615,183,183
  183 IF (NOAT-NA(I))615,184,184
  184 CONTINUE
  186 DO 189 I=1,10
      IF (KOOOFX(I))615,188,188
  188 IF (NCOR-KOOOFX(I))615,189,189
  189 CONTINUE
  190 DO 193 I=1,13
      IF (NFOR(I))615,192,192
  192 IF (NF-NFOR(I))615,193,193
```

```
  193 CONTINUE
  200 MX=NCOD
      GO TO (210,220,230,240),MX
  210 CALL EVGEM
      IF (JOKE)172,172,620
  220 CALL ETETRA
      IF (JOKE)172,172,620
  230 CALL EVCIS
      IF (JOKE)172,172,620
  240 CALL EVCISP
      IF (JOKE)172,172,620
  410 CONTINUE
  400 WRITE(6,53)IND,NOPROB,NZ
   53 FORMAT (1HL13,17H Z MATRIX PROBLEMI8,5H  NZ=I6)
  402 WRITE(6,54)(NC1(I),NC2(I),NFO(I),DATINZ(I),I=1,NZ)
      DO 1001 IK=1,IFTC
 1001 WRITE(7,54)(NC1(I),NC2(I),NFO(I),DATINZ(I),I=1,NZ)
      IF(INDZ.EQ.0)  GO TO 462
      NZ2=NZ+1
      NC1(NZ2)=-6
      NC2(NZ2)=0
      NFO(NZ2)=0
      DATINZ(NZ2)=0
      DO 461 IJ=1,IFTC
      NZ4=1
      NZ8=4
  433 WRITE(17) (NC1(L),NC2(L),NFO(L),DATINZ(L),L=NZ4,NZ8)
      DO 435 L=NZ4,NZ8
      IF(NC1(L).EQ.-6)  GO TO 461
  435 CONTINUE
      NZ4=NZ4+4
      NZ8=NZ8+4
      GO TO 433
   54 FORMAT(4(3I4,F8.5))
   53 FORMAT (2H  2I3,F12.6,2I3,F12.6,2I3,F12.6,2I3,F12.6)
  461 CONTINUE
  462 DO 470 I=1,NOAT
      DO 470 J=1,NOAT
      DSQ=0.0
  466 DO 468 M=1,3
      R(M)=X(M,J)-X(M,I)
  468 DSQ=DSQ+R(M)*R(M)
  470 D(I,J)=SQRT(DSQ)
  471 WRITE(6,60)NOPROB
   60 FORMAT (28H1ATOM DISTANCE CHECK PROBLEMI8)
  472 DO 474 I=1,NOAT
  474 WRITE(6,62)I,(D(I,J),J=1,NOAT)
   62 FORMAT (5HOATOMI3/(1CF12.6))
      GO TO 90
  605 WRITE(6,70)NOPROB
   70 FORMAT (24HO X MATRIX ERROR PROBLEMI8)
      GO TO 90
  610 WRITE(6,72)NOPROB
```

```
 72 FORMAT (38HODIAGONAL FORCE CONSTANT ERROR PROBLEMI8)
    GO TO 90
615 WRITE(6,74)NOPROB,NOPT,NCCC,I
 74 FORMAT (14HOERROR PROBLEMI8,5H NOPTI3,5H CODE I3,3H I=I3)
    GO TO 90
626 WRITE(6,76)NOPROB,NOPT,NCCC,JUKE,(NA(I),I=1,5),(KOOOFX(J),J=1,10)
   1,(NFOR(K),K=1,13)
 76 FORMAT (28HOERROR IN SUBROUTINE PROBLEMI8,5H NOPTI3,5H CODEI3,5H J
   1UKEI3/28I3)
    GO TO 90
900 CALL EXIT
    END
```

```
      SUBROUTINE EVGEM
      DIMENSION NC1(2000),NC2(3000)
      DIMENSION NFO(2000),CATINZ(2000)
      DIMENSION NA(5),KCOCFX(10)
      DIMENSION NFOR(400),RKI(3)
      DIMENSION RKJ(3),EI(3)
      DIMENSION EJ(3),D(100,100)
      DIMENSION X(3,100),GEM(6,2)
      COMMON D,IND,NOPRCB,NOAT,NCOR,NF,NOPT,NCOD,NA,KOOOFX,NFOR
      COMMON NZ,JOKE,INFRA,X
      EQUIVALENCE (D(1),NC1(1)),(D(3001),NC2(1)),(NFO(1),D(6002)),(
     1D(9003),DATINZ(1))
  100 I=NA(1)
      J=NA(3)
      K=NA(2)
      DIS=0.0
      DJS=0.0
  106 DO 114 M=1,3
      RKI(M)=X(M,I)-X(M,K)
      DIS=DIS+RKI(M)*RKI(M)
      RKJ(M)=X(M,J)-X(M,K)
  114 DJS=DJS+RKJ(M)*RKJ(M)
      DI=SQRT(DIS)
      DJ=SQRT(DJS)
      COIJ=0.0
  120 DO 124 M=1,3
      EI(M)=RKI(M)/DI
      EJ(M)=RKJ(M)/DJ
  124 COIJ=COIJ+EI(M)*EJ(M)
      IF (1.0-ABS(COIJ))180,180,130
  130 SINIJ=SQRT(1.0-COIJ*COIJ)
      GO TO (132,134,136,138),NOPT
  132 DX=1.0
      GO TO 140
  134 DX=DI
      GO TO 140
  136 DX=DJ
      GO TO 140
  138 DX=SQRT(DI*DJ)
  140 QIJ=SQRT(DI*DI+DJ*DJ-2.0*DI*DJ*COIJ)
      SIJ=(DI-DJ*COIJ)/QIJ
      SJI=(DJ-DI*COIJ)/QIJ
      TIJ=DJ*SINIJ/QIJ
      TJI=DI*SINIJ/QIJ
      GEM(1,1)=SIJ*SIJ
      GEM(1,2)=TIJ*TIJ
      GEM(2,1)=SIJ*SJI
      GEM(2,2)=-TIJ*TJI
      GEM(3,1)=SIJ*SQRT(TIJ*TJI*DJ*CI)/DX
      GEM(3,2)=TIJ*SJI*DJ/DX
      GEM(4,1)=SJI*SJI
      GEM(4,2)=TJI*TJI
      GEM(5,1)=SJI*SQRT(TIJ*TJI*DJ*CI)/DX
```

```
      GEM(5,2)=TJI*SIJ*DI/DX
      GEM(6,1)=(TIJ*TJI*DJ*DI)/(DX*DX)
      GEM(6,2)=-(SIJ*SJI*DJ*DI)/(DX*DX)
  150 IF (INFRA)155,155,151
  151 WRITE(6,32)NOPRCB,NCPT
   32 FORMAT (13H1 GEM PRCBLEM18,10H OPTION   13)
  152 DO 154 I=1,6
  154 WRITE(6,34)I,(GEM(I,J),J=1,2)
   34 FORMAT (4HOROW13/(2F12.6))
  155 IF (NFOR(1)-NFOR(2))160,156,160
  156 DO 158 I=1,6
      GEM(I,1)=GEM(I,1)-0.1*GEM(I,2)
  158 GEM(I,2)=0.0
  160 DO 174 I=1,3
      DO 174 J=1,3
      K=7-I-(J*(J-1))/2
      DO 174 L=1,2
      IF (0.0001-ABS(GEM(K,L)))165,165,174
  165 NZ=NZ+1
  166 IF (KOOOFX(J)-KOOOFX(I))167,170,170
  167 NC1(NZ)=KOOOFX(J)
      NC2(NZ)=KOOOFX(I)
      GO TO 172
  170 NC1(NZ)=KOOOFX(I)
      NC2(NZ)=KOOOFX(J)
  172 NFO(NZ)=NFOR(L)
      DATINZ(NZ)=GEM(K,L)
  174 CONTINUE
      GO TO 182
  180 JOKE=1
  182 RETURN
      END
      SUBROUTINE ETETRA
      DIMENSION NC1(2000),NC2(3000)
      DIMENSION NFO(2000),DATINZ(2000)
      DIMENSION NA(5),KOOOFX(10)
      DIMENSION NFOR(400),RI(3)
      DIMENSION RJ(3),RK(3)
      DIMENSION RL(3),EI(3)
      DIMENSION EJ(3),EK(3)
      DIMENSION EL(3),D(100,100)
      DIMENSION X(3,100),TETRA(55,13)
      COMMON D,IND,NOPRCB,NCAT,NCOR,NF,NOPT,NCOD,NA,KOOOFX,NFOR
      COMMON NZ,JOKE,INFRA,X
      EQUIVALENCE (D(1),NC1(1)),(D(3001),NC2(1)),(NFO(1),D(6002)),(
     1D(9003),DATINZ(1))
  100 I=NA(1)
      J=NA(2)
      K=NA(3)
      L=NA(4)
      MC=NA(5)
  106 DO 108 N=1,55
      DO 108 M=1,13
```

```
108 TETRA(N,M)=0.0
109 DIS=0.0
    DJS=0.0
    DKS=0.0
    DLS=0.0
114 DO 120 M=1,3
    RI(M)=X(M,I)-X(M,MC)
    RJ(M)=X(M,J)-X(M,MC)
    RK(M)=X(M,K)-X(M,MC)
    RL(M)=X(M,L)-X(M,MC)
    DIS=DIS+RI(M)*RI(M)
    DJS=DJS+RJ(M)*RJ(M)
    DKS=DKS+RK(M)*RK(M)
120 DLS=DLS+RL(M)*RL(M)
121 DI=SQRT(DIS)
    DJ=SQRT(DJS)
    DK=SQRT(DKS)
124 DL=SQRT(DLS)
125 DO 130 M=1,3
126 EI(M)=RI(M)/DI
    EJ(M)=RJ(M)/DJ
    EK(M)=RK(M)/DK
130 EL(M)=RL(M)/DL
131 COSIJ=0.0
    COSIK=0.0
    COSIL=0.0
    COSJK=0.0
    COSJL=0.0
137 COSKL=0.0
140 DO 148 M=1,3
    COSIJ=COSIJ+EI(M)*EJ(M)
    COSIK=COSIK+EI(M)*EK(M)
142 COSIL=COSIL+EI(M)*EL(M)
    COSJK=COSJK+EJ(M)*EK(M)
    COSJL=COSJL+EJ(M)*EL(M)
148 COSKL=COSKL+EK(M)*EL(M)
149 IF (1.0-ABS(COSIJ))300,300,150
150 IF (1.0-ABS(COSIK))300,300,151
151 IF (1.0-ABS(COSIL))300,300,152
152 IF (1.0-ABS(COSJK))300,300,153
153 IF (1.0-ABS(COSJL))300,300,154
154 IF (1.0-ABS(COSKL))300,300,155
155 SINIJ=SQRT(1.0-COSIJ*COSIJ)
    SINIK=SQRT(1.0-COSIK*COSIK)
    SINIL=SQRT(1.0-COSIL*COSIL)
    SINJK=SQRT(1.0-COSJK*COSJK)
    SINJL=SQRT(1.0-COSJL*COSJL)
292 SINKL=SQRT(1.0-COSKL*COSKL)
162 QIJ=SQRT(DI*DI+DJ*DJ-2.0*DI*DJ*COSIJ)
163 QIK=SQRT(DI*DI+DK*DK-2.0*DI*DK*COSIK)
    QIL=SQRT(DI*DI+DL*DL-2.0*DI*DL*COSIL)
    QJK=SQRT(DJ*DJ+DK*DK-2.0*DJ*DK*COSJK)
    QJL=SQRT(DJ*DJ+DL*DL-2.0*DJ*DL*COSJL)
```

```
      QKL=SQRT(DK*DK+DL*DL-2.0*DK*DL*COSKL)
      SIJ=(DI-DJ*COSIJ)/QIJ
      SJI=(DJ-DI*COSIJ)/QIJ
      TIJ=DJ*SINIJ/QIJ
      TJI=DI*SINIJ/QIJ
      SIK=(DI-DK*COSIK)/QIK
      SKI=(DK-DI*COSIK)/QIK
      TIK=DK*SINIK/QIK
      TKI=DI*SINIK/QIK
      SIL=(DI-DL*COSIL)/QIL
      SLI=(DL-DI*COSIL)/QIL
      TIL=DL*SINIL/QIL
      TLI=DI*SINIL/QIL
      SJK=(DJ-DK*COSJK)/QJK
      SKJ=(DK-DJ*COSJK)/QJK
      TJK=DK*SINJK/QJK
      TKJ=DJ*SINJK/QJK
      SJL=(DJ-DL*COSJL)/QJL
      SLJ=(DL-DJ*COSJL)/QJL
      TJL=DL*SINJL/QJL
      TLJ=DJ*SINJL/QJL
      SKL=(DK-DL*COSKL)/QKL
      SLK=(DL-DK*COSKL)/QKL
      TKL=DL*SINKL/QKL
      TLK=DK*SINKL/QKL
      GO TO (192,194,196,196),NOPT
  192 DX1=1.0
      DX2=1.0
      DX3=1.0
      GO TO 200
  194 DX1=DJ
      DX2=DK
      DX3=DL
      GO TO 200
  196 DX1=DI
      DX2=DI
      DX3=DI
  200 THEIJ=COSIJ*(SINKL**2)-COSIK*(COSJK-COSJL*COSKL)+COSIL*(COSJK*
     1COSKL-COSJL)
      THEJK=COSJK*(SINIL**2)-COSIJ*(COSIK-COSKL*COSIL)+COSJL*(COSIK*
     1COSIL-COSKL)
      THEIK=COSIK*(SINJL**2)-COSIJ*(COSJK-COSKL*COSJL)+COSIL*(COSJK*
     1COSJL-COSKL)
      THEIL=COSIL*(SINJK**2)-COSIJ*(COSJL-COSKL*COSJK)+COSIK*(COSJL*
     1COSJK-COSKL)
      THEJL=COSJL*(SINIK**2)-COSIJ*(COSIL-COSKL*COSIK)+COSJK*(COSIL*
     1COSIK-COSKL)
      THEKL=COSKL*(SINIJ**2)-COSIK*(COSIL-COSJL*COSIJ)+COSJK*(COSIL*
     1COSIJ-COSJL)
      XIJ=COSIJ*THEIJ-(SINIJ**2)*(SINKL**2)
      XIK=COSIK*THEIK-(SINIK**2)*(SINJL**2)
      XIL=COSIL*THEIL-(SINIL**2)*(SINJK**2)
      XJK=COSJK*THEJK-(SINJK**2)*(SINIL**2)
```

```
      XJL=COSJL*THEJL-(SINJL**2)*(SINIK**2)
      XKL=COSKL*THEKL-(SINKL**2)*(SINIJ**2)
      ZIJIK=SINIJ*SINIK*(COSJK-COSJL*COSKL)
      ZIJIL=SINIJ*SINIL*(COSJL-COSJK*COSKL)
      ZIJJK=SINIJ*SINJK*(COSIK-COSIL*COSKL)
      ZIJJL=SINIJ*SINJL*(COSIL-COSIK*COSKL)
      ZIKKL=SINIK*SINKL*(COSIL-COSIJ*COSJL)
      ZIKIL=SINIK*SINIL*(COSKL-COSJK*COSJL)
      ZIKJK=SINIK*SINJK*(COSIJ-COSIL*COSJL)
      ZILJL=SINIL*SINJL*(COSIJ-COSIK*COSJK)
      ZJKJL=SINJK*SINJL*(COSKL-COSIK*COSIL)
      ZILKL=SINIL*SINKL*(COSIK-COSIJ*COSJK)
      ZJKKL=SINJK*SINKL*(COSJL-COSIL*COSIJ)
      ZJLKL=SINJL*SINKL*(COSJK-COSIJ*COSIK)
      YIJKL=SINIJ*SINKL*(2.0*COSIJ*COSKL-COSIK*COSJL-COSIL*COSJK)
      YIKJL=SINIK*SINJL*(2.0*COSIK*COSJL-COSIJ*COSKL-COSIL*COSJK)
      YILJK=SINIL*SINJK*(2.0*COSIL*COSJK-COSIJ*COSKL-COSIK*COSJL)
      TETRA(1,1)=SIJ*SIJ
      TETRA(1,2)=SIK*SIK
      TETRA(1,3)=SIL*SIL
      TETRA(1,7)=TIJ*TIJ
      TETRA(1,8)=TIK*TIK
      TETRA(1,9)=TIL*TIL
      TETRA(2,1)=SIJ*SJI
      TETRA(2,7)=-TIJ*TJI
      TETRA(3,2)=SIK*SKI
      TETRA(3,8)=-TIK*TKI
      TETRA(4,3)=SIL*SLI
      TETRA(4,9)=-TIL*TLI
      TETRA(5,1)=SIJ*SQRT(TIJ*TJI*DI*CJ)/DX1
      TETRA(5,7)=TIJ*SJI*DJ/DX1
      TETRA(6,2)=SIK*SQRT(TIK*TKI*CI*CK)/DX2
      TETRA(6,8)=TIK*SKI*DK/DX2
      TETRA(7,3)=SIL*SQRT(TIL*TLI*CI*CL)/DX3
      TETRA(7,9)=TIL*SLI*DL/DX3
      TETRA(11,1)=SJI*SJI
      TETRA(11,4)=SJK*SJK
      TETRA(11,5)=SJL*SJL
      TETRA(11,7)=TJI*TJI
      TETRA(11,10)=TJK*TJK
      TETRA(11,11)=TJL*TJL
      TETRA(12,4)=SJK*SKJ
      TETRA(12,10)=-TJK*TKJ
      TETRA(13,5)=SJL*SLJ
      TETRA(13,11)=-TJL*TLJ
      TETRA(14,1)=SJI*SQRT(TIJ*TJI*CI*DJ)/DX1
      TETRA(14,7)=TJI*SIJ*DI/DX1
      TETRA(17,4)=SJK*SQRT(TJK*TKJ*DK*DJ)/DX1
      TETRA(17,10)=TJK*SKJ*DK/DX1
      TETRA(19,5)=SJL*SQRT(TJL*TLJ*DL*DJ)/DX1
      TETRA(19,11)=TJL*SLJ*DL/DX1
      TETRA(20,2)=SKI*SKI
      TETRA(20,4)=SKJ*SKJ
```

```
      TETRA(20,6)=SKL*SKL
      TETRA(20,8)=TKI*TKI
      TETRA(20,10)=TKJ*TKJ
      TETRA(20,12)=TKL*TKL
      TETRA(21,6)=SKL*SLK
      TETRA(21,12)=-TKL*TLK
      TETRA(23,2)=SKI*SQRT(TIK*TKI*DI*DK)/DX2
      TETRA(23,8)=TKI*SIK*DI/DX2
      TETRA(25,4)=SKJ*SQRT(TJK*TKJ*DK*CJ)/DX1
      TETRA(25,10)=TKJ*SJK*DJ/DX1
      TETRA(26,6)=SKL*SQRT(TLK*TKL*DL*DK)/DX2
      TETRA(26,12)=TKL*SLK*CL/DX2
      TETRA(28,3)=SLI*SLI
      TETRA(28,5)=SLJ*SLJ
      TETRA(28,6)=SLK*SLK
      TETRA(28,9)=TLI*TLI
      TETRA(28,11)=TLJ*TLJ
      TETRA(28,12)=TLK*TLK
      TETRA(31,3)=SLI*SQRT(TIL*TLI*CI*DL)/DX3
      TETRA(31,9)=TLI*SIL*DI/DX3
      TETRA(33,6)=SLK*SQRT(TLK*TKL*CL*CK)/DX2
      TETRA(33,12)=TLK*SKL*DK/DX2
      TETRA(34,5)=SLJ*SQRT(TLJ*TJL*CL*CJ)/DX1
      TETRA(34,11)=TLJ*SJL*DJ/DX1
      TETRA(35,1)=TIJ*TJI*DI*CJ/(DX1*DX1)
      TETRA(35,7)=-SIJ*SJI*DI*DJ/(CX1*DX1)
      TETRA(35,13)=XIJ/(CX1*DX1)
      TETRA(36,13)=ZIJIK/(DX1*DX2)
      TETRA(37,13)=ZIJIL/(CX1*DX3)
      TETRA(38,13)=ZIJJK/(CX1*DX1)
      TETRA(39,13)=YIJKL/(CX1*DX2)
      TETRA(40,13)=ZIJJL/(DX1*DX1)
      TETRA(41,2)=TIK*TKI*DI*CK/(DX2*DX2)
      TETRA(41,8)=-SIK*SKI*DI*CK/(DX2*DX2)
      TETRA(41,13)=XIK/(DX2*DX2)
      TETRA(42,13)=ZIKIL/(CX2*DX3)
      TETRA(43,13)=ZIKJK/(CX2*DX1)
      TETRA(44,13)=ZIKKL/(CX2*DX2)
      TETRA(45,13)=YIKJL/(CX2*DX1)
      TETRA(46,3)=TIL*TLI*DI*CL/(CX3*DX3)
      TETRA(46,9)=-SIL*SLI*DI*CL/(DX3*DX3)
      TETRA(46,13)=XIL/(DX3*DX3)
      TETRA(47,13)=YILJK/(CX3*DX1)
      TETRA(48,13)=ZILKL/(DX3*DX2)
      TETRA(49,13)=ZILJL/(DX3*DX1)
      TETRA(50,4)=TJK*TKJ*DK*DJ/(DX1*CX1)
      TETRA(50,10)=-SJK*SKJ*DK*CJ/(DX1*DX1)
      TETRA(50,13)=XJK/(CX1*DX1)
      TETRA(51,13)=ZJKKL/(CX1*DX2)
      TETRA(52,13)=ZJKJL/(DX1*DX1)
      TETRA(53,6)=TKL*TLK*DL*CK/(DX2*CX2)
      TETRA(53,12)=-SKL*SLK*DL*CK/(DX2*CX2)
      TETRA(53,13)=XKL/(CX2*DX2)
```

```
      TETRA(54,13)=ZJLKL/(DX2*DX1)
      TETRA(55,5)=TJL*TLJ*DL*DJ/(DX1*DX1)
      TETRA(55,11)=-SJL*SLJ*DL*DJ/(DX1*DX1)
      TETRA(55,13)=XJL/(DX1*DX1)
  260 IF (INFRA)264,264,261
  261 WRITE(6,30)NOPROB,NOPT
   30 FORMAT (15H1 TETRA PROBLEM18,10H OPTION   I3)
  262 DO 263 I=1,55
  263 WRITE(6,32)I,(TETRA(I,J),J=1,13)
   32 FORMAT (4HOROWI3/(13F9.5))
  264 DO 270 J=1,6
      K=J+6
  265 IF (NFOR(J)-NFOR(K))270,266,270
  266 DO 269 I=1,55
      TETRA(I,J)=TETRA(I,J)-0.1*TETRA(I,K)
  269 TETRA(I,K)=0.0
  270 CONTINUE
  271 DO 285 I=1,10
      DO 285 J=I,10
      K=56-I-(J*(J-1))/2
      DO 285 L=1,13
      IF (0.0001-ABS(TETRA(K,L)))276,276,285
  276 NZ=NZ+1
  277 IF (KOOOFX(J)-KOOOFX(I))278,280,280
  278 NC1(NZ)=KOOOFX(J)
      NC2(NZ)=KOOOFX(I)
      GO TO 282
  280 NC1(NZ)=KOOOFX(I)
      NC2(NZ)=KOOOFX(J)
  282 NFO(NZ)=NFOR(L)
      DATINZ(NZ)=TETRA(K,L)
  285 CONTINUE
      GO TO 302
  300 JOKE=1
  302 RETURN
      END
      SUBROUTINE EVCIS
      DIMENSION NC1(2000),NC2(3000)
      DIMENSION NFO(2000),DATINZ(2000)
      DIMENSION NA(5),KOOOFX(10)
      DIMENSION NFOR(400),RI(3)
      DIMENSION RJ(3),RK(3)
      DIMENSION EI(3),EJ(3)
      DIMENSION EK(3),CRIJ(3)
      DIMENSION CRJK(3),DIK(3)
      DIMENSION D(100,100),X(3,100)
      DIMENSION CIS(15,2)
      COMMON D,IND,NOPROB,NCAT,NCOR,NF,NOPT,NCOD,NA,KOOOFX,NFOR
      COMMON NZ,JOKE,INFRA,X
      EQUIVALENCE (D(1),NC1(1)),(D(3001),NC2(1)),(NFO(1),D(6002)),(
     1D(9003),DATINZ(1))
  425 I=NA(1)
      J=NA(2)
```

```
      L=NA(3)
      K=NA(4)
  426 DIS=0.0
      DJS=0.0
  427 DKS=0.0
  428 DO 434 M=1,3
      RI(M)=X(M,J)-X(M,I)
  430 RJ(M)=X(M,L)-X(M,J)
      RK(M)=X(M,K)-X(M,L)
  432 DIS=DIS+RI(M)*RI(M)
      DJS=DJS+RJ(M)*RJ(M)
  434 DKS=DKS+RK(M)*RK(M)
  435 DI=SQRT(DIS)
      DJ=SQRT(DJS)
      DK=SQRT(DKS)
  438 DO 442 M=1,3
      EI(M)=RI(M)/DI
      EJ(M)=RJ(M)/DJ
  442 EK(M)=RK(M)/DK
  445 COSIJ=0.0
      COSJK=0.0
  444 DO 446 M=1,3
      COSIJ=COSIJ-EI(M)*EJ(M)
  446 COSJK=COSJK-EJ(M)*EK(M)
  447 IF (1.0-ABS(COSIJ))502,502,448
  448 IF (1.0-ABS(COSJK))502,502,449
  449 SINIJ=SQRT(1.0-COSIJ*COSIJ)
  450 SINJK=SQRT(1.0-COSJK*COSJK)
  451 CRIJ(1)=EI(2)*EJ(3)-EI(3)*EJ(2)
      CRIJ(2)=EI(3)*EJ(1)-EI(1)*EJ(3)
      CRIJ(3)=EI(1)*EJ(2)-EI(2)*EJ(1)
  452 CRJK(1)=EJ(2)*EK(3)-EJ(3)*EK(2)
      CRJK(2)=EJ(3)*EK(1)-EJ(1)*EK(3)
      CRJK(3)=EJ(1)*EK(2)-EJ(2)*EK(1)
  453 CP=0.0
  454 DO 455 M=1,3
  455 CP=CP+CRIJ(M)*CRJK(M)
  456 COST=CP/(SINIJ*SINJK)
      QIKS=0.0
  458 DO 460 M=1,3
      DIK(M)=X(M,I)-X(M,K)
  460 QIKS=QIKS+DIK(M)*DIK(M)
  461 QIK=SQRT(QIKS)
  462 GO TO (464,466,468,469),NOPT
  464 D1=1.0
      D2=1.0
      GO TO 470
  466 D1=DI
      D2=DK
      GO TO 470
  468 D1=DI
      D2=DJ
      GO TO 470
```

```
409  D1=SQRT(DI*DJ)
     D2=SQRT(DJ*DK)
470  GAM1=COSIJ*COSJK-SINIJ*SINJK*CCST
     GAM2=SINIJ*SINJK-COSIJ*COSJK*CCST
     SIG1=SINIJ*COSJK+COSIJ*SINJK*COST
     SIG2=COSIJ*SINJK+SINIJ*COSJK*COST
     VIK=(DI-DJ*COSIJ+DK*COSIJ*COSJK-DK*SINIJ*SINJK*COST)/QIK
     VKI=(DK-DJ*COSJK+DI*COSIJ*COSJK-DI*SINIJ*SINJK*COST)/QIK
     AIK=(DJ-DI*COSIJ-DK*COSJK)/QIK
     UIK=(DI*DJ*SINIJ-DI*DK*SINIJ*COSJK-DI*DK*COSIJ*SINJK*COST)/QIK
     UKI=(DK*DJ*SINJK-DI*DK*COSIJ*SINJK-DI*DK*SINIJ*COSJK*COST)/QIK
471  CIS(1,1)=VIK*VIK
     CIS(1,2)=(1.0-VIK*VIK)
     CIS(2,1)=VIK*VKI
     CIS(2,2)=GAM1-VIK*VKI
     CIS(3,1)=VIK*AIK
     CIS(3,2)=-(COSIJ+AIK*VIK)
     CIS(4,1)=VIK*UIK/D1
     CIS(4,2)=UIK*(QIK/DI-VIK)/D1
     CIS(5,1)=VIK*UKI/D2
     CIS(5,2)=-(DK*SIG2+UKI*VIK)/D2
472  CIS(6,1)=VKI*VKI
     CIS(6,2)=(1.0-VKI*VKI)
     CIS(7,1)=VKI*AIK
     CIS(7,2)=-(COSJK+AIK*VKI)
     CIS(8,1)=VKI*UIK/D1
     CIS(8,2)=-(DI*SIG1+UIK*VKI)/D1
     CIS(9,1)=VKI*UKI/D2
     CIS(9,2)=UKI*(QIK/DK-VKI)/D2
473  CIS(10,1)=AIK*AIK
     CIS(10,2)=(1.0-AIK*AIK)
     CIS(11,1)=AIK*UIK/D1
     CIS(11,2)=(DI*SINIJ-UIK*AIK)/D1
     CIS(12,1)=AIK*UKI/D2
     CIS(12,2)=(DK*SINJK-UKI*AIK)/C2
474  CIS(13,1)=(UIK*UIK)/(D1*D1)
     CIS(13,2)=(DI*DI-UIK*UIK-DI*VIK*QIK)/(D1*D1)
     CIS(14,1)=(UIK*UKI)/(D1*D2)
     CIS(14,2)=(DI*DK*GAM2-UIK*UKI)/(D1*D2)
475  CIS(15,1)=(UKI*UKI)/(D2*D2)
476  CIS(15,2)=(DK*DK-UKI*UKI-DK*VKI*QIK)/(D2*D2)
477  IF (INFRA)481,481,478
478  WRITE(6,34)NCPRCB,NOPT
 34  FORMAT (23H1THE CIS MATRIX PRCBLEM16,1CH OPTION   I3)
479  DO 480 I=1,15
480  WRITE(6,32)I,(CIS(I,J),J=1,2)
 32  FORMAT (4HOROWI3/(2F12.6))
481  IF (NFOR(1)-NFOR(2))486,482,486
482  DO 484 I=1,15
     CIS(I,1)=CIS(I,1)-0.1*CIS(I,2)
484  CIS(I,2)=0.0
486  DO 500 I=1,5
     DO 500 J=1,5
```

```
      K=16-I-(J*(J-1))/2
      DO 500 L=1,2
      IF (0.0001-ABS(CIS(K,L)))492,492,500
  492 NZ=NZ+1
      IF (KOOOFX(J)-KOOOFX(I))494,496,496
  494 NC1(NZ)=KOOOFX(J)
      NC2(NZ)=KOOOFX(I)
      GO TO 498
  496 NC1(NZ)=KOOOFX(I)
      NC2(NZ)=KOOOFX(J)
  498 NFO(NZ)=NFOR(L)
      DATINZ(NZ)=CIS(K,L)
  500 CONTINUE
      GO TO 504
  502 JOKE=1
  504 RETURN
      END
      SUBROUTINE EVCISP
      DIMENSION NC1(2000),NC2(3000)
      DIMENSION NFO(2000),DATINZ(2000)
      DIMENSION NA(5),KOOOFX(10)
      DIMENSION NFOR(400),RI(3)
      DIMENSION RJ(3),RK(3)
      DIMENSION EI(3),EJ(3)
      DIMENSION EK(3),CRIJ(3)
      DIMENSION CRJK(3),CIK(3)
      DIMENSION D(100,100),X(3,100)
      DIMENSION CIS(21,2)
      COMMON D,IND,NOPROB,NOAT,NCOR,NF,NOPT,NCOD,NA,KOOOFX,NFOR
      COMMON NZ,JOKE,INFRA,X
      EQUIVALENCE (D(1),NC1(1)),(D(3001),NC2(1)),(NFO(1),D(6002)),(
     1D(9003),DATINZ(1))
  634 I=NA(1)
      J=NA(2)
      L=NA(3)
      K=NA(4)
  636 DIS=0.0
      DJS=0.0
  638 DKS=0.0
  639 DO 642 M=1,3
      RI(M)=X(M,J)-X(M,I)
  640 RJ(M)=X(M,L)-X(M,J)
      RK(M)=X(M,K)-X(M,L)
  641 DIS=DIS+RI(M)*RI(M)
      DJS=DJS+RJ(M)*RJ(M)
  642 DKS=DKS+RK(M)*RK(M)
      DI=SQRT(DIS)
      DJ=SQRT(DJS)
      DK=SQRT(DKS)
      GO TO (643,644,645,646),NOPT
  643 D1=1.0
      D2=1.0
      D3=1.0
```

```
      GO TO 647
  644 D1=DI
      D2=DK
      D3=DJ
      GO TO 647
  645 D1=DI
      D2=DJ
      D3=DJ
      GO TO 647
  646 D1=DI
      D2=DK
      D3=DI
  647 COSIJ=0.0
      COSJK=0.0
      DO 652 M=1,3
  648 EI(M)=RI(M)/DI
      EJ(M)=RJ(M)/DJ
  650 EK(M)=RK(M)/DK
      COSIJ=COSIJ-EI(M)*EJ(M)
  652 COSJK=COSJK-EJ(M)*EK(M)
  653 IF (1.0-ABS(COSIJ))729,729,654
  654 IF (1.0-ABS(COSJK))729,729,655
  655 SINIJ=SQRT(1.0-COSIJ*COSIJ)
      SINJK=SQRT(1.0-COSJK*COSJK)
  657 CRIJ(1)=EI(2)*EJ(3)-EI(3)*EJ(2)
      CRIJ(2)=EI(3)*EJ(1)-EI(1)*EJ(3)
      CRIJ(3)=EI(1)*EJ(2)-EI(2)*EJ(1)
  658 CRJK(1)=EJ(2)*EK(3)-EJ(3)*EK(2)
      CRJK(2)=EJ(3)*EK(1)-EJ(1)*EK(3)
      CRJK(3)=EJ(1)*EK(2)-EJ(2)*EK(1)
      CP=0.0
  660 CPD=0.0
  661 QIKS=0.0
  662 DO 665 M=1,3
      CP=CP+CRIJ(M)*CRJK(M)
  664 CPD=CPD+CRIJ(M)*EK(M)
      DIK(M)=X(M,I)-X(M,K)
  665 QIKS=QIKS+DIK(M)*DIK(M)
  666 COST=CP/(SINIJ*SINJK)
  667 SINT=CPD/(SINIJ*SINJK)
  668 QIK=SQRT(QIKS)
  669 GAM1=COSIJ*COSJK-SINIJ*SINJK*COST
  670 GAM2=SINIJ*SINJK-COSIJ*COSJK*COST
  671 SIG1=SINIJ*COSJK+COSIJ*SINJK*COST
  672 SIG2=COSIJ*SINJK+SINIJ*COSJK*COST
  673 A1=COSIJ*SINJK*SINT
  674 A2=SINIJ*COSJK*SINT
  675 A3=SINIJ*SINJK*COST
  676 XIK=(DI*DK*SINIJ*SINJK*SINT)/QIK
  677 AIK=(DJ-DI*COSIJ-DK*COSJK)/QIK
  678 VIK=(DI-DJ*COSIJ+DK*COSIJ*COSJK-DK*SINIJ*SINJK*COST)/QIK
  679 VKI=(DK-DJ*COSJK+DI*COSIJ*COSJK-DI*SINIJ*SINJK*COST)/QIK
  680 UIK=(DI*DJ*SINIJ-DI*DK*SINIJ*COSJK-DI*DK*COSIJ*SINJK*COST)/QIK
```

```
      UKI=(DK*DJ*SINJK-DI*DK*COSIJ*SINJK-DI*DK*SINIJ*COSJK*COST)/QIK
      CIS(1,1)=VIK*VIK
      CIS(1,2)=1.0-VIK*VIK
      CIS(2,1)=VIK*VKI
      CIS(2,2)=GAM1-VIK*VKI
      CIS(3,1)=VIK*AIK
      CIS(3,2)=-(COSIJ+AIK*VIK)
      CIS(4,1)=VIK*UIK/D1
      CIS(4,2)=UIK*(QIK/DI-VIK)/D1
      CIS(5,1)=VIK*UKI/D2
      CIS(5,2)=-(DK*SIG2+UKI*VIK)/D2
      CIS(6,1)=VIK*XIK/D3
      CIS(6,2)=XIK*(QIK/DI-VIK)/D3
      CIS(7,1)=VKI*VKI
      CIS(7,2)=(1.0-VKI*VKI)
      CIS(8,1)=VKI*AIK
      CIS(8,2)=-(COSJK+AIK*VKI)
      CIS(9,1)=VKI*UIK/D1
      CIS(9,2)=-(DI*SIG1+UIK*VKI)/D1
      CIS(10,1)=VKI*UKI/D2
      CIS(10,2)=UKI*(QIK/DK-VKI)/D2
      CIS(11,1)=VKI*XIK/D3
      CIS(11,2)=XIK*(QIK/DK-VKI)/D3
      CIS(12,1)=AIK*AIK
      CIS(12,2)=1.0-AIK*AIK
      CIS(13,1)=AIK*UIK/D1
      CIS(13,2)=(DI*SINIJ-UIK*AIK)/D1
      CIS(14,1)=AIK*UKI/D2
      CIS(14,2)=(DK*SINJK-UKI*AIK)/D2
      CIS(15,1)=AIK*XIK/D3
      CIS(15,2)=-AIK*XIK/D3
      CIS(16,1)=(UIK*UIK)/(D1*D1)
      CIS(16,2)=(DI*DI-UIK*UIK-DI*VIK*QIK)/(D1*D1)
      CIS(17,1)=(UIK*UKI)/(D1*D2)
      CIS(17,2)=(DI*DK*GAM2-UIK*UKI)/(D1*D2)
      CIS(18,1)=(UIK*XIK)/(D1*D3)
      CIS(18,2)=(DI*DK*A1-XIK*UIK)/(D1*D3)
      CIS(19,1)=(UKI*UKI)/(D2*D2)
      CIS(19,2)=(DK*DK-UKI*UKI-DK*VKI*QIK)/(D2*D2)
      CIS(20,1)=(UKI*XIK)/(D2*D3)
      CIS(20,2)=(DI*DK*A2-XIK*UKI)/(D2*D3)
      CIS(21,1)=(XIK*XIK)/(D3*D3)
      CIS(21,2)=(DI*DK*A3-XIK*XIK)/(D3*D3)
      IF (INFRA)709,709,705
      WRITE(6,34)NCPRCB,NCPT
   34 FORMAT (23H1THE CIS MATRIX PROBLEMI6,10H OPTION   I3)
      DO 707 I=1,21
      WRITE(6,32)I,(CIS(I,J),J=1,2)
   32 FORMAT (4HOROWI3/(2F12.6))
      IF (NFOR(2)-NFOR(1))714,710,714
      DO 712 I=1,21
      CIS(I,1)=CIS(I,1)-0.1*CIS(I,2)
  712 CIS(I,2)=0.0
```

```
714 DO 726 I=1,6
    DO 726 J=I,6
    K=22-I-(J*(J-1))/2
    DO 726 L=1,2
    IF (0.0001-ABS(CIS(K,L)))720,720,726
720 NZ=NZ+1
721 IF (KOOOFX(J)-KCCOFX(I))722,724,724
722 NC1(NZ)=KOOOFX(J)
    NC2(NZ)=KCOOFX(I)
    GO TO 725
724 NC1(NZ)=KCOOFX(I)
    NC2(NZ)=KCCOFX(J)
725 NFO(NZ)=NFOR(L)
    DATINZ(NZ)=CIS(K,L)
726 CONTINUE
    GO TO 730
727 JOKE=1
730 RETURN
    END
```

4. ZSYM

The only changes in this program affecting the input data are on the control card.

Card Column Field	Values	Options
1-3	-09	problem indicator
4-7	NINT	number of internal coordinates
8-11	NF	number of force constants
12-15	NS	number of symmetry coordinates
16-19	NB	number of factor blocks plus 1
20-27	1	punch symmetrized Z matrix
28-31	1	read U matrix from disk
	0	read U matrix from cards
32-35	1	write symmetry blocks on disk
36-47	-	ignore
48-51	1	read Z matrix from disk
	0	read Z matrix from cards

```
      DIMENSION NR(1200),NC(1200),NFO(1200),DZ(1200),NRU(1200),
     1 NCU(1200),DU(1200),NR1(1200),NC1(1200),DU1(1200),NRZ(500),
     2 NCZ(500),Z(500),NBL(101),NRS(101),NCS(101),NFC(101),FS(101),
     3NB1(2000),DA(500),U(500),FU(500),UF(500),RECORD(40),NB(20),NRO(4),
     4 NCO(4),NPI(4),DAT(4)
      DIMENSION NSB1(10)
      COMMON NR,NC,NFO,DZ,NRU,NCU
      COMMON DU,NR1,NC1,CU1
      EQUIVALENCE (DA,U,UF),(NB1,NRZ),(NB1(501),NCZ),(NB1(1002),Z)
      REWIND 16
      REWIND 17
   90 READ (5,10) IND
   10 FORMAT(I3)
      IF(IND+9)90,92,90
   92 READ(5,12) IND,NC,NF,NS,NSB,IND1,IND2,INDU,IFNSB,IFSK,IFREP,NST,
     1 INDZ
   12 FORMAT(I3,12I4)
      IF(IND) 93,94,93
   94 CALL EXIT
   93 READ(5,14) (RECORD(I),I=1,40)
   14 FORMAT(20A4)
      REWIND 1
      NE=0
      NOZ=0
      NREC=0
      IF(INDZ.EQ.0)  GO TO 105
  104 READ (5,16)(NRO(L),NCO(L),NPI(L),DAT(L),L=1,4)
      GO TO 106
  105 READ(17) (NRO(L),NCO(L),NPI(L),DAT(L),L=1,4)
   16 FORMAT(4(3I4,F8.5))
  106 DO 120 L=1,4
      IF(NRO(L))122,120,108
  108 IF(NRO(L).GT.NQ)  GO TO 600
  109 IF(NRO(L).GT.NCO(L))  GO TO 600
  110 IF(NPI(L).GT.NF)  GO TO 600
  111 IF(DAT(L).NE.0.0)  GO TO 113
  112 DAT(L)=1.0
  113 NOZ=NOZ+1
      NR(NOZ)=NRO(L)
      NC(NOZ)=NCO(L)
      NFO(NOZ)=NPI(L)
  119 DZ(NOZ)=DAT(L)
  120 CONTINUE
      IF(INDZ.EQ.0)  GO TO 105
      GO TO 104
  122 IF(NRO(L).EQ.-6)  GO TO 124
      GO TO 600
  124 IF(IFREP)126,126,125
  125 NO=NST
      GO TO 186
  126 WRITE (6,50)NOZ,(RECORD(I),I=1,40)
   50 FORMAT(27H1 Z MATRIX SYMMETRIZE. NOZ=I4 /(1X,20A4))
      WRITE(6,620)
```

```
620 FORMAT('-',10X,'THE INPUT Z MATRIX IS'/11X,21('-')//)
    WRITE(6,621) (NR(I),NC(I),NFO(I),DZ(I),I=1,NOZ)
621 FORMAT(6(3X,3I3,F9.5))
    NOU=0
    NX=1
    DSQ=0.0
    WRITE(6,622)
    IF(INDU.EQ.0) GO TO 130
129 READ(16)(NRO(L),NCO(L),DAT(L),L=1,4)
    GO TO 131
130 READ (5,18)(NRO(L),NCO(L),DAT(L),L=1,4)
 18 FORMAT(4(2I3,F12.6))
622 FORMAT('-',10X,'THE UNNORMALIZED U-MATRIX IS'/11X,28('-')//)
    WRITE(6,623) (NRO(L),NCO(L),DAT(L),L=1,4)
623 FORMAT(20X,4(2I4,F10.5))
131 DO 150 L=1,4
    IF(NRO(L))152,150,140
140 IF(NS-NRO(L))605,141,141
141 IF(NRO(L)-NX)605,145,142
142 DA(NX)=1.0/SQRT(DSQ)
    NX=NX+1
    DSQ=0.0
    GO TO 141
145 DSQ=DSQ+DAT(L)**2
    NCU=NOU+1
    NRU(NOU)=NRO(L)
    NCU(NOU)=NCO(L)
    DU(NOU)=DAT(L)
150 CONTINUE
    IF(INDU.GT.0) GO TO 129
    GO TO 130
152 IF(3+NRO(L))605,154,605
154 DA(NX)= 1.0 / SQRT(DSQ)
    IF(NS-NX)605,156,605
156 DO 158 I=1,NOU
    J=NRU(I)
158 DU(I)=DA(J)*DU(I)
    NCU=NOU+1
    NRU(NOU)=-3
    NCU(NOU)=0
    DU(NOU)=0.0
180 NU=NOU-1
    DO 184 K=1,NU
    NR1(K)= NRU(K)
    NC1(K)=NCU(K)
184 DU1(K)=DU(K)
    IF(IFNSB.EQ.0)  GO TO 185
    READ(5,20) (NSB1(I),I=1,NSB)
185 READ (5,20)(NB(I),I=1,NSB)
 20 FORMAT(24I3)
    IF(NB(NSB).EQ.0)  GO TO 619
    NO=1
186 NZ=0
```

```
      DO 190 K=1,NOZ
      IF(NO-NFO(K))190,188,190
  188 NZ=NZ+1
      NRZ(NZ)=NR(K)
      NCZ(NZ)=NC(K)
      Z(NZ)=DZ(K)
  190 CONTINUE
      IF(NZ)600,192,220
  192 NO=NO+1
      IF(NO-NF)186,186,295
  220 NL=1
      NX=2
      NUT=1
      NUB=1
      NJ=1
  230 NP=NB(NL)
      NT=NB(NX)
  236 DO 238 I=1,NQ
      FU(I)=0.0
  238 U(I)=0.0
      DO 250 K=NUB,NOU
      IF(NRO(K)-NJ)240,248,240
  240 DO 246 L=1,NZ
      I=NRZ(L)
      J=NCZ(L)
      FU(I)=FU(I)+Z(L)*U(J)
      IF(I-J)244,246,244
  244 FU(J)=FU(J)+Z(L)*U(I)
  246 CONTINUE
      GO TO 252
  248 JU=NCU(K)
  250 U(JU)=DU(K)
  252 NUB=K
      DO 254 I=NJ,NS
  254 UF(I)=0.0
      ASSIGN 262 TO JCKE
      DO 265 L=NUT,NU
      GO TO JUKE,(262,264)
  262 IF(NR1(L)-NJ)619,264,263
  263 ASSIGN 264 TO JUKE
      NWY=L
  264 I=NR1(L)
      J=NC1(L)
  265 UF(I)=UF(I)+DU1(L)*FU(J)
      NUT=NWY
      DO 280 J=NJ,NS
      IF(0.00005-ABS(UF(J)))270,280,280
  270 IF(NT-J)271,271,272
  271 WRITE (6,72)NJ,J
   72 FORMAT(40HO ERROR,ERRCR,ERROR- Z NOT FACTORING.ROW14,7H COLUMN14)
  272 NE=NE+1
      IF(101-NE)273,273,274
  273 WRITE (1)(NBL(I),NRS(I),NCS(I),NFC(I),FS(I),I=1,100)
```

```
      NREC=NREC+1
      NE=1
  274 NRS(NE)=NJ-NP+1
      NCS(NE)=J-NP+1
      NBL(NE)=NL
      NFC(NE)=NC
      FS(NE)=UF(J)
  280 CONTINUE
      NJ=NJ+1
      IF(NT-NJ)284,284,236
  284 NL=NL+1
      NX=NX+1
      IF(NSB-NX)290,230,230
  290 NC=NC+1
      IF(NF-NC)295,186,186
  295 IF(NREC)296,296,298
  296 NOZ=0
      GO TO 321
  298 WRITE (1)(NBL(I),NRS(I),NCS(I),NFC(I),FS(I),I=1,NE)
  300 REWIND 1
  302 DO 312 L=1,NREC
      READ (1)(NBL(I),NRS(I),NCS(I),NFC(I),FS(I),I=1,100)
      DO 312 K=1,100
      NZ=100*(L-1)+K
      NB1(NZ)=NBL(K)
      NR(NZ)=NRS(K)
      NC(NZ)=NCS(K)
      NFO(NZ)=NFC(K)
  312 DZ(NZ)=FS(K)
      NOZ=NZ
  315 IF(NE)330,330,320
  320 READ (1)(NBL(I),NRS(I),NCS(I),NFC(I),FS(I),I=1,NE)
  321 DO 324 K=1,NE
      NZ=NOZ+K
      NB1(NZ)=NBL(K)
      NR(NZ)=NRS(K)
      NC(NZ)=NCS(K)
      NFO(NZ)=NFC(K)
  324 DZ(NZ)=FS(K)
  330 NSO=1
      IJQ=1
  331 NT=0
      NX=0
  332 WRITE (6,64)IND,NSO,(RECORD(I),I=1,12)
   64 FORMAT(2HW0I3,15H Z MATRIX BLOCK(3,12A4)
      IF(IFNSB.EQ.0)  GO TO 335
      IF(NSO.NE.NSB1(IJQ))  GO TO 335
      NZ2=NZ+1
      NR(NZ2) = -5
      NC(NZ2) = 0
      NFO(NZ2) =0
      DZ(NZ2) =0.0
      NZ4 = 1
```

```
      NZ8 = 4
  334 WRITE(15) (NR(I),NC(I),NFO(I),DZ(I),I=NZ4,NZ8)
      DO 333 I=NZ4,NZ8
      IF(NR(I).LT.0)  GO TO 335
  333 CONTINUE
      NZ4 = NZ4 + 4
      NZ8 = NZ8 + 4
      GO TO 334
  335 DO 340 I=1,NZ
      IF(NSO-NB1(I))340,336,340
  336 NX=NX+1
      IF(101-NX)337,337,338
  337 WRITE (6,66)(NRS(L),NCS(L),NFC(L),FS(L),L=1,100)
  609 IF(IND2.EQ.0)  GO TO 607
      WRITE(7,66)(NRS(L),NCS(L),NFC(L),FS(L),L=1,100)
   66 FORMAT(4(3I3,F11.6))
  607 NT=NT+100
      NX=1
  338 NRS(NX)=NR(I)
      NCS(NX)=NC(I)
      NFC(NX)=NFO(I)
      FS(NX)=DZ(I)
  340 CONTINUE
      IF(NX)344,344,342
  342 WRITE (6,66)(NRS(L),NCS(L),NFC(L),FS(L),L=1,NX)
      NX2=NX+1
      NRS(NX2)=-5
      NCS(NX2)=0
      NFC(NX2)=0
      FS(NX2)=0.0
 1608 IF(IND2.EQ.0)  GO TO 608
      WRITE(7,66)(NRS(I),NCS(I),NFC(I),FS(I),I=1,NX2)
  608 NT=NT+NX
  344 WRITE (6,76)NT
   76 FORMAT(2Hw0,5H NOZ=I4)
      IF(NX.GT.0) GO TO 606
      NRS(1)=-5
      NCS(1)=0
      NFC(1)=0
      FS(1)=0.0
 1609 IF(IND2.EQ.0)  GO TO 606
      WRITE(7,66) NRS(1),NCS(1),NFC(1),FS(1)
  606 NSO=NSO+1
      IJQ=IJQ+1
      IF(NSB-NSO)90,90,331
  600 WRITE (6,56)L,NRO(L),NCO(L),NPI(L),DAT(L)
   56 FORMAT(23HO  Z MATRIX ERROR FIELDI3,6H READS3I4,F12.6)
      GO TO 90
  605 WRITE (6,58)L,NRC(L),NCO(L),DAT(L)
   58 FORMAT(23HO  U MATRIX ERRCR FIELDI3,6H READS2I4,F12.6)
      GO TO 90
  619 WRITE(6,659)
  659 FORMAT('-',5X,'THERE IS AN ERROR ASSOCIATED WITH THE U-MATRIX, PRO
```

```
18ABLY THE NUMBERS OF ROWS STARTING SYMMETRY BLOCKS'/6X,100('-')/)
 GO TO 90
 END
```

5. BRADPERT

The input data for this program is explained below.

a. Control Card

Card Column Field	Values	Options
1-2	-1	terminate program
	+1	write L matrix
3-4	1	write out result of $L^{-1}GFL$
5-6	0	read Z matrix from cards
	1	read Z matrix from disk
7-8	0	read G matrix from cards
	1	read G matrix from disk
9-10	0	read in difference limits
	1	assume limits = 1.0 cm^{-1}
11-12	1	form significance matrix
13-14	1	read in force constant numbers to be used in the significance matrix
	0	use all force constants in the significance matrix

b. Read NOZ — I4

NOZ -- the number of Z matrix elements

c. Read RECORD — 20A4

RECORD -- literal data

d. Read N, LL, NPERT, NFO — 4I3

N -- number of normal coordinates

LL -- number of force constants entered into J matrix

NPERT -- maximum number of perturbations allowed

NFO -- number of force constants

e.	Read row number starting each symmetry block	I3
f.	Read force constant numbers to be entered into J matrix	20I4
g.	NR, NC, NOP, Z	4(3I3,F11.6)

NR -- row number of F matrix

NC -- column number of F matrix

NOP -- Urey-Bradley force constant number

Z -- Z matrix element

h.	Read initial force constants	8F10.6
i.	Read force constant labels	10A8
j.	Read PHEEP, ISOP, NFREQ, AMT	3I4,F10.6

PHEEP -- force constant number, to be incremented if ISOP > 1

ISOP -- number of increments for a given force constant PHEEP

NFREQ -- number of observed frequencies

AMT -- amount by which force constant PHEEP is to be incremented

k.	Read symmetry coordinate labels	2(10A4)
l.	Read G matrix	8F10.6
m.	Read difference limits	8F10.6
n.	Read observed frequencies	8F10.6
o.	Read force constant numbers to be used in the significance matrix	20I4

The main program listing is followed by all of the subroutines it calls. Many of these subroutines are written both in Fortran and in Basic Assembly Language. The listings of the B.A.L. subroutines are in Appendix 1B.

```
      REAL *8LABPHE
      DIMENSION NFC(100),PHEE(100),NOPHEE(1000),Z(1000),NRF(1000)
      DIMENSION NCF(1000),LABPHE(100),PHEE1(100)
      DIMENSION RECORD(20),Z1(30,30),SYM(30,30),F(30,30),G(900)
      DIMENSION E(900)  ,FREQ(30),XL(30),EXFREQ(30),B(30),XM(30)
      DIMENSION XX(30),XY(30),FM2(30,30)
      DIMENSION FN1(30),FN2(30),FREQ1(30),FREQ2(30),FREQ3(30)
      DIMENSION XLX(30,30),QMM2(30),FREQ4(30),EPOT(30,30),EG(30,30)
      DIMENSION ALFG(30,30),ALFGL(30,30),CMLFGL(30,30),FG(30,30)
      DIMENSION XLX3(30,30) ,ALIM(30)
      DIMENSION AJ(30,30),XJ(30,30),BJ(30,30),B1(30,30) ,B2(30,30)
      DIMENSION B3(30,30),B5(30,1),QMM1(30),QMM(30),XLX1(30,30)
      DIMENSION FM3(900)
      DIMENSION NROW(5)
      DIMENSION IFINC(100)
      NUMB=1
      NDIM=30
      REWIND 15
      REWIND 10
   11 READ(5,5) IND1,IND2,IND3,INDG,INDL,NTEST1,NTEST2
    5 FORMAT(10I2)
      IF(IND1.LT.0)  CALL EXIT
      IF(IND3.GT.0) GO TO 606
  500 READ(5,36) NOZ
      NOZ1=NOZ + 1
  600 READ(5,5000) (RECORD(I),I=1,20)
 5000 FORMAT(20A4)
      READ(5,15) N,LL,NPERT,NFD
   15 FORMAT(5I3)
      READ(5,15) (NROW(I),I=1,5)
      WRITE(6,802) NUMB
  802 FORMAT('1  THIS IS THE MOLECULE NUMBER',I3)
      NUMB=NUMB+1
      READ(5,36) (NFC(I),I=1,LL)
   36 FORMAT(10(2I4))
      IF(IND3.EQ.0)  GO TO 34
      NOZ = 0
      NZ4 = 1
      NZ8 = 4
  131 READ(15) (NRF(I),NCF(I),NOPHEE(I),Z(I),I=NZ4,NZ8)
      DO 133 I=NZ4,NZ8
      IF(NRF(I).EQ.-5)  GO TO 38
      NOZ = NOZ + 1
  133 CONTINUE
      IF(NOZ.GT.500) GO TO 132
      NZ4 = NZ4 + 4
      NZ8 = NZ8 + 4
      GO TO 131
   34 READ(5,134) (NRF(I),NCF(I),NOPHEE(I),Z(I),I=1,NOZ1)
  134 FORMAT(4(3I3,F11.6))
   39 DO 33 I=1,NOZ1
      IF(NRF(I).EQ.-5)  GO TO 38
   33 CONTINUE
```

```
  132 WRITE(6,37)
   37 FORMAT(///,'    Z MATRIX READING ERROR, JOB TERMINATED',//)
      CALL EXIT
   38 CONTINUE
      NOZ1 = NOZ + 1
      READ(5,45) (PHEE(I),I=1,NFO)
      READ(5,5001) (LABPHE(I),I=1,NFO)
 5001 FORMAT(10A8)
      READ(5,200) PHEEP,ISOP,NFREQ,AMT
  200 FORMAT(3I4,F10.6)
      READ(5,846) ((SYM(I,J),J=1,10),I=1,N)
  846 FORMAT(2(10A4))
      IF(INDG.EQ.0)  GO TO 601
      READ(10)((EG(I,J),J=1,N),I=1,N)
      GO TO 602
  601 READ(5,45)((EG(I,J),J=1,N),I=1,N)
  602 CALL ARAY(2,N,N,NDIM,EG)
      NN=N*N
      DO 830 I=1,NN
  830 G(I)=EG(I,1)
      CALL ARAY(1,N,N,NDIM,EG)
   45 FORMAT(8F10.6)
      CALL MINV (G,N,D,FN1,FN2)
      CALL FCONST(NRF,NCF,NCPHEE,PHEE,Z,NOZ,N,NROW,F)
      DO 905 I=1,NN
      E(I)=G(I)
      FM2(I,1)=F(I,1)
  905 FM3(I)=F(I,1)
      DO 858 I=1,NFREQ
  858 ALIM(I)=1.0
      IF(INDL.NE.0)  GO TO 857
      READ(5,2)  (ALIM(I),I=1,NFREQ)
  857 READ(5,2) (EXFREQ(I),I=1,NFREQ)
    2 FORMAT(8F10.6)
  210 DO 900 IJK=1,ISOP
      PHEE(PHEEP)=PHEE(PHEEP)+AMT
      IF(IJK.EQ.1)GO TO 854
      CALL FCONST(NRF,NCF,NCPHEE,PHEE,Z,NOZ,N,NROW,F)
      DO 73 I=1,NN
      FM2(I,1)=F(I,1)
   73 CONTINUE
      READ(5,36) (IFINC(I),I=1,NFO)
      DO 75 I=1,NFO
      IF(IFINC(I).EQ.0)  IFINC(I)=NFO+1
   75 CONTINUE
      DO 76 I=1,NFO
      DO 76 J=1,NFO
      IF(IFINC(I).LE.IFINC(J))  GO TO 76
      IT=IFINC(I)
      IFINC(I)=IFINC(J)
      IFINC(J)=IT
   76 CONTINUE
  854 CONTINUE
```

```
      WRITE(6,7001) (RECORD(III),III=1,20)
 7001 FORMAT(///,2X,20A4)
      WRITE(6,760)
  760 FORMAT(//,'   THE SYMMETRIZED Z MATRIX IS'/)
      WRITE(6,761) (NRF(I),NCF(I),NOPHEE(I),Z(I),I=1,NOZ1)
  761 FORMAT(6(3I3,F11.6))
      WRITE(6,801)
  801 FORMAT(//,'  THE G MATRIX IS',/)
      DO  804 I=1,N
  804 WRITE(6,803) (EG(I,J),J=1,N)
  803 FORMAT(5X,15F8.5)
      WRITE(6,706)
  706 FORMAT(///,'   THE TRIAL UREY-BRADLEY FORCE CONSTANTS WITH APPROPR
     1IATE LABELS ARE',/)
      WRITE(6,707)  (LABPHE(I),PHEE(I),I=1,NFO)
  707 FORMAT(4X,'*',2X,A8,F10.6,4X,'*',2X,A8,F10.6,4X,'*',2X,A8,F10.6,
     1 4X,'*',2X,A8,F10.6,4X,'*',2X,A8,F10.6/4X,'*',24X,'*',24X,'*',24X,
     2 '*', 24X,'*',1X)
      CALL ARAY(1,N,N,NDIM,F)
      WRITE(6,805)
  805 FORMAT(///,'   THE TRIAL F MATRIX  LABELED WITH SYMMETRY COORDINAT
     1ES IS',/)
      DO  806 I=1,N
  806 WRITE(6,848) (SYM(I,KJ),KJ=1,10),(F(I,J),J=1,N)
  848 FORMAT(1X,10A4,15F6.3/41X,15F6.3/41X,15F6.3)
      DO 850 I=1,N
      IF(0.0+F(I,I))10,850,850
  850 CONTINUE
   74 CALL ARAY(2,N,N,30,F)
      CALL NROOTE(N,NROW,F,G,XL,XLX)
      DO 65 I=1,NN
      G(I)=E(I)
      F(I,1)=FM2(I,1)
   65 CONTINUE
      DO 651 I=1,N
      IF(XL(I).LE.0.0)  GO TO 652
  651 CONTINUE
      GO TO 653
  652 WRITE(6,654) (XL(I),I=1,N)
  654 FORMAT(///,'    THE RUN ON THIS MOLECULE WILL TERMINATE HERE DUE T
     1O A NEGATIVE EIGENVALUE OF THE FG SECULAR EQUATION'/'    THE EIGEN
     2VALUES ARE'/(10F12.6))
      CALL ARAY(1,N,N,NDIM,XLX)
      CALL ARAY(1,N,N,NDIM,F)
      WRITE(6,656)
  656 FORMAT(/,'    THE EIGENVECTORS ARE',/)
      DO 655 I=1,N
  655 WRITE(6,803)  (XLX(I,J),J=1,N)
      DO 670 I=1,N
      DO 670 J=1,N
  670 EPOT(I,J)=F(I,I)*(XLX(I,J)**2)
      WRITE(6,818)
      DO 671 I=1,N
```

```
 671 WRITE(6,803)  (EPOT(I,J),J=1,N)
     GO TO 10
 653 CONTINUE
     DO 6031 I=1,N
     FREQ(I)=1303.16*SQRT(XL(I))
6031 CONTINUE
     DO 811 I=1,NFREQ
 811 QMM2(I)=EXFREQ(I)-FREQ(I)
     IF(N-NFREQ)226,226,215
 215 NF=NFREQ+1
     DO 220 I=NF,N
     EXFREQ(I)=0.0
     QMM2(I)=0.0
     QMM1(I)=0.0
 220 XX(I)=0.0
 226 WRITE(6,807)
 807 FORMAT(///,'  THE RESULT USING THE TRIAL F MATRIX IS',/)
     WRITE(6,808)
 808 FORMAT(25X,'OBSERVED',25X,'CALCULATED',25X,'DIFFERENCE',7X,'DIFF.L
    1IMIT',/)
     DO 810 I=1,N
 810 WRITE(6,809)I,EXFREQ(I),FREQ(I),QMM2(I),ALIM(I)
 809 FORMAT(15X,I2,4('-'),F12.6,23X,F12.6,23X,F12.6,7X,F10.5)
 225 DO 681 I=1,N
     XY(I) = ((EXFREQ(I))/1303.16)**2
 681 CONTINUE
     WRITE(6,915) NPERT
 915 FORMAT('0  THE MAXIMUM NUMBER OF ITERATIONS IS',I4)
     CALL ITER(NRF,NCF,NCPHEE,PHEE,Z,NCZ,N,NROW,F,G,XM,XLX3,AJ,
    1NDIM,XL,LL,E,NFREQ,NFC,BJ,B2,FN1,FN2,B3,NPERT,XX,XY,FREQ3,
    2FREQ2,QMM,NTEST,XLX1,FREQ4,QMM1,NFC,PHEE1,ALIM,FM2,B5,JQ1,
    3 XLX,JQ)
     CALL ARAY(1,N,N,NDIM,FM2)
     CALL ARAY(1,N,N,NDIM,XLX1)
 491 WRITE(6,831) JQ1
 831 FORMAT(/,'  THE NUMBER OF ITERATIVE CYCLES ACTUALLY PERFORMED IS',
    1I4)
  54 WRITE(6,812) JQ
 812 FORMAT(//,' THE BEST FIT  OBTAINED ON ITERATION NUMBER',I4)
     WRITE(6,808)
     DO 813 I=1,N
 813 WRITE(6,809)I,EXFREQ(I),FREQ4(I),QMM1(I),ALIM(I)
     WRITE(6,814)
 814 FORMAT(///,'    THE CORRESPONDING F MATRIX WITH SYMMETRY COORDINATE
    1S IS',/)
     DO 815 I=1,N
 815 WRITE(6,848)  (SYM(I,KJ) ,KJ=1,10),(FM2(I,J),J=1,N)
     IF (IND1)842,842,841
 841 WRITE(6,816)
 816 FORMAT(///,'    THE CORRESPONDING L MATRIX IS',/)
     DO 817 I=1,N
 817 WRITE(6,803)(XLX1(I,J),J=1,N)
 842 IF(IND2)843,843,844
```

```
  844 CALL MATM2(NDIM,EG,FM2,FG,N,N,N)
      DO 870 I=1,N
      DO 870 J=1,N
  870 XLX3(I,J)=XLX1(I,J)
      CALL ARAY(2,N,N,NDIM,XLX3)
      CALL MINV(XLX3,N,D,FN1,FN2)
      CALL ARAY(1,N,N,NDIM,XLX3)
      CALL MATM2(NDIM,XLX3,FG,ALFG,N,N,N)
      CALL MATM2(NDIM,ALFG,XLX1,ALFGL,N,N,N)
      DO 827 I=1,N
      DO 827 J=1,N
  827 CMLFGL(I,J)=1303.16*SQRT(ABS(ALFGL(I,J)))
      WRITE(6,837)
  837 FORMAT(//,'     THE LFGL MATRIX IS',/)
      DO  838 I=1,N
  838 WRITE(6,7803) (CMLFGL(I,J),J=1,N)
 7803 FORMAT(5X,15F8.2)
  843 DO 825 I=1,N
      DO 825 J=1,N
      TEMP=(FREQ4(J)/1303.16)**2
  825 EPOT(I,J)=FM2(I,I)*(XLX1(I,J)**2)/TEMP
      WRITE(6,818)
  818 FORMAT(///,'  THE POTENTIAL ENERGY DISTRIBUTION IS ',/)
      DO 819 I=1,N
  819 WRITE(6,7084) I,(EPOT(I,J),J=1,N)
 7084 FORMAT(3X,I2,15(F8.3)/5X,15(F8.3))
      WRITE(6,851)
  851 FORMAT(//,'   THE BEST FIT UREY-BRADLEY FORCE CONSTANTS WITH THE A
     1PPROPRIATE LABELS ARE'//5(4X,'LABEL',8X,'CONSTANT')/)
      WRITE(6,707) (LABPHE(I),PHEE1(I),I=1,NFO)
      DO 853 I=1,NFO
  853 PHEE(I)=PHEE1(I)
      IF(NTEST1.EQ.0)  GO TO 878
      CALL SIGNIF(NOPHEE,PHEE,Z,NRF,NCF,F,N,NOZ,NFO,NFREQ,FREQ4,
     1 G,E,XL,XLX,XY,NTEST1,LABPHE,NROW,IFINC,QMM2,NTEST2)
  878 WRITE(6,852)
  852 FORMAT(///,2X,110('-')/2X,110('*')/2X,110('-')/)
  900 CONTINUE
   10 CONTINUE
      GO TO 11
      END
```

```
      SUBROUTINE ITER(NRF,NCF,NCPHEE,PHEE,Z,NOZ,N,NROW,F,G,XM,XLX3,AJ,
     1 NDIM,XL,LL,E,NFREQ,NFC,B4,B2,FN1,FN1,B3,NPERT,XX,XY,
     2FREQ3,FREQ2,QMM,NTEST,XLX1,FREQ4,QMM1,NFC,PHEE1,ALIM,
     3 FM2,B5,JQ1,XLX,JC)
      DIMENSION NRF(26),NCF(26),NCPHEE(26),PHEE(7),Z(26),F(1),G(1),
     1  XM(6),XLX3(  6),AJ(  6),XL(6),E(  6),NFC(6),BJ(  6),B2(  6),
     2  FN1(6),FN2(6),B3(  6),XX(6),XY(6),FREQ3(6),FREQ2(6),QMM(6),
     3 XLX1(  6),FREQ4(6),QMM1(6),PHEE1(7),ALIM(6),FM2(  6),B5(  1),
     4 XLX(1)
      DIMENSION NROW(5)
      NN=N*N
      JQ=0
      DO 49 KK = 1,NPERT
      CALL JMAT(NRF,NCF,NCPHEE,PHEE,Z,NOZ,N,NROW,F,G,XM,XLX3,
     1AJ,NDIM,XL,LL, E,NFREQ,NFC)
      CALL FCONST(NRF,NCF,NCPHEE,PHEE,Z,NOZ,N,NROW,F)
      CALL MTRA(AJ,BJ,NFREQ,LL,0)
      CALL MATM(NDIM,BJ,AJ,B2,LL,LL,NFREQ)
      CALL MINV(B2,LL,D,FN1,FN2)
      CALL MATM(NDIM,B2,BJ,B3,LL,NFREQ,LL)
      CALL XMAT(XL,N,NFREQ,NDIM,XX,XY,FREQ3,FREQ2,QMM,NTEST)
      IF(NTEST.LT.0) GO TO 54
  660 IF(KK.NE.1)  GO TO 6003
      DO 6004 I=1,NN
 6004 XLX1(I)=XLX(I)
      DO 6091 I=1,N
      FREQ4(I)=FREQ3(I)
 6091 QMM1(I)=QMM(I)
      DO 6016 I=1,NFO
      PHEE1(I)=PHEE(I)
 6016 CONTINUE
      GO TO 6006
 6003 DO 6007 I=1,NFREQ
      IF(ALIM(I).GT.ABS(QMM(I)))  GO TO 6007
 6009 IF(ABS(QMM(I))-ABS(QMM1(I))) 6007,6006,6006
 6007 CONTINUE
      JQ=KK
      DO 6008 I=1,NN
      XLX1(I)=XLX(I)
 6008 FM2(I)=F(I)
      DO 6017 I=1,N
      QMM1(I)=QMM(I)
 6017 FREQ4(I)=FREQ3(I)
      DO 6014 I=1,NFO
      PHEE1(I)=PHEE(I)
 6014 CONTINUE
 6006 CONTINUE
      JQ1=KK
      DO 51 I=1,NFREQ
      IF(ALIM(I).LT.ABS(QMM1(I)))  GO TO 1250
   51 CONTINUE
      GO TO 54
 1250 CALL MATM(NDIM,B3,XX,B5,LL,1,NFREQ)
```

```
1003 DO 1002 I=1,LL
     IF(0.1-ABS(B5(I))) 1001,1002,1002
1002 CONTINUE
     GO TO 1241
1001 DO 1000 I=1,LL
1000 B5(I)=(B5(I))*0.1
     DO 1004 I=1,LL
     IF(0.1-ABS(B5(I))) 1003,1004,1004
1004 CONTINUE
1241 DO 63 I=1,LL
     PHEE(NFC(I))=PHEE(NFC(I))+B5(I)
  63 CONTINUE
     CALL FCONST(NRF,NCF,NCPHEE,PHEE,Z,NOZ,N,NROW,F)
     DO 64 I=1,NN
  64 XLX3(I)=F(I)
     CALL NRCOTE(N,NROW,F,G,XL,XLX)
     DO 66 I=1,NN
     F(I)=XLX3(I)
  66 G(I)=E(I)
  49 CONTINUE
  54 RETURN
     END
```

```
      SUBROUTINE JMAT1(NRF,NCF,NOPHEE,PHEE,Z,NOZ,N,F,G,XM,XLX,AJ,NDIM,XL
     1 ,LL,E,NFREQ,NFC)
      DIMENSION NOPHEE(500),PHEE(100),Z(500),NFC(100),NRF(500),NCF(500)
      DIMENSION  E(NDIM,NDIM)
      DIMENSION F(NDIM,NCIM)
      DIMENSION XM(NDIM)
      DIMENSION XL(NDIM)
      DIMENSION AJ(NDIM,NDIM)
      DIMENSION G(NCIM,NDIM)
      DIMENSION XLX(NCIM,NDIM)
      MQ = LL + 1
      JJ = 0
      II = 1
   11 TEMP=PHEE(NFC(II))
      PHEE(NFC(II))=PHEE(NFC(II))+0.01
      CALL FCONST(NRF,NCF,NOPHEE,PHEE,Z,NOZ,N,F)
      PHEE(NFC(II))=TEMP
      CALL NROOT(N, F, G, XM, XLX)
      DO 67 I = 1,N
      DO 67 J = 1,N
      G(I,J) = E(I,J)
   67 CONTINUE
      JJ = JJ + 1
      DO 13 JI=1,NFREQ
      AJ(JI,JJ)=ALOG(XM(JI))-ALOG(XL(JI))
   13 CONTINUE
      II = II + 1
      IF(MQ.GT.II)  GO TO 11
      RETURN
      END
```

```
      SUBROUTINE XMAT(XL,N,NFREQ,NDIM,XX,XY,FREQ3,FREQ2,QMM,NTEST)
      DIMENSION XX(NDIM)
      DIMENSION XL(NDIM)
      DIMENSION XY(NDIM)
      DIMENSION FREQ3(NDIM),FREQ2(NDIM)
      DIMENSION QMM(NDIM)
      NTEST=1
      DO 31 I=1,N
      FREQ3(I)=1303.16*SQRT(ABS(XL(I)))
      FREQ2(I)=1303.16*SQRT(ABS(XY(I)))
      QMM(I)=FREQ2(I)-FREQ3(I)
   31 CONTINUE
      DO 10 I=1,NFREQ
      IF(XL(I).LE.0.0)  GO TO 12
   10 CONTINUE
      GO TO 15
   12 WRITE(6,14) I,XL(I)
   14 FORMAT(//,'    THE VALUE OF AN INTERMEDIATE EIGENVALUE WAS LESS TH
     1AN OR EQUAL TO ZERO AND THE ITERATIONS WERE DISCONTINUED'/'    THE
     2VALUE OF XL(',I2,') WAS',F12.6)
      NTEST=-1
      RETURN
   15 CONTINUE
      DO 6032 I=1,NFREQ
 6032 XX(I)=ALOG(XY(I))-ALOG(XL(I))
      RETURN
      END
```

```
      SUBROUTINE NROOTE(M,NRCW,A,B,XL,X)
      DIMENSION A(1),B(1),XL(1),X(1)
      DIMENSION NROW(1)
      K=1
      DO 100 J=2,M
      L=M*(J-1)
      DO 100 I=1,J
      L=L+1
      K=K+1
  100 B(K)=B(L)
C
C        THE MATRIX B IS A REAL SYMMETRIC MATRIX.
C
      MV=0
      CALL EIGENE(B,X,M,MV,NROW)
C
C     FORM RECIPROCALS OF SQUARE ROOT OF EIGENVALUES.  THE RESULTS
C     ARE PREMULTIPLIED BY THE ASSOCIATED EIGENVECTORS.
C
      L=0
      DO 110 J=1,M
      L=L+J
  110 XL(J)=1.0/SQRT(ABS(B(L)))
      K=0
      DO 115 J=1,M
      DO 115 I=1,M
      K=K+1
  115 B(K)=X(K)*XL(J)
C
C     FORM (B**(-1/2))PRIME * A * (B**(-1/2))
C
      DO 120 I=1,M
      N2=0
      DO 120 J=1,M
      N1=M*(I-1)
      L=M*(J-1)+I
      X(L)=0.0
      DO 120 K=1,M
      N1=N1+1
      N2=N2+1
  120 X(L)=X(L)+B(N1)*A(N2)
      L=0
      DO 130 J=1,M
      DO 130 I=1,J
      N1=I-M
      N2=M*(J-1)
      L=L+1
      A(L)=0.0
      DO 130 K=1,M
      N1=N1+M
      N2=N2+1
  130 A(L)=A(L)+X(N1)*B(N2)
C
```

```
C       COMPUTE EIGENVALUES AND EIGENVECTORS OF A
C
        CALL EIGENE(A,X,M,MV,NROW)
        L=0
        DO 140 I=1,M
        L=L+I
  140   XL(I)=A(L)
C
C       COMPUTE THE NORMALIZED EIGENVECTORS
C
        DO 150 I=1,M
        N2=0
        DO 150 J=1,M
        N1=I-M
        L=M*(J-1)+I
        A(L)=0.0
        DO 150 K=1,M
        N1=N1+M
        N2=N2+1
  150   A(L)=A(L)+B(N1)*X(N2)
        MM=M*M
        DO 160 I=1,MM
  160   X(I)=A(I)
        RETURN
        END
```

```
      SUBROUTINE EIGENE(A,R,N,MV,NC)
      DIMENSION A(1),R(1),NC(1)
      IF(MV-1) 10,25,10
   10 IQ=-N
      DO 20 J=1,N
      IQ=IQ+N
      DO 20 I=1,N
      IJ=IQ+I
      R(IJ)=0.0
      IF(I-J) 20,15,20
   15 R(IJ)=1.0
   20 CONTINUE
C
C        COMPUTE INITIAL AND FINAL NORMS (ANORM AND ANORMX)
C
   25 ANORM=0.0
      DO 35 I=1,N
      DO 35 J=I,N
      IF(I-J) 30,35,30
   30 IA=I+(J*J-J)/2
      ANORM=ANORM+A(IA)*A(IA)
   35 CONTINUE
      IF(ANORM) 165,165,40
   40 ANORM=1.414*SQRT(ANORM)
      ANRMX=ANORM*1.0E-12/FLOAT(N)
C
C        INITIALIZE INDICATORS AND COMPUTE THRESHOLD, THR
C
      IND=0
      THR=ANORM
   45 THR=THR/FLOAT(N)
   50 L=1
   55 M=L+1
C
C        COMPUTE SIN AND COS
C
   60 MQ=(M*M-M)/2
      LQ=(L*L-L)/2
      LM=L+MQ
   62 IF(ABS(A(LM))-THR) 130,65,65
   65 IND=1
      LL=L+LQ
      MM=M+MQ
      X=0.5*(A(LL)-A(MM))
   68 Y=-A(LM)/SQRT(A(LM)*A(LM)+X*X)
      IF(X) 70,75,75
   70 Y=-Y
   75 SINX=Y/SQRT(2.0*(1.0+(SQRT(1.0-Y*Y))))
      SINX2=SINX*SINX
   78 COSX=SQRT(1.0-SINX2)
      COSX2=COSX*COSX
      SINCS =SINX*COSX
C
```

```
C         ROTATE L AND M COLUMNS
C
      ILQ=N*(L-1)
      IMQ=N*(M-1)
      DO 125 I=1,N
      IQ=(I*I-I)/2
      IF(I-L) 80,115,80
   80 IF(I-M) 85,115,90
   85 IM=I+MQ
      GO TO 95
   90 IM=M+IQ
   95 IF(I-L) 100,105,105
  100 IL=I+LQ
      GO TO 110
  105 IL=L+IQ
  110 X=A(IL)*COSX-A(IM)*SINX
      A(IM)=A(IL)*SINX+A(IM)*COSX
      A(IL)=X
  115 IF(MV-1) 120,125,120
  120 ILR=ILQ+I
      IMR=IMQ+I
      X=R(ILR)*COSX-R(IMR)*SINX
      R(IMR)=R(ILR)*SINX+R(IMR)*COSX
      R(ILR)=X
  125 CONTINUE
      X=2.0*A(LM)*SINCS
      Y=A(LL)*COSX2+A(MM)*SINX2-X
      X=A(LL)*SINX2+A(MM)*COSX2+X
      A(LM)=(A(LL)-A(MM))*SINCS+A(LM)*(COSX2-SINX2)
      A(LL)=Y
      A(MM)=X
C
C         TESTS FOR COMPLETION
C
C         TEST FOR M = LAST COLUMN
C
  130 IF(M-N) 135,140,135
  135 M=M+1
      GO TO 60
C
C         TEST FOR L = SECOND FROM LAST COLUMN
C
  140 IF(L-(N-1)) 145,150,145
  145 L=L+1
      GO TO 55
  150 IF(IND-1) 160,155,160
  155 IND=0
      GO TO 50
C
C         COMPARE THRESHOLD WITH FINAL NORM
C
  160 IF(THR-ANRMX) 165,165,45
C
```

```
C         SORT EIGENVALUES ANC EIGENVECTORS
C
  165 IQ=-N
      I=1
 1100 I1=I+1
      N2=NC(I1)-2
      IF(NC(I1).EQ.0) N2=N-1
      N1=NC(I)
      IF(N2.LT.N1)  GO TO 111
      N4=N2+1
      DO 1110 J=N1,N2
      K2=J
      KT=(J+J*J)/2
      J2=KT
      N3=J+1
      DO 104 K=N3,N4
      K1=(K+K*K)/2
      IF(A(KT).GT.A(K1)) GO TO 104
      KT=K1
      K2=K
  104 CONTINUE
      TEMP=A(J2)
      A(J2)=A(KT)
      A(KT)=TEMP
      N5=(J-1)*N+1
      N6=(K2-1)*N+1
      DO 106 II=1,N
      TEMP =R(N5)
      R(N5)=R(N6)
      R(N6)=TEMP
      N5=N5+1
  106 N6=N6+1
 1110 CONTINUE
  111 I=I+1
      IF(NC(I).NE.0)  GO TO 1100
      RETURN
      END
```

```
      SUBROUTINE FCON(NRF,NCF,NOPHEE,PHEE,Z,F,N,NOZ)
      DIMENSION NRF(500),NCF(500),NOPHEE(500),PHEE(500),Z(500),F(20,20)
      DO 4 I=1,N
      DO 4 J=1,N
    4 F(I,J) = 0.0
      DO 5 I=1,NOZ
    5 F(NRF(I),NCF(I))= F(NRF(I),NCF(I))+Z(I)*PHEE(NOPHEE(I))
      DO 10 I=1,N
      DO 10 J=1,N
   10 F(J,I)=F(I,J)
      RETURN
      END
```

```
      SUBROUTINE ARRAY (MODE,I,J,N,M,S,D)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION S(1),D(1)
C
      NI=N-I
C
C        TEST TYPE OF CONVERSION
C
      IF(MODE-1) 100, 100, 120
C
C        CONVERT FROM SINGLE TO DOUBLE DIMENSION
C
  100 IJ=I*J+1
      NM=N*J+1
      DO 110 K=1,J
      NM=NM-NI
      DO 110 L=1,I
      IJ=IJ-1
      NM=NM-1
  110 D(NM)=S(IJ)
      GO TO 140
C
C        CONVERT FROM DOUBLE TO SINGLE DIMENSION
C
  120 IJ=0
      NM=0
      DO 130 K=1,J
      DO 125 L=1,I
      IJ=IJ+1
      NM=NM+1
  125 S(IJ)=D(NM)
  130 NM=NM+NI
C
  140 RETURN
      END
```

```
      SUBROUTINE SIGNIF(NCPHEE,PHEE,Z,NRF,NCF,F,N,NOZ,NFO,NFREQ,FREQ4,
     1 G,E,XL,XLX,XY,NTEST1,LABPHE,NROW,IFINC,QMM2,NTEST2,NPUN)
      REAL *8LABPHE
      DIMENSION PHEE(100),Z(500),NCPHEE(500),NRF(500),NCF(500),F(30,30),
     1G(900),E(900),XL(30),XLX(30,30),XY(30),LABPHE(40),FREQ4(30)
      DIMENSION SIGNF(30),NROW(5)
      DIMENSION IFINC(1),QMM2(1)
      NN=N*N
   45 WRITE(6,50)
   50 FORMAT(///5X,'THE NUMBERS IN THIS SIGNIFICANCE MATRIX ARE THE CHAN
     1GES IN THE FREQUENCES DUE TO A CHANGE OF 0.01 IN THE U.B. F. CONST
     2ANTS'//15X,'FREQUENCES',/)
      WRITE(6,685)
      WRITE(6,65) (FREQ4(I),I=1,N)
  685 FORMAT(17X,'1',6X,'2',6X,'3',6X,'4',6X,'5',6X,'6',6X,'7',6X,
     1 '8',6X,'9',5X,'10',5X,'11',5X,'12',5X,'13',5X,'14',5X,'15',1X)
   65 FORMAT(T120,'U.B.F.C.',T15,15(F6.1,1X)/14X,15(F6.1,1X))
      WRITE(6,686) (QMM2(I),I=1,N)
  686 FORMAT(2X,'DIFFERENCES'/T15,15(F6.1,1X)/14X,15(F6.1,1X))
      IZ=1
      DO 10 IK=1,NFO
      IN=0
      IF(NTEST2.EQ.0)  GO TO 13
      IF(IFINC(IZ).NE.IK)  GO TO 10
      IZ=IZ+1
   13 TEMP=PHEE(IK)
      IF(PHEE(IK).GT.0) GO TO 15
      PHEE(IK)=PHEE(IK)+0.01
   15 CALL FCONST(NRF,NCF,NCPHEE,PHEE,Z,NOZ,N,NROW,F)
      CALL NROOTE(N,NROW,F,G,XL,XLX)
      DO 20 I=1,NN
   20 G(I)=E(I)
   21 PHEE(IK)=PHEE(IK)+0.01
      CALL FCONST(NRF,NCF,NCPHEE,PHEE,Z,NOZ,N,NROW,F)
      CALL NROOTE(N,NROW,F,G,XY,XLX)
      DO 25 I=1,NN
   25 G(I)=E(I)
      DO 35 I=1,N
      SIGNF(I)=1303.61*(SQRT(ABS(XY(I)))-SQRT(ABS(XL(I))))
      IF(XL(I).LT.0.0) XL(I)=-XL(I)
      IF(XY(I).LT.0.0) XY(I)=-XY(I)
   35 CONTINUE
      IN=IN+1
      IF(IN.GT.1) GO TO 66
   61 WRITE(6,70)
      WRITE(6,60) TEMP,IK,LABPHE(IK),(SIGNF(J),J=1,N)
      IF(NPUN.EQ.0) GO TO 67
      WRITE(7,71) (SIGNF(J),J=1,15)
   71 FORMAT(8F10.6)
      IF(N.EQ.15)  GO TO 67
      WRITE(7,71) (SIGNF(J),J=16,30)
      GO TO 67
   66 WRITE(6,62) (SIGNF(J),J=1,N)
```

```
67 IF(IN.EQ.NTEST1)  GO TO 30
   GO TO 21
60 FORMAT(T120,F8.5,T2,I2,1X,A8,' I',15(6X,'I'),T15,15(F6.2,'I')/13X,
  1 'I',15(6X,'I'),T15,15(F6.2,'I'))
62 FORMAT(13X,'I',15(6X,'I'),T15,15(F6.2,'I')/13X,
  1'I',15(6X,'I'),T15,15(F6.2,'I'))
70 FORMAT(13X,'*',15(6('-'),'*'))
30 PHEE(IK) = TEMP
10 CONTINUE
   RETURN
   END
```

6. SORT

This program is used to initially sort out the potential energy distribution weightings of the normal coordinates. The input data is identical to that of BRADPERT.

```
      REAL *8LABPHE
      DIMENSION G(900),PHEE(100),NRF(1000),NCF(1000),NOPHEE(1000)
      DIMENSION Z(1000),NROW(5),FN1(30),FN2(30),E(900)
      DIMENSION F(30,30),XL(30),XLX(30,30),FREQ(30)
      DIMENSION NFC(100),LABPHE(100),PHEE1(100)
      DIMENSION RECORD(20),Z1(30,30),SYM(30,30),EXFREQ(30),B(30),XM(30)
      DIMENSION XX(30,1),XY(30),Y(30,30),YZ(30,30),FM2(30,30)
      DIMENSION FREQ1(30),FREQ2(30),FREQ3(30)
      DIMENSION QMM2(30),FREQ4(30),EPOT(30,30),EG(30,30)
      DIMENSION ALFG(30,30),ALFGL(30,30),CMLFGL(30,30),FG(30,30)
      DIMENSION XLX2(30,30) ,ALIM(30)
      DIMENSION IFINC(100)
      NOIM=30
      NUMB=1
      REWIND 15
      REWIND 10
   11 READ(5,5) IND1,IND2,IND3,INDG,INDL,NTEST1,NTEST2,NPUN
    5 FORMAT(10I2)
      IF(IND1.LT.0)  CALL EXIT
      IF(IND3.GT.0)  GO TO 606
  506 READ(5,36) NOZ
      NOZ1 = NOZ + 1
  606 READ(5,5000) (RECORD(I),I=1,20)
 5000 FORMAT(20A4)
      READ(5,15) N,LL,NPERT,NFC
   15 FORMAT(5I3)
      NN=N*N
         READ(5,15) (NROW(I),I=1,5)
      WRITE(6,802) NUMB
  802 FORMAT('1  THIS IS THE MOLECULE NUMBER',I3)
      NUMB=NUMB+1
      READ(5,36) (NFC(I),I=1,LL)
   36 FORMAT(10(2I4))
      IF(IND3.EQ.0)  GO TO 34
      NOZ = 0
      NZ4 = 1
      NZ8 = 4
  131 READ(15) (NRF(I),NCF(I),NOPHEE(I),Z(I),I=NZ4,NZ8)
      DO 133 I=NZ4,NZ8
      IF(NRF(I).EQ.-5)  GO TO 38
      NOZ = NOZ + 1
  133 CONTINUE
      IF(NOZ.GT.500) GO TO 132
      NZ4 = NZ4 + 4
      NZ8 = NZ8 + 4
      GO TO 131
   34 READ(5,134) (NRF(I),NCF(I),NOPHEE(I),Z(I),I=1,NOZ1)
  134 FORMAT(4(3I3,F11.6))
   39 DO 33 I=1,NOZ1
      IF(NRF(I).EQ.-5)  GO TO 38
   33 CONTINUE
  132 WRITE(6,37)
   37 FORMAT(///,'   Z MATRIX READING ERROR, JOB TERMINATED',//)
```

```
      CALL EXIT
   33 CONTINUE
      NOZ1 = NCZ + 1
      READ(5,45) (PHEE(I),I=1,NFC)
      READ(5,5001) (LABPHE(I),I=1,NFO)
5001  FORMAT(10A8)
      READ(5,200) PHEEP,ISOP,NFREQ,AMT
  200 FORMAT(3I4,F10.6)
      READ(5,846) ((SYM(I,J),J=1,10),I=1,N)
  846 FORMAT(2(10A4))
      IF(INDG.EQ.0)  GO TO 601
      READ(10) ((EG(I,J),J=1,N),I=1,N)
      GO TO 602
  601 READ(5,25) ((EG(I,J),J=1,N),I=1,N)
   25 FORMAT(8F10.6)
  602 CALL ARAY(2,N,N,NDIM,EG)
      DO 830 I=1,NN
  830 G(I)=EG(I,1)
      CALL ARAY(1,N,N,NDIM,EG)
   45 FORMAT(8F10.6)
      CALL MINV(G,N,D,FN1,FN2)
      CALL FCONST(NRF,NCF,NCPHEE,PHEE,Z,NOZ,N,NROW,F)
      DO 905 I=1,NN
      E(I)=G(I)
  905 FM2(I,1)=F(I,1)
      DO 958 I=1,NFREQ
  858 ALIM(I)=1.0
      IF(INDL.NE.0)  GO TO 857
      READ(5,2)  (ALIM(I),I=1,NFREQ)
  857 READ(5,2) (EXFREQ(I),I=1,NFREQ)
    2 FORMAT(8F10.6)
      READ(5,36) (IFINC(I),I=1,NFC)
      DO 75 I=1,NFO
      IF(IFINC(I).EQ.0) IFINC(I)=NFO+1
   75 CONTINUE
      DO 76 I=1,NFO
      DO 76 J=I,NFO
      IF(IFINC(I).LE.IFINC(J))  GO TO 76
      IT=IFINC(I)
      IFINC(I)=IFINC(J)
      IFINC(J)=IT
   76 CONTINUE
  854 CONTINUE
      WRITE(6,7001) (RECORD(III),III=1,20)
7001  FORMAT(///,2X,20A4)
      WRITE(6,760)
  760 FORMAT(//,'   THE SYMMETRIZED Z MATRIX IS'/)
      WRITE(6,761) (NRF(I),NCF(I),NCPHEE(I),Z(I),I=1,NOZ1)
  761 FORMAT(6(3I3,F11.6))
      WRITE(6,801)
  801 FORMAT(//,'  THE G MATRIX IS',/)
      DO  804 I=1,N
  804 WRITE(6,803) (EG(I,J),J=1,N)
```

```
 803 FORMAT(5X,15F8.5)
     WRITE(6,706)
 706 FORMAT(///,'    THE TRIAL UREY-BRADLEY FORCE CONSTANTS WITH APPROPR
    1IATE LABELS ARE',/)
     WRITE(6,707)  (LABPHE(I),PHEE(I),I=1,NFO)
 707 FORMAT(4X,'*',2X,A8,F10.6,4X,'*',2X,A8,F10.6,4X,'*',2X,A8,F10.6,
    1 4X,'*',2X,A8,F10.6,4X,'*',2X,A8,F10.6/4X,'*',24X,'*',24X,'*',24X,
    2 '*', 24X,'*',1X)
     WRITE(6,805)
     CALL ARAY(1,N,N,NDIM,F)
 805 FORMAT(///,'    THE TRIAL F MATRIX  LABELED WITH SYMMETRY COORDINAT
    1ES IS',/)
     IF(NPUN.EQ.0)  GO TO 6807
     WRITE(7,6806) ((F(I,J),J=1,N),I=1,N)
6806 FORMAT(8F10.6)
6807  DO  806 I=1,N
 806 WRITE(6,849) (SYM(I,KJ),KJ=1,10),(F(I,J),J=1,N)
 849 FORMAT(1X,10A4,15F6.3/41X,15F6.3/41X,15F6.3)
     DO 850 I=1,N
     IF(F(I,I).LT.0.0)  GO TO 10
 850 CONTINUE
  74 CALL ARAY(2,N,N,NDIM,F)
     CALL NRGOTE(N,NRCW,F,G,XL,XLX)
     DO 65 I=1,NN
     G(I)=E(I)
     F(I,1)=FM2(I,1)
  65 CONTINUE
     DO 651 I=1,N
     IF(XL(I).LE.0.0)  GO TO 652
 651 CONTINUE
     GO TO 653
 652 WRITE(6,654) (XL(I),I=1,N)
 654 FORMAT(///,'     THE RUN ON THIS MOLECULE WILL TERMINATE HERE DUE T
    1O A NEGATIVE EIGENVALUE OF THE FG SECULAR EQUATION'/'    THE EIGEN
    2VALUES ARE'/(10F12.6))
     CALL ARAY(1,N,N,NDIM,F)
     CALL ARAY(1,N,N,NDIM,XLX)
     WRITE(6,656)
 656 FORMAT(/,'     THE EIGENVECTORS ARE',/)
     DO 655 I=1,N
 655 WRITE(6,803)  (XLX(I,J),J=1,N)
     DO 7002 I=1,N
7002 FREQ(I)=1303.61*SQRT(ABS(XL(I)))
     WRITE(6,6008) (FREQ(I),I=1,N)
6008 FORMAT(5X,15F8.3)
     DO 670 I=1,N
     DO 670 J=1,N
 670 EPOT(I,J)=F(I,I)*(XLX(I,J)**2)/XL(J)
     WRITE(6,818)
     GO TO 853
 653 CONTINUE
     DO 6081 I=1,N
     FREQ(I)=1303.16*SQRT(XL(I))
```

```
 6081 CONTINUE
      DO 811 I=1,NFREQ
  811 QMM2(I)=EXFREQ(I)-FREQ(I)
      IF(N-NFREQ)226,226,215
  215 NF=NFREQ+1
      DO 220 I=NF,N
      EXFREQ(I)=0.0
      QMM2(I)=0.0
  220 XX(I,1)=0.0
  226 WRITE(6,807)
  807 FORMAT(///,'  THE RESULT USING THE TRIAL F MATRIX IS',/)
      WRITE(6,808)
  808 FORMAT(25X,'OBSERVED',25X,'CALCULATED',25X,'DIFFERENCE',7X,'DIFF.L
     1IMIT',/)
      DO 810 I=1,N
  810 WRITE(6,809)I,EXFREQ(I),FREQ(I),QMM2(I),ALIM(I)
  809 FORMAT(15X,I2,4('-'),F12.6,23X,F12.6,23X,F12.6,7X,F10.5)
      IF(NPUN.EQ.0)  GO TO 841
      DO 873 I=1,N
  873 WRITE(7,872) EXFREQ(I),FREQ(I),QMM2(I)
  872 FORMAT(3F10.2)
  841 WRITE(6,816)
  816 FORMAT(///,'   THE CORRESPONDING L MATRIX IS',/)
      CALL ARAY(1,N,N,NDIM,XLX)
      DO 817 I=1,N
  817 WRITE(6,803)(XLX (I,J),J=1,N)
      IF(NPUN.EQ.0) GO TO 842
      WRITE(7,6806) ((XLX(I,J),J=1,15),I=1,15)
      IF(N.EQ.15) GO TO 842
      WRITE(7,6806) ((XLX(I,J),J=16,30),I=16,30)
  842 IF(IND2)843,843,844
  844 CALL ARAY(2,N,N,NDIM,EG)
      CALL MATM(NDIM,EG,FM2,FG,N,N,N)
      CALL ARAY(2,N,N,NDIM,XLX)
      DO 870 I=1,NN
  870 XLX2(I,1)=XLX(I,1)
      CALL MINV(XLX2,N,D,FN1,FN2)
      CALL MATM(30,XLX2,FG,ALFG,N,N,N)
      CALL MATM(30,ALFG,XLX ,ALFGL,N,N,N)
      CALL ARAY(1,N,N,NDIM,ALFGL)
      DO 827 I=1,N
      DO 827 J=1,N
  827 CMLFGL(I,J)=1303.16*SQRT(ABS(ALFGL(I,J)))
      WRITE(6,837)
  837 FORMAT(//,'     THE LFGL MATRIX IS',/)
      DO  838 I=1,N
  838 WRITE(6,7803) (CMLFGL(I,J),J=1,N)
 7803 FORMAT(5X,15F8.2)
      CALL ARAY(1,N,N,NDIM,XLX)
  843 CALL ARAY(1,N,N,NDIM,FM2)
      DO 825 I=1,N
      DO 825 J=1,N
      TEMP=(FREQ (J)/1303.16)**2
```

```
  825 EPOT(I,J)=FM2(I,I)*(XLX (I,J)**2)/TEMP
      WRITE(6,818)
  818 FORMAT(///,'  THE POTENTIAL ENERGY DISTRIBUTION IS ',/)
  853 DO 819 I=1,N
  819 WRITE(6,7084) I,(EPOT(I,J),J=1,N)
      IF(NPUN.EQ.0) GO TO 863
      WRITE(7,6806) ((EPOT(I,J),J=1,N),I=1,N)
 7084 FORMAT(3X,I2,15(F8.3)/5X,15(F8.3))
  863 IF(NTEST1.EQ.0)  GO TO 851
      CALL SIGNIF(NOPHEE,PHEE,Z,NRF,NCF,F,N,NOZ,NFC,NFREQ,FREQ ,
     1 G,E,XL,XLX,XY,NTEST1,LABPHE,NROW,IFINC,QMM2,NTEST2,NPUN)
  851 WRITE(6,852)
  852 FORMAT(///,2X,130('-')/2X,130('*')/2X,130('-')/)
  900 CONTINUE
   10 CONTINUE
      GO TO 11
      END
```

7. ZMAT and GMAT COMBINE

This program is used to renumber the Z matrix and reform the G matrix in such a way that two isotopic molecules can be treated simultaneously.

```
      DIMENSION NUM(2,30)
      DIMENSION NOZF(2)
      DIMENSION NR1(2,600),NC1(2,660),NOP1(2,600),Z1(2,600)
      DIMENSION NR(1200),NC(1200),NOP(1200),Z(1200),NRZ(1200),NCZ(1200)
      DIMENSION NOPZ(1200),ZZ(1200)
   11 READ(5,500) N,NCOP,NOZ1,NOZ2
      IF(N.LT.0)  CALL EXIT
      READ(5,501) (NR1(1,I),NC1(1,I),NOP1(1,I),Z1(1,I),I=1,NOZ1)
      READ(5,501) (NR1(2,I),NC1(2,I),NOP1(2,I),Z1(2,I),I=1,NOZ2)
      READ(5,500)(NUM(1,I),I=1,N)
      READ(5,500) (NUM(2,I),I=1,N)
  500 FORMAT(24I3)
  501 FORMAT(4(3I3,F11.6))
      NOZF(1)=NOZ1
      NOZF(2)=NOZ2
      N1=0
      N2=0
      DO 110 IZ=1,2
      N1=N2+1
      N2=NOZF(IZ)+N2
      J=1
      DO 110 I=N1,N2
      NR(I)=NUM(IZ,NR1(IZ,J))
      NC(I)=NUM(IZ,NC1(IZ,J))
      NOP(I)=NOP1(IZ,J)
      Z(I)=Z1(IZ,J)
  110 J=J+1
      N21=N2-1
      DO 120 I=1,N21
      NT=NOP(I)
      I1=I+1
      DO 120 J=I1,N2
      IF(NT.GT.NOP(J))  GO TO 115
      GO TO 120
  115 NT=NOP(J)
      NTEMP=NR(I)
      NOP(J)=NOP(I)
      NOP(I)=NT
      NR(I)=NR(J)
      NR(J)=NTEMP
      NTEMP=NC(I)
      NC(I)=NC(J)
      NC(J)=NTEMP
      TEMP=Z(I)
      Z(I)=Z(J)
      Z(J)=TEMP
  120 CONTINUE
      KT=0
      DO 130 J=1,N2
      IF(Z(J).EQ.0.0)  GO TO 130
      KT=KT+1
      NRZ(KT)=NR(J)
      NCZ(KT)=NC(J)
```

```
      NOPZ(KT)=NOP(J)
      NZ2=NR(J)
      NZ3=NC(J)
      NZ1=NOP(J)
      ZZ(KT)=Z(J)
      J1=J+1
      IF(J1.GT.N2)  GO TO 130
      DO 125 K=J1,N2
      IF(NZ1.LT.NOP(K))  GO TO 130
      IF(NZ2.NE.NR(K))  GO TO 125
      IF(NZ3.NE.NC(K))  GO TO 125
      ZZ(KT)=ZZ(KT)+Z(K)
      Z(K)=0.0
  125 CONTINUE
  130 CONTINUE
      WRITE(6,601) (NRZ(I),NCZ(I),NOPZ(I),ZZ(I),I=1,KT)
      DO 101 J=1,NCOP
  101 WRITE(7,501) (NRZ(I),NCZ(I),NOPZ(I),ZZ(I),I=1,KT)
  601 FORMAT(6(3I3,F11.6))
      GO TO 11
      END
```

```
      DIMENSION G1(30,30),G2(30,30),G(60,60),NUM1(30),NUM2(30)
      WRITE(6,610)
   11 READ(5,500) N,NCOP
      IF(N.LT.0) CALL EXIT
      IF(NCOP.EQ.0) NCOP=1
      READ(5,501) ((G1(I,J),J=1,N),I=1,N)
      READ(5,500) (NUM1(I),I=1,N)
  501 FORMAT(8F10.6)
      READ(5,501) ((G2(I,J),J=1,N),I=1,N)
      READ(5,500) (NUM2(I),I=1,N)
  500 FORMAT(24I3)
      NN = N+N
      DO 10 I=1,NN
      DO 10 J=1,NN
   10 G(I,J)=0.0
      DO 20 I=1,N
      DO 20 J=1,N
      G(NUM1(I),NUM1 (J)) =G1(I,J)
   20 G(NUM2(I),NUM2(J)) = G2(I,J)
      DO 30 I=1,NN
      WRITE(6,600)
   30 WRITE(6,601) (G(I,J),J=1,NN)
  610 FORMAT('1')
  600 FORMAT('0')
  601 FORMAT(10X,15F8.5)
      DO 101 J=1,NCOP
      WRITE(7,501) ((G(I,K),K=1,NN),I=1,NN)
  101 CONTINUE
      GO TO 11
      END
```

B. Basic Assembly Language -- Subroutines

Following are several subroutines called in BRADPERT and SORT and written in B.A.L. to speed up the computational process. The most important subroutines with respect to saving computation time are the two iterative diagonalization routines NROOTE and EIGENE.

```
ITER     START
         SAVE    (14,12),,*
         BALR    2,0
         USING   *,2
         LR      12,13
         LA      13,SAVAR
         ST      12,4(13)
         ST      13,8(12)
         ST      1,SAVARG          SAVE ADD. OF ARG. LIST
         LA      3,0
         L       4,164(1)
         ST      3,0(4)
         LA      4,1
         ST      4,KK
         L       4,48(1)
         ST      4,ARG             ARG IS ARG. LIST FOR MTRA
         L       7,76(1)
         ST      7,ARG+4
         L       8,68(1)
         ST      8,ARG+8
         L       6,60(1)
         ST      6,ARG+12
         L       9,52(1)
         LA      3,ZERO
         ST      3,ARG+16
         ST      9,ARG1            ARG1 IS ARG. LIST OF MATM
         ST      7,ARG1+4
         ST      4,ARG1+8
         L       10,30(1)
         ST      10,ARG1+12
         ST      6,ARG1+16
         ST      6,ARG1+20
         ST      8,ARG1+24
         ST      10,ARG2
         ST      6,ARG2+4
         LA      5,DET
         ST      5,ARG2+8
         LA      5,84(1)
         LA      12,ARG2
         MVC     12(8,12),0(5)
         ST      9,ARG3            ARG3 IS ARG. LIST FOR MATM ALSO
         ST      10,ARG3+4
         ST      7,ARG3+8
         L       5,92(1)
         ST      5,ARG3+12
         ST      6,ARG3+16
         ST      8,ARG3+20
         ST      6,ARG3+24
         L       5,56(1)
         ST      5,ARG4            ARG4 IS ARG. LIST FOR  XMAT
         L       5,24(1)
         ST      5,ARG4+4
         ST      8,ARG4+8
```

```
         ST      9,ARG4+12
         LA      5,100(1)
         LA      12,ARG4+16
         MVC     0(24,12),0(5)
         ST      9,ARG5              ARG5 IS ARG. LIST FOR MATM
         L       5,92(1)
         ST      5,ARG5+4
         L       5,152(1)
         ST      5,ARG5+12
         L       5,100(1)
         ST      5,ARG5+8
         ST      6,ARG5+16
         LA      5,ONE
         ST      5,ARG5+20
         ST      3,ARG5+24
         LA      5,24(1)
         LA      12,ARG6             ARG6 IS ARG. LIST FOR NROOT
         MVC     0(16,12),0(5)
         L       5,160(1)
         ST      5,ARG6+20
         L       5,56(1)
         ST      5,ARG6+16
         L       5,24(1)
         L       5,0(5)
         LR      9,5
         SR      4,4
         MR      4,5
         LR      12,5
         LA      11,256
         LA      3,1
         L       5,136(1)
         L       5,0(5)
         SLL     5,2
         SR      4,4
         DR      4,11
         SR      4,3
         SR      5,3
         ST      5,NF04
         ST      4,REM2
         LR      5,12
         SLL     5,2
         SR      4,4
         DR      4,11
         SR      5,3
         ST      5,NSQ4
         SR      4,3
         ST      4,REM
         SLL     9,2
         SR      8,8
         DR      8,11
         SR      9,3
         ST      9,N4
         SR      8,3
```

```
         ST      8,REM1
         L      4,96(1)
         L       4,0(4)
         SR      4,3
LOOP     ST      4,NPERT
         L       15,JMA
         BALR    14,15
         L       15,FCON
         BALR    14,15              CALL FCONST
         LA      1,ARG
         L       15,MTR
         BALR    14,15
         LA      1,ARG1
         L       15,MAT
         BALR    14,15
         LA      1,ARG2
         L       15,MIN
         BALR    14,15
         LA      1,ARG3
         L       15,MAT
         BALR    14,15
         LA      1,ARG4
         L       15,XMA
         BALR    14,15
         L       1,SAVARG
         L      5,120(1)
         LA      4,0
         CR      5,4
         BC      4,RET
         L       5,KK
         LA      3,1
         CR      5,3
         BC      7,GT1
         L       4,NSQ4
         L       8,REM
         LNR     5,3
         LA      6,0
         L      7,160(1)
         L      9,124(1)
         CR      4,6
         BC      4,XLXA
         LA      3,256
XLX      MVC     0(256,9),0(7)
         AR      7,3
         AR      9,3
         BXH     4,5,XLX
XLXA     STC     8,MVCINS1+1
MVCINS1  MVC     0(1,9),0(7)
         L      7,128(1)
         L      9,108(1)
         L       4,N4
         L       8,REM1
         LR      10,4
```

```
         CR      4,6
         BC      4,FREQA
FREQ     MVC     0(256,9),0(7)
         AR      7,3
         AR      9,3
         BXH     4,5,FREQ
FREQA    STC     8,MVCINS2+1
MVCINS2  MVC     0(1,9),0(7)
         LR      4,10
         L      7,116(1)
         L      9,132(1)
         CR      4,6
         BC      4,QMMA
QMM      MVC     0(256,9),0(7)
         AR      7,3
         AR      9,3
         BXH     4,5,QMM
QMMA     STC     8,MVCINS3+1
MVCINS3  MVC     0(1,9),0(7)
         L       7,12(1)
         L      9,140(1)
         L       4,NFG4
         L       8,REM2
         CR      4,6
         BC      4,PHEEA
PHEE     MVC     0(256,9),0(7)
         AR      7,3
         AR      9,3
         BXH     4,5,PHEE
PHEEA    STC     8,MVCINS4+1
MVCINS4  MVC     0(1,9),0(7)
         BC     15,BB
GT1      L      4,68(1)
         L       4,0(4)              GR4=NFREQ
         L      7,144(1)
         L       5,=F'-1'
         L      9,132(1)
         L      8,116(1)
         LA      11,0
         LA      12,4
TEST1    LE      4,0(11,8)
         LPER    2,4                 FPR2=ABS(QMM(I))
         CE      2,0(11,7)
         BC      13,AA
         LE      4,0(11,9)
         LPER    0,4
         CER     0,2
         BC      13,BB
AA       AR      11,12
         BXH     4,5,TEST1
         L       3,KK
         L      4,164(1)
         ST      3,0(4)
```

```
         L      4,NSQ4
         L      7,REM
         L      3,124(1)
         L      8,160(1)
         LR     9,4
         CR     4,6
         BC     4,A2
         LA     11,256
A1       MVC    0(256,3),0(8)
         AR     3,11
         AR     8,11
         BXH    4,5,A1
A2       STC    7,A3+1
A3       MVC    0(1,3),0(8)
         LR     4,9
         L      3,148(1)
         L      8,32(1)
         CR     4,6
         BC     4,A5
A4       MVC    0(256,3),0(8)
         AR     3,11
         AR     8,11
         BXH    4,5,A4
A5       STC    7,A6+1
A6       MVC    0(1,3),0(8)
         L      3,132(1)
         L      8,116(1)
         L      4,N4
         L      7,REM1
         LR     9,4
         CR     4,6
         BC     4,A8
A7       MVC    0(256,3),0(8)
         AR     3,11
         AR     8,11
         BXH    4,5,A7
A8       STC    7,A9+1
A9       MVC    0(1,3),0(8)
         L      3,128(1)
         L      8,104(1)
         LR     4,9
         CR     4,6
         BC     4,A11
A10      MVC    0(256,3),0(8)
         AR     3,11
         AR     8,11
         BXH    4,5,A10
A11      STC    7,A12+1
A12      MVC    0(1,3),0(8)
         L      4,NFO4
         L      7,REM2
         L      8,12(1)
         L      3,140(1)
```

```
         CR      4,6
         BC      4,A14
A13      MVC     0(256,3),0(8)
         AR      3,11
         AR      3,11
         BXH     4,5,A13
A14      STC     7,A15+1
A15      MVC     0(1,3),0(8)
BB       L       3,KK
         L       4,156(1)
         ST      3,0(4)              JQ1=KK
         LE      6,PT1
         L       4,60(1)
         L       4,0(4)
         AR      4,5
         LR      10,4
         L       3,144(1)
         L       8,132(1)
         LA      7,0
         LA      9,4
A16      LE      0,0(7,8)            FPR0=QMM
         LPER    2,0
         CE      2,0(7,3)
         BC      11,CC
         AR      7,9
         BXH     4,5,A16
         BC      15,RET
CC       L       15,MAT
         LA      1,ARG5
         BALR    14,15
         L       1,SAVARG
         LE      6,PT1
A20      LR      4,10
         LA      7,0
A17      LE      0,0(7,3)
         LPER    2,0
         CER     2,6
         BC      2,DD
         AR      7,9
         BXH     4,5,A17
         BC      15,EE
DD       LR      4,10
         LA      7,0
A18      LE      2,0(7,3)
         MER     2,6
         STE     2,0(7,3)
         AR      7,9
         BXH     4,5,A18
         LR      4,10
         LA      7,0
A19      LE      0,0(7,3)
         LPER    2,0
         CER     2,6
```

```
         BC      2,A20
         AR      7,9
         BXH     4,5,A19
EE       LR      4,10
         LA      7,0
         L       10,72(1)
         L       8,12(1)
A21      L       11,0(7,10)
         AR      11,5
         SLL     11,2
         LE      0,0(11,8)
         AE      0,0(7,3)
         STE     0,0(11,8)
         AR      7,9
         BXH     4,5,A21
         L       15,FCCN
         BALR    14,15
         L       4,NSQ4
         L       10,REM
         L       8,32(1)
         L       3,44(1)
         LA      11,256
         CR      4,6
         BC      4,FF1
FF2      MVC     0(256,3),0(8)
         AR      3,11
         AR      8,11
         BXH     4,5,FF2
FF1      STC     10,FF4+1
FF4      MVC     0(1,3),0(8)
         LA      1,ARG6
         L       15,NRG
         BALR    14,15
         L       1,SAVARG
         L       4,NSQ4
         L       10,REM
         L       3,32(1)
         L       8,44(1)
         CR      4,6
         BC      4,FF5
FF6      MVC     0(256,3),0(8)
         AR      3,11
         AR      8,11
         BXH     4,5,FF6
FF5      STC     10,*+5
         MVC     0(1,3),0(8)
         L       4,NSQ4
         L       10,REM
         L       3,36(1)
         L       8,64(1)
         CR      4,6
         BC      4,FF
A22      MVC     0(256,3),0(8)
```

```
         AR      3,11
         AR      8,11
         BXH     4,5,A22
FF       STC     10,A23+1
A23      MVC     0(1,3),0(8)
         L       4,KK
         SR      4,5
         ST      4,KK
         L       4,NPERT
         BXH     4,5,LOOP
RET      L       13,4(13)
         RETURN  (14,12)
FCON     DC      V(FCONST)
JMA      DC      V(JMAT)
MTR      DC      V(MTRA)
MAT      DC      V(MATM)
MIN      DC      V(MINV)
XMA      DC      V(XMAT)
NRO      DC      V(NROOTE)
SAVAR    DS      18F
ARG      DS      5F
ARG1     DS      7F
ARG2     DS      5F
ARG3     DS      7F
ARG4     DS      10F
ARG5     DS      7F
ARG6     DS      6F
JJ       DS      1F
JJ1      DS      1F
KK       DS      1F
ZERO     DC      F'0'
SAVARG   DS      1F
PT1      DC      E'0.1'
DET      DS      1F
NFU4     DS      1F
REM2     DS      1F
ONE      DC      F'1'
NSW4     DS      1F
REM      DS      1F
N4       DS      1F
REM1     DS      1F
NPERT    DS      1F
         LTORG
         END     ITER
```

```
NRTE     TITLE 'SINGLE PRECISION VERSION OF SSP PROGRAM NROOT'
         LCLC  &T,&TT
         LCLA  &A,&S
NROOTE   START 0
*        CALL NRCCTE(N,NROW,A,B,XL,X(,J))
*        THE ONLY DIFFERENCE IN THE CALLING SEQUENCES BETWEEN THIS
*        ROUTINE AND NRCCT IS THAT THE PRESENCE OF A SIXTH ELEMENT IN THE
*        LIST WILL CAUSE NRCCTE TO PESS AN ARGUMENT TO EIGENE INSTRUCTING
*        EIGENE NOT TO SORT THE EIGENVECTORS AND EIN
*        EIGENE NOT TO SORT THE EIGENVECTORS AND EIGENVALUES. %THE VALUE
*        OF J IS IRRELEVANT<.
*
*        PROGRAMMING CONSIDERATIONS..
*           THIS PROGRAM EXPECTS FORTRAN TO FLAG THE LAST ITEM IN ITS
*        ARGUMENT LIST WITH A X'80'. IF IF THIS X'80' IS NOT IN THE
*        BYTE OF X BUT IS IN FACT PLACED FOUR BYTES LATER IN THE ARGUMENT
*        LIST NROOTE WILL DECIDE THAT A SIXTH ARGUMENT IS PRESENT AND
*        NOT PERMIT THE EIGENVALUES % AND EIGENVECTORS < TO BE SORTED.
           PRINT NOGEN
*
*          BAL PROGRAM TO SUBSTITUTE FOR NROOT  TO CONSERVE TIME
*
&T       SETC  'E'                    EXPAND SHORT FORM
&TT      SETC  'E'
&A       SETA  4
&S       SETA  2
         B     84(15)
         DC    AL1(6),C'NRCCTE',18F'0'
         STM   14,12,12(13)
         LR    12,13
         LA    13,12(15)
         ST    12,4(13)
         ST    13,8(12)
         USING NROOTE+12,13
         SPACE
*        POINTER CONVENSICNS USED FOR ACCRESSING THE 4 ARRAYS
         SPACE
*        GR 9  A
*        GR 10 B
*        GR 11 XL
*        GR 12 X
         SPACE 2
         L     5,4(0,1)
         ST    5,ARG+16
         LM    9,12,8(1)
         LTR   12,12
         BL    *+18
         CLI   24(1),X'80'
         BNE   *+10
         MVC   MV,FTWO
         L     1,0(1)
         L     8,0(1)
         ST    8,M
```

```
         LR    4,8                    STORE IN R 4 FOR NEXT STEP
*        COMPUTE THE CONSTANTS WHICH ARE DEPENDANT ON M FOR LATER USE
         SLL   8,&S
         ST    8,M4
         LR    7,8
         S     7,FOUR
         ST    7,M4M4
         SPACE
*        CONVERT THE GENERAL MATRIX B TO SYMMETRIC MODE USING MVC INSTR
         SPACE
         LR    2,10                   ADDB IN GR 2
         LA    2,&A.(2)
         LA    3,0(8,10)
         LA    5,&A+&A-1
*                                     MINUS 1 (BECAUSE OF THE EXECUTE INSTRUC-
*                                     TION WHICH WILL BE USED LATER).
         BCTR  4,0                       C( R4 )= M-1
MOVE     LR    7,5
         LR    0,3
         SR    6,6
         D     6,F256                 THE NUMBER OF CHARACTERS TO BE MOVED C(R
*                                     DIVIDED BY 256 YIELDS IN GR 7 THE NUMBER
*                                     THAT 256 CHARACTERS MUST BE MOVED AND IN
*                                     THE RESIDUE WHICH WILL BE MOVED BY THE
*                                     EXECUTE INSTRUCTION.
         LTR   7,7
         BE    *+22
         MVC   0(256,2),0(3)
         LA    2,256(2)
         LA    3,256(3)
         BCT   7,*-14
         LTR   6,6
         BE    *+12
         EX    6,MVC
         LA    2,1(2,6)
         LR    3,0
         AR    3,8
         LA    5,&A.(5)
         BCT   4,MOVE
         ST    10,ARG
         ST    12,ARG+4
         LA    1,ARG
         L     15,AEIGEN
         BALR  14,15
*        FORM RECIPROCALS
         SR    2,2
         LR    3,2
         LA    4,&A
         L     5,M4M4
RECIP    EQU   *
         LE&T  0,0(10,2)
         LPE&T.R 0,0
         STE&T 0,TEMP
```

```
                LA      1,ARG2
                L       15,ASQRT
                BALR    14,15
                L&T     4,ONE
                D&T.R   4,0
                LA      2,&A+&A.(2,3)
                ST&T    4,0(11,3)
                BXLE    3,4,RECIP
                SR      3,3
                LR      2,3
LOADO           L&T     0,0(11,3)
                L       1,M
LOAD4           L&T     4,0(12,2)
                M&T.R   4,0
                ST&T    4,0(10,2)
                LA      2,&A.(2)
                BCT     1,LOAD4
                BXLE    3,4,LOADO
                LM      1,3,LOOPER
ILOOP1          LR      8,9
                SR      0,0
JLOOP1          LR      7,1
                SR      6,6
                M       6,M
                S&T.R   0,0
                L       5,M
KLOOP1          L&T     4,0(8)
                M&T     4,0(10,7)
                A&T.R   0,4
                LA      7,&A.(7)
                LA      8,&A.(8)
                BCT     5,KLOOP1
                LR      7,0
                M       6,M
                AR      7,1
                ST&T    0,0(12,7)
                BXLE    0,2,JLOOP1
                BXLE    1,2,ILOOP1
                LR      8,9
                LR      5,3
                SR      3,3
                LA      4,&A
                LR      2,4
JLOOP2          SR      1,1
                LR      15,3
                M       14,M
ILOOP2          S&T.R   0,0
                LR      7,15
                LR      6,1
                L       0,M
KLOOP2          L&T     4,0(10,7)
                M&T     4,0(12,6)
                A&T.R   0,4
```

```
         LA     7,&A.(7)
         A      6,M4
         BCT    0,KLOOP2
         ST&T   0,0(8)
         LA     8,&A.(8)
         BXLE   1,2,ILOOP2
         BXLE   3,4,JLOOP2
         ST     9,ARG
         LA     1,ARG
         L      15,AEIGEN
         BALR   14,15
         SR     2,2
         LR     3,2
LOOP     EQU    *
         L&T    0,0(9,2)
         ST&T   0,0(11,3)
         LA     2,&A+&A.(2,3)
         BXLE   3,4,LOOP
         LM     1,3,LOOPER
ILOOP3   LR     8,12
         SR     0,0
         LR     7,1
JLOOP3   LR     5,1
         S&T.R  0,0
         L      6,M
KLOOP3   L&T    4,0(8)
         M&T    4,0(5,10)
         A&T.R  0,4
         LA     8,&A.(8)
         A      5,M4
         BCT    6,KLOOP3
         ST&T   0,0(9,7)
         A      7,M4
         BXLE   0,2,JLOOP3
         BXLE   1,2,ILOOP3
         LR     6,12
         L      2,M
         LR      5,2
         MR      4,5
         SLL     5,2
         LA      3,256
         DR      4,3
         LA      11,1
         SR      4,11
         CR      11,5
         BC      2,BB
         LNR     11,11
         AR      5,11
B        MVC     0(256,6),0(9)
         AR      6,3
         AR      9,3
         BXH     5,11,B
BB       STC     4,BB1+1
```

```
BB1       MVC    0(1,6),0(9)
          XC     MV,MV
          L      13,4(13)
          LM     14,12,12(13)
          BR     14
ASQRT     DC     V(SQRT)
ARG2      DC     A(TEMP)
TEMP      DS     &T
J         DS     0F
JINDEX    DS     3F
I         DS     0F
IINDEX    DS     3F
M         DS     F
MV        DC     F'0'
FTWO      DC     F'2'
F256      DC     F'256'
ARG       DS     2F
          DC     A(M,MV)
          DS     1F
AEIGEN    DC     V(EIGENE)
ONE       DC     &T'1.'
M4        DS     F
LOOPER    DC     F'0,4'
FOUR      EQU    LOOPER+4
M4M4      DS     F
MVC       MVC    0(1,2),0(3)
          END    NROOTE
```

```
FONE     TITLE 'SINGLE PRECISION VERSION OF SSP PROGRAM EIGEN'
         LCLC  &T,&TT
         LCLA  &A,&S
EIGENE   START 0
*
*       THE FOLLOWING MODIFICATION HAS BEEN MADE
*
*       MV = 0 IMPLIES THE SAME AS THE SSP VERSION (EIGENVECTORS AND A
*              SORT OF THE EIGENVALUES AT THE END OF THE COMPUTATIONS)
*
*       MV = 1 IMPLIES THE SAME AS THE SSP VERSION (NO EIGENVECTORS BUT
*              SORT THE EIGENVALUES)
*
*       MV = 2 IS THE SAME AS ( MV = 0 ) BUT NO SORT WILL BE PERFORMED.
*
*       MV = 3 IS THE SAME AS ( MV = 1 ) BUT NO SORT WILL BE PERFORMED.
*
&T       SETC  'E'
&TT      SETC  'G'
&A       SETA  4
&S       SETA  2
F         EQU   3
         B     84(0,15)
         DC    AL1(6),C'EIGENE',18F'0'
         STM   14,12,12(13)
         LR    12,13
         LA    13,12(15)
         ST    13,8(12)
         ST    12,4(13)
         USING EIGENE+12,13
         LM    11,12,0(1)          R 11 PTS TO A  R 12 PTS TO R
         LM    2,3,8(1)
         ST    1,SAVARG
         L     2,0(2)
         L     3,0(3)
         SR    0,0
         LA    8,&A                R8 WILL CONTAIN THE WORD LENGTH
         ST    3,MV2
         C     3,FTWO
         BL    *+8
         S     3,FTWO
         C     3,FONE
         BE    *+6
         LR    3,0
         STM   2,3,N
         ST    2,FN
         OI    FN,X'46'            CONVERT N TO UNNORMALIZED REAL NUMBR
         LR    1,2
         SLL   1,&S
         ST    1,N4
         BCTR  2,0
         ST    2,NM1
         LR    1,2
```

```
         SLL   1,&S
         ST    1,NM1T4
         S     1,FOUR
         ST    1,NM2T4
         CR    3,0
         BNE   N25
         L&T   0,EONE
         L&T   4,EO
         LR    10,12
         ST&T  0,0(10)
         LA    10,&A.(10)
         LA    3,1(2)
LOOP     LR    4,3
         ST&T  4,0(10)
         LA    10,&A.(10)
         BCT   4,LOOP+2
         ST&T  0,0(10)
         LA    10,&A.(10)
         BCT   2,LOOP
N25      EQU   *
         S&T.R 0,0
*        FOLLOWING LOOPS ARE TO SUM THE SQUARES OF THE OFF DIAGONAL
*        ELEMENTS OF A TO FORM A CONVERGENCE CRITERION.
         LR    10,11
         L     2,NM1
         LA    3,1
LOOP2    LR    4,3
         LA    10,&A.(10)
         L&T   4,0(10)
         M&T.R 4,4
         A&T.R 0,4
         BCT   4,LOOP2+2
         LA    10,&A.(10)
         LA    3,1(3)
         BCT   2,LOOP2
         M&T   0,ETWO
         ST&T  0,TEMP
         LA    1,ARG
         L     15,ASQRT
         BALR  14,15
         SR     0,0
         ST&T  0,ANORM
         LE    0,ANORM
         L&T.R 4,0
         M&T   4,RANGE
         D&T   4,FN
         ST&T  4,ANRMX
         ST    0,IND
N45      D&T   0,FN
         ST&T  0,THR
*        INITIALIZE LOOPS
N50      LR    6,0
         LR    5,6
```

```
         LR     7,6
LLOOP    STM    5,7,ILQ
N55      LA     6,&A.(6,7)
         LA     7,&A.(7)
         A      5,N4
MLOOP    STM    5,7,IMQ
         A      6,L
         L&T    0,0(6,11)
         LP&T.R                      0,0
         C&T    0,THR
         BL     N130
         ST     11,IND               STORE NON ZERO IN IND
         ST     6,LM
         L      2,L
         A      2,LQ
         L      3,M
         A      3,MQ
         STM    2,3,LL
         L&T    4,0(2,11)
         S&T    4,0(3,11)
         M&T    4,HALF
         ST&T   4,X
         M&T.R  4,4
         M&T.R  0,0
         A&T.R  0,4
         ST&T   0,TEMP               STORE ARGUMENT AND LOAD
         LA     1,ARG                ARGUMENT LIST POINTER
         L      15,ASQRT             ADDR OF SQUARE ROOT ROUTINE
         BALR   14,15
         L&T    4,0(6,11)
         D&T.R  4,0
         L&T    0,X
         LT&T.R                      0,0
         BL     *+6                  IF X.LT.0 THEN Y = + C( FR 4 )
*                                                 ELSE Y = - C( FR 4 )
         LC&T.R                      4,4
         ST&T   4,Y
         M&T.R  4,4
         L&T    0,EONE
         S&T.R  0,4
         ST&T   0,TEMP               STORE ARGUMENT AND LOAD
         LA     1,ARG                ARGUMENT LIST POINTER
         L      15,ASQRT             ADDR OF SQUARE ROOT ROUTINE
         BALR   14,15
         A&T    0,EONE
         M&T    0,ETWO
         ST&T   0,TEMP
         LA     1,ARG
         L      15,ASQRT
         BALR   14,15
         L&T    4,Y
         D&T.R  4,0
         ST&T   4,SINX
```

```
         M&T.R 4,4
         ST&T  4,SINX2
         L&T   0,EONE
         S&T.R 0,4
         ST&T  0,TEMP              STORE ARGUMENT AND LOAD
         LA    1,ARG               ARGUMENT LIST POINTER
         L     15,ASQRT            ADDR OF SQUARE ROOT ROUTINE
         BALR  14,15
         SR     0,0
         ST&T  0,COSX
         L&T.R 4,0
         M&T.R 0,0
         ST&T  0,COSX2
         M&T   4,SINX
         ST&T  4,SINCS
*        SET UP DO 125
         L     9,NMIT4
         LR    7,0
         LR    6,7                 R 6 = IQ
ILOOP    C     7,L
         BE    N115
         BH    *+14
         LR    5,7                 IL
         A     5,LQ                IN GR 5
         B     *+10
         LR    5,6
         A     5,L
         C     7,M
         BE    N115
         BH    *+14
         LR    4,7                 IM
         A     4,MQ                IN GR 4
         B     *+10
         LR    4,6
         A     4,M
N110     L&T   0,0(5,11)
         L&T   4,0(4,11)
         L&T.R 2,0
         L&T.R 6,4
         M&T   0,COSX
         M&T   2,SINX
         M&T   4,SINX
         M&T   6,COSX
         S&T.R 0,4
         A&T.R 2,6
         ST&T  0,0(5,11)
         ST&T  2,0(4,11)
N115     EQU   *
         C     0,MV
         BNE   N125
         L     5,ILQ
         AR    5,7
         L     4,IMQ
```

```
                AR      4,7
                L&T     0,0(5,12)
                L&T     4,0(4,12)
                L&T.R   2,0
                L&T.R   6,4
                M&T     0,COSX
                M&T     2,SINX
                M&T     4,SINX
                M&T     6,COSX
                S&T.R   0,4
                A&T.R   2,6
                ST&T    0,0(5,12)
                ST&T    2,0(4,12)
N125            EQU     *
                LA      6,&A.(6,7)
                BXLE    7,8,ILCCP
                LM      4,6,LM                  LM,LL,MM
                AR      4,11
                AR      5,11
                AR      6,11
                L&T     0,0(5)
                L&T     2,0(6)
                L&T.R   4,0
                L&T.R   6,2
                M&T     0,COSX2
                M&T     2,SINX2
                M&T     4,SINX2
                M&T     6,COSX2
                A&T.R   0,2
                A&T.R   4,6
                L&T     6,ETWO
                L&T     2,0(4)
                M&T.R   6,2
                M&T     6,SINCS
                S&T.R   0,6                     Y
                A&T.R   4,6                     X
                L&T     6,COSX2
                S&T     6,SINX2
                M&T.R   2,6
                L&T     6,0(5)
                S&T     6,0(6)
                M&T     6,SINCS
                A&T.R   2,6
                ST&T    2,0(4)
                ST&T    0,0(5)
                ST&T    4,0(6)
N130            LM      5,9,IMQ
                A       5,N4
                LA      6,&A.(6,7)
                BXLE    7,8,MLOOP
N140            LM      5,9,ILQ
                A       5,N4
                LA      6,&A.(6,7)
```

```
         BXLE   7,8,LLOOP
         C      0,IND
         BNE    *+12
         ST     0,IND
         B      N50
         L&T    0,THR
         C&T    0,ANRMX
         BH     N45
         CLC    MV2,FTWO
         BE     RETURN
N165     EQU    *
         SR     0,0
         L      1,SAVARG
         L      4,16(1)          GR4=ADD OF NROW VECTOR
         L      2,N
*  GR11  IS ADD OF A VECTOR MATRIX
*  GR12 IS ADD OF B VECTOR MATRIX
         LA     5,0
         LA     6,1
         LA     3,2              GR3=2
         ST     5,I              STORE VALUE OF I
N100     LR     10,5             GR10=I
         SLL    10,2             R10=I*4
         L      10,0(10,4)       R10=NROW(I) = N1
         AR     5,6              R5=I1 = I+1
         SLL    5,2              R5=I1*4
         L      5,0(5,4)         R5=NROW(I1)
         CR     5,0              COMPARE NROW(I1) TO 0
         BC     8,*+10           BRANCH IF EQUAL
         SR     5,3              R5=N2=NROW(I1)-2
         BC     15,*+8           UNCONDITIONAL BRANCH
         LR     5,2              R5=N
         SR     5,6              R5=N2=N-1
         CR     5,10             COMPARE N2 TO N1
         BC     4,N111           BRANCH ON N2.LT.N1
         LR     8,5              R8=N2
         AR     8,6              R8=N4=N2+1
         ST     8,N4             STORE N4
         ST     5,N2             STORE N2
L110     LR     9,10             R9=J
         ST     9,J              STORE J
         ST     9,K2             STORE K2
         MR     8,9              R9=J*J
         AR     9,10             R9=J+J*J
         SRL    9,1              R9=(J+J*J)/2=KT
         SR     9,6              J2=KT=KT-1  (FOR INDEXING)
         ST     9,J2             STORE J2
         AR     10,6             R10=J+1=N3
         LR     7,9              R7=KT
         SLL    7,2              R7=KT*4
L104     LR     9,10             R9=K
         MR     8,9              R9=K*K
         AR     9,10             R9=K+K*K
```

```
         SR     9,3              USED FOR INDEXING
         SLL    9,1              R9=((K+K*K)/2)4=K1*4
         LE     2,0(7,11)        FPR2=A(KT)
         LE     4,0(9,11)        FPR4=A(K1)
         CER    2,4              COMPAREA(KT) TO A(K1)
         BC     2,N104           BRANCH ON A(KT).GT.A(K1)
         LR     7,9              KT=K1
         ST     10,K2            K2=K
N104     LR     8,6              INDEXER
         L      9,N4             R9=N4
         BXLE   10,8,L104        BRANCH TO L104 IF K.LE.N4
         L      8,J2             R8=J2
         SLL    8,2              R8=J2*4
         LE     6,0(8,11)        FPR6=A(J2)
         LE     4,0(7,11)        FPR4=A(KT)
         STE    4,0(8,11)        A(J2)=A(KT)
         STE    6,0(7,11)        A(KT)=TEMP
         L      9,J              R9=J
         SR     9,6              R9=J-1
         MR     8,2              R9=(J-1)*N
         LR     7,9              R7=(J-1)*N
         L      9,K2             R9=K2
         SR     9,6              R9=K2-1
         MR     8,2              R9=(K2-1)*N
         SLL    7,2              R7=(J-1)*N*4 = N5
         LR     15,9             R15= (K2-1)*N
         SLL    15,2             R15= (K2-1)*N*4 = N6
         LR     9,2              R9=N
         LA     10,1             R10=1
         LR     8,6              INDEXER
L106     LE     6,0(7,12)        FPR6=B(N5)
         LE     4,0(15,12)       FPR4=B(N6)
         STE    6,0(15,12)       B(N6)=B(N5)   (TEMP)
         STE    4,0(7,12)        B(N5)=B(N6)
         LA     7,4(7)           N5=N5+1
         LA     15,4(15)         N6=N6+1
         BXLE   10,8,L106        BRANCH TO L106 IF II.LE.N
         L      10,J             R10=J
         LR     8,6              INDEXER
         L      9,N2             R9=N2
         BXLE   10,8,L110        BRANCH TO L110 IF J.LE.N2
N111     L      8,I              R8=I
         AR     8,6              R8=I+1
         ST     8,I              R8=I=I+1
         LR     5,8              R5=NEW I
         SLL    8,2              R8=I+1)*4
         L      9,0(8,4)         R9=NROW(I)
         CR     9,0              COMPARE NROW(I) TO 0
         BC     7,N100           IF(NROW(I).NE.0) BRANCH TO N100
RETURN   EQU    *
         L      13,4(13)
         LM     14,12,12(13)
         BR     14
```

```
RANGE    DC    &TT'1.E-6'
ZERO     DC    &TT'0.'
HALF     DC    &TT'.5'
ONE      DC    &TT'1.'
TWO      DC    &TT'2.'
FN       DC    &TT'0'
ANORM    EQU   *
THR      DS    &TT
TEMP     DS    &TT
ANRMX    DS    &TT
X        DS    &TT
Y        DS    &TT
SINX     DS    &TT
COSX     DS    &TT
SINX2    DS    &TT
COSX2    DS    &TT
SINCS    DS    &TT
ARG      DC    A(TEMP)
ASQRT    DC    V(SQRT)
N        DS    F
MV       DS    F
NM1      DS    F
IND      DS    F
FONE     DC    F'1'
ILO      DS    F
LO       DS    F
L        DS    F
FOUR     DC    F'&A'
NM2I4    DS    F
IHI      DS    F
MU       DS    F
M        DS    F
         DC    F'&A'
NM1I4    DS    F
N4       DS    F
LM       DS    F
LL       DS    F
MM       DS    F
MV2      DS    F
FTWO     DC    F'2'
I        DS    1F
N2       DS    1F
J        DS    1F
K2       DS    1F
J2       DS    1F
SAVARG   DS    F
         END
```

```
JMAT     START
         SAVE    (14,12),,*
         BALR    2,0              REDUCE REG 2 BY 1
         USING   *,2
         LR      12,13
         LA      13,SAVAREA
         ST      12,4(13)
         ST      13,8(12)
         LA      10,1             GR10 = 1
         LNR     10,10            GR10=-1
         ST      1,SAVARG         STORE ADDRESS OF ARGUMENT LIST
         L       9,24(1)          GR9 = VALUE OF N
         L       9,0(9)
         ST      9,NN
         LA      11,0
         LR      5,9              GR5=N
         LR      12,9
         SLL     5,2              GR5=N*4
         BCTR    5,0
         STC     5,E+1            STORE N*4-1 IN MVC INSTRUCTION
         L       6,56(1)
         LA      5,XL
E        MVC     0(1,5),0(6)
         LA      5,4              GR5=4
         LA      6,XL             GR6=ADDRESS OF TEMP XL VECTOR
         LA      7,0              GR7=0
F        LA      3,0(7,6)
         LA      1,ARG
         ST      3,ARG
         MVI     ARG,X'80'
         AR      7,5
         L       15,AL            GET ADDRESSS OF ALCG FROM V CONSTANT
         BALR    14,15
         STE     0,0(3)
         BXH     9,10,F
         L       1,SAVARG         GR1=ADDRESS OF ARGUMENT LIST
         LR      9,12
         MR      8,9              GR9=N**2
         SLL     9,2              GR9=N**2*4
         LA      3,256            GR3=256
         DR      8,3              GR9=(N**2)*4/256  GR8=REMAINDER
         AR      8,10
         ST      9,NSQ            STORE (N**2)*4/256 IN NSQ
         ST      8,REMAIN         STORE REMAINDER IN REMAIN
         L       3,60(1)
         L       3,0(3)
         LA      0,1
         AR      3,0              GR3=MQ = LL+1
         ST      3,S2             STORE MQ IN S2
         LA      10,0             GR10=JJ
         LA      11,1             GR11GR11=II
         ST      11,S3            >3=II
         L       7,68(1)
```

```
         L      7,0(7)
         LA     4,0
         ST     4,S4
A        LR     4,11              GR4=II
         LA     0,1               GR0=1
         SR     4,0               GR4=II-1
         SLL    4,2               GR4=(II-1)*4
         ST     10,S1             S1=JJ
         L     5,72(1)
         L      5,0(4,5)
         SR     5,0               GR5=NFC(II)-1
         SLL    5,2               GR5=NFC(II)-1)*4
         L      6,12(1)
         LE     2,0(5,6)
         STE    2,TEMP
         AE     2,PT01            FPR2=PHEE + 0.01
         STE    2,0(5,6)
         L      15,FCON           LOAD ADDRESS OF FCONST
         BALR   14,15             CALL FCONST
         LE     0,TEMP
         STE    0,0(5,6)
         LA     1,24(1)
         L      15,NRO            LOAD ADDRESS OF NROOT
         BALR   14,15             CALL NROOT
         L      1,SAVARG
         L      8,REMAIN
         L      9,NSQ
         LA     10,1
         L     5,64(1)
         L     6,36(1)
         CR     10,9              COMPARE 1 TO NSQ/256
         BC     2,B               IF NSQ/256.EQ.0 BRANCH TO B
         LA     3,256             GR3=256
         LA     10,1
         LNR    10,10             GR10=-GR10
         LA     11,0
LOOPG    MVC    0(256,6),0(5)
         AR     5,3               INDEX FOR E + 256
         AR     6,3               INDEX FOR G + 256
         BXH    9,10,LOOPG        BRANCH TO LOOPG
B        STC    8,C+1
C        MVC    0(1,6),0(5)
         LA     10,1
         LNR    10,10
         LA     11,0
         L     6,48(1)
         LA     5,0
         LA     8,XL              GR8=ADDRESS OF XL VECTOR
         LA     3,4
         L      4,S4
         L     7,40(1)
         L      9,NN
D        LA     14,0(5,7)
```

```
                ST      14,ARG
                LA      1,ARG
                L       15,AL
                MVI     ARG,X'80'
                BALR    14,15           ALOG
                LE      2,0(5,8)
                SER     0,2
                STE     0,0(4,6)
                AR      4,3
                AR      5,3
                BXH     9,10,D
                ST      4,S4
                L       1,SAVARG
                LA      11,1
                L       10,S1
                AR      10,3
                L       4,S2            GR4=MQ
                L       5,S3
                AR      5,11
                ST      5,S3
                LR      11,5
                CR      4,5             COMPARE MQ TO 11
                BC      2,A
                L       13,4(13)
                RETURN  (14,12)
NN              DS      1F
S2              DS      1F
S3              DS      1F
S1              DS      1F
S4              DS      1F
SAVARG          DS      1F
PTO1            DC      E'0.01'
FCON            DC      V(FCONST)
NRO             DC      V(NROOTE)
AL              DC      V(ALOG)
XL              DS      04F
TEMP            DS      1F
REMAIN          DS      1F
NSQ             DS      1F
SAVAREA         DS      18F
                DS      0F
ARG             DS      1F
                LTORG
                END     JMAT
```

```
FCONST   START
         SAVE   (14,12),,*
         BALR  2,0
         USING *,2
         LR     12,13
         LA     13,SAVEAREA
         ST     12,4(13)
         ST     13,8(12)
*   CALL FCONST(NRZ,NCZ,NOPHEE,PHEE,NOZ,N,NROW,F)
         LM     3,9,0(1)
         L      10,32(1)
         MVI    0(10),X'00'
         LA     15,1
         LR     11,10
         L      13,0(9)            GR13=N
         LR     9,13               GR9=N
         MR     12,13
         SLL    13,2               GR13=N**N *4
         LA     14,256
         LR     0,14                 GR0=256
         DR     12,14              GR13=N**2 , GR12=REMAINDER
         CR     15,13
         BC     2,G
         LNR    14,15
         LA     15,0
LOOPC    MVC    1(256,11),0(11)      PUT 0'S IN F MATRIX
         AR     11,0               GR11 = GR11 + 256  LOOP INDEXER
         BXH    13,14,LOOPC
G        S      12,=F'2'
         STC    12,H+1
H        MVC    1(1,11),0(11)      FINISH MOVING 0'S
         L      11,0(8)            GR11=NOZ
         LA     1,0                GR1=0  = INDEX REG.
         LA     0,4                GR0=4
I        LE     0,0(1,7)           FPR0=Z(I)
         L      12,0(1,5)          GR12=NOPHEE(I)
         SLL    12,2               GR12=NOPHEE(I)*4
         SR     12,0               GR12=NOPHEE(I)*4-4
         LE     2,0(12,6)          FPR2=PHEE(NOPHEE(I))
         MER    0,2                FPR0=Z(I)*PHEE(NOPHEE(I))
         L      14,0(1,3)          GR14=NRF(I)
         L      15,0(1,4)          GR15=NCF(I)
         SLL    14,2               GR14=NRF(I)*4
         SLL    15,2               GR15=NRF(I)*4
         SR     15,0               GR15=NCF(I)*4-4
         SR     14,0               GR14=NRF(I)*4-4
         LR     13,9               GR13=N
         MR     12,15               GR13=N*NCF(I)*4
         AR     13,14               GR13=N*NCF(I)*4 + NRF(I)*4
         AE     0,0(13,10)         ADD OLD VALUE OF F(I,J) TO REG.
         STE    0,0(13,10)          STORE ELEMENT IN F MATRIX
         LR     13,9               GR13=N
         MR     12,14              GR13=N*NRF(I)*4
```

```
          AR      13,15                GR13=N*NRF(I)*4 + NCF(I)*4
          STE     C,0(13,10)           FORM SYMMETRIC ELEMENT
          AR      1,0                  GR1 = GR1 + 4  INDEXING
          LA      13,0
          L       12,=F'-1'
          BXH     11,12,I
          LA       13,SAVEAREA
          L        13,4(13)
          RETURN  (14,12)
SAVEAREA  DS      18F
          LTORG
          END     FCONST
```

```
ARAY     START
         STM   14,12,12(13)
         BALR  2,0
         USING *,2
         ST    13,SAVAD1
         LA    12,1              GR12 = 1
         LA    10,1              GR10 = 1
         LM    3,7,0(1)
         L     3,0(3)            GR2 = INDICATOR VALUE
         LA    13,2
         CR    3,13
         BC    4,ONETWO          IF IND. LT. TWO BRANCH TO ONETWO
         L     3,0(4)            GR3 = VALUE OF N
         L     11,0(5)
         SLL   3,2               GR3 = VALUE OF N*4
         SR    11,10             GR11 = N-1
         LR    13,3
         LR    8,3               GR8 = N*4
         BCTR  13,0
         STC   13,M+1
         LA    3,0(3,7)
         L     13,0(6)
         SLL   13,2
         LR    9,13
         AR    13,7
M        MVC   0(1,3),0(13)
         AR    3,8               INCREASE GR3 BY N*4
         AR    13,9
         BXLE  12,10,M           BRANCH TO M FOR LOOP
         BC    15,L              UNCONDITIONAL BRANCH TO RETURN
ONETWO   L     3,0(4)            GR3 = VALUE OF N
         L     9,0(5)
         SR    9,10              GR9 = N-1
         LR    1,9               GR1 = N-1
         LR    11,9              GR11 = N-1
         MR    8,3               GR9 = N*(N-1)
         SLL   9,2               GR9 = (N*(N-1))*4
         LR    8,3               GR8 = N
         SLL   8,2               GR8 = N*4
         LR    13,8
         SR    8,10              GR8 = N*4-1
         STC   8,MM+1            ADD N*4-1 IN DISP. OF MVC INST.
         STC   8,MM1+1
         LA    8,C(9,7)
         L     3,0(6)
         SLL   3,2               GR3 = NDIM*4
         MR    0,3               GR1 = (NDIM*4)*(N-1)
         LA    6,X
         AR    1,7
MM1      MVC   C(1,6),C(8)
MM       MVC   0(1,1),0(6)
         SR    8,13
         SR    1,3               ADDRESS OF NEW VECTOR - NDIM*4
```

```
            BXLE   12,10,MM1
L           L      13,SAVAD1
            LM     14,12,12(13)
            BCR    15,14
SAVAD1      DS     1F
X           DS     64F
            END    ARAY
```

```
MATM     START
         STM    14,12,12(13)
         BALR   2,0
         USING  *,2
         ST     13,SAVADD
         L      4,4(0,1)
         L      12,8(0,1)
         L      3,12(0,1)
         L      11,16(0,1)
         L      11,0(11)        R11 = VALUE OF N
         L       7,0(1)
         L       7,0(7)               GR7=NDIM
         SLL    7,2             GR7 = NDIM*4
         LA     6,1             GR6 = 1
         LA     10,1            GR10 = 1
LOOP1    ST     6,L1            L1 = VALUE OF I
         ST     11,LL1
         L      11,20(0,1)
         L      11,0(0,11)
         LA     6,1             GR6 = 1
LOOP2    ST     6,L2            L2 = VALUE OF J
         ST     11,LL2
         SER    0,0             FPR0 = 0.0
         LR     9,6             GR9 = VALUE OF J
         SR     9,10            GR9 = J-1
         LA     6,1             GR6 = 1
         MR     8,7             GR9 = (NDIM*4)*(J-1)
         ST     9,L5            L5 = GR9
         LA     9,4             GR9 = 4
         M      8,L1            GR9 = 4*I
         S      9,=F'4'         GR9 = I*4-4
         ST     9,L6            L6 = GR9
         L      8,L5            GR8 = L5
         L      11,24(0,1)
         L      11,0(11)
LOOP3    LE     2,0(9,4)        FPR2 = A(I,K)
         AR     9,7             ADD 4*NDIM TO INDEX R9
         LE     4,0(8,12)       FPR4 = B(K,J)
         LA     8,4(8)          INCREASE INDEX R8 BY 4
         MER    2,4             FPR2 = A(I,K)*B(K,J)
         AER    0,2             TEMP = TEMP + A*B
         BXLE   6,10,LOOP3      BRANCH TO LOOP3
         L      6,L6            GR6 = I*4-4
         A      6,L5            GR6 = I*4-4 +(NDIM*4)*(J-1)
         STE    0,0(6,3)        STORE TEMP IN C(I,J)
         L      6,L2            GR6 = COUNTER LOOP2
         L      11,LL2
         BXLE   6,10,LOOP2      BRANCH TO LOOP2
         L      6,L1            GR6 = COUNTER LOOP1
         L      11,LL1
         BXLE   6,10,LOOP1      BRANCH TO LOOP1
         L      13,SAVADD
         LM     14,12,12(13)
```

```
         BCR    15,14
SAVADC   DS     1F
L1       DS     1F
L2       DS     1F
L3       DS     1F
L5       DS     1F
L6       DS     1F
LL1      DS     1F
LL2      DS     1F
         LTORG
         END    MATM
```

2. Data Tables -- Computer Output

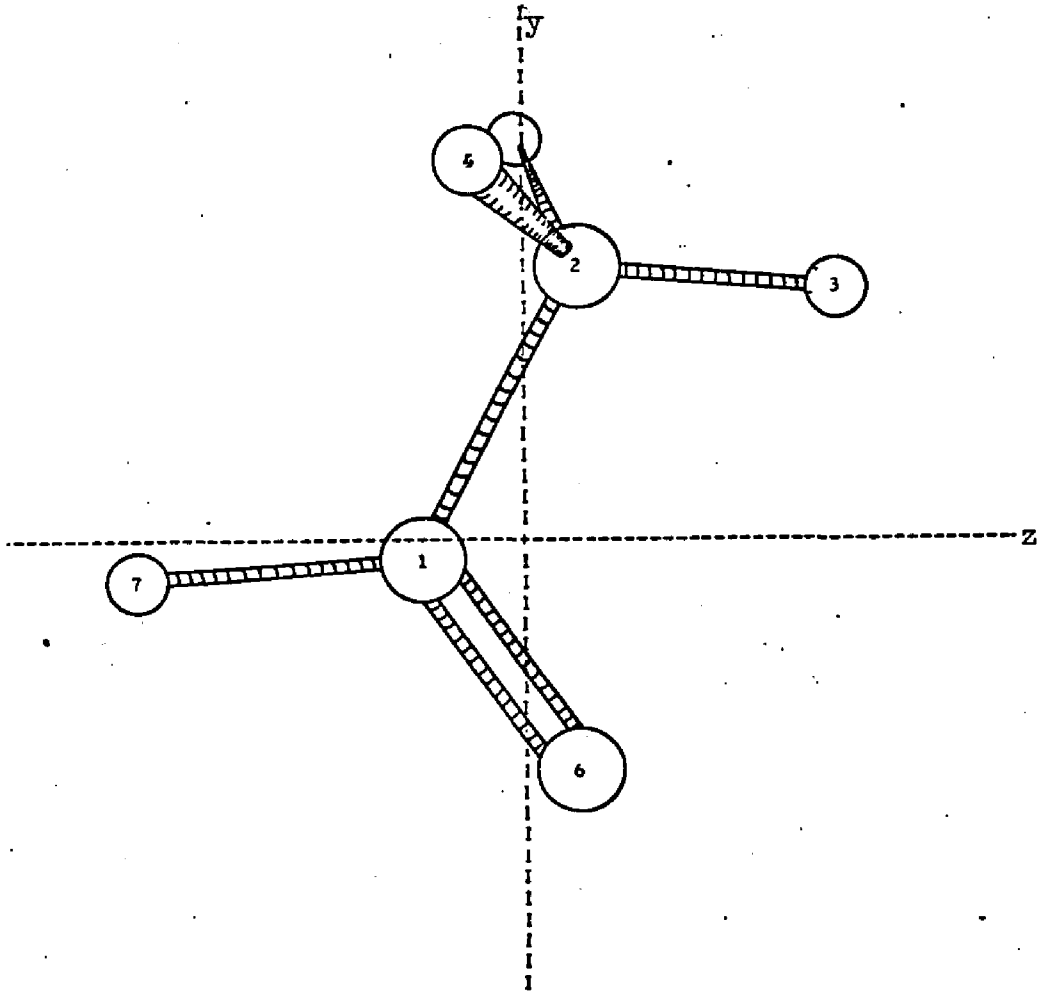
A. PREIGEN

1. Principal Cartesian Coordinates and Plots

The Cartesian coordinates are listed on the following pages. Below each list is a two-dimensional plot of the molecule, looking down the x-axis. All fourteen molecules including isotopic species are listed.

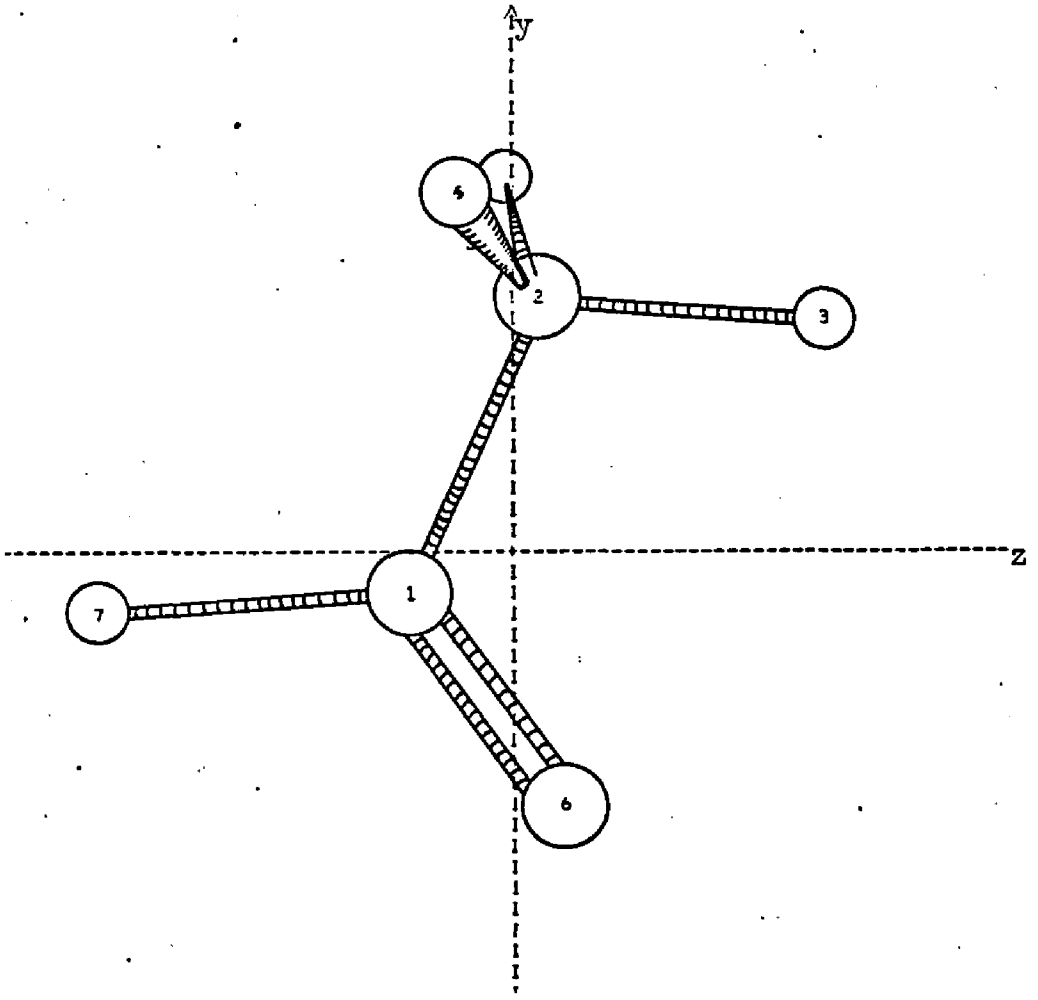
PRINCIPAL CARTESIAN COORDINATES ---- CH3-COH

ATOM NO.	X	Y	Z
1 ---	0.0	-0.42586	-0.12306
2 ---	0.0	0.16144	1.25773
3 ---	0.0	1.24623	1.20644
4 ---	-0.88189	-0.15938	1.80430
5 ---	0.88189	-0.15938	1.80430
6 ---	0.0	0.23687	-1.14199
7 ---	0.0	-1.53652	-0.20915



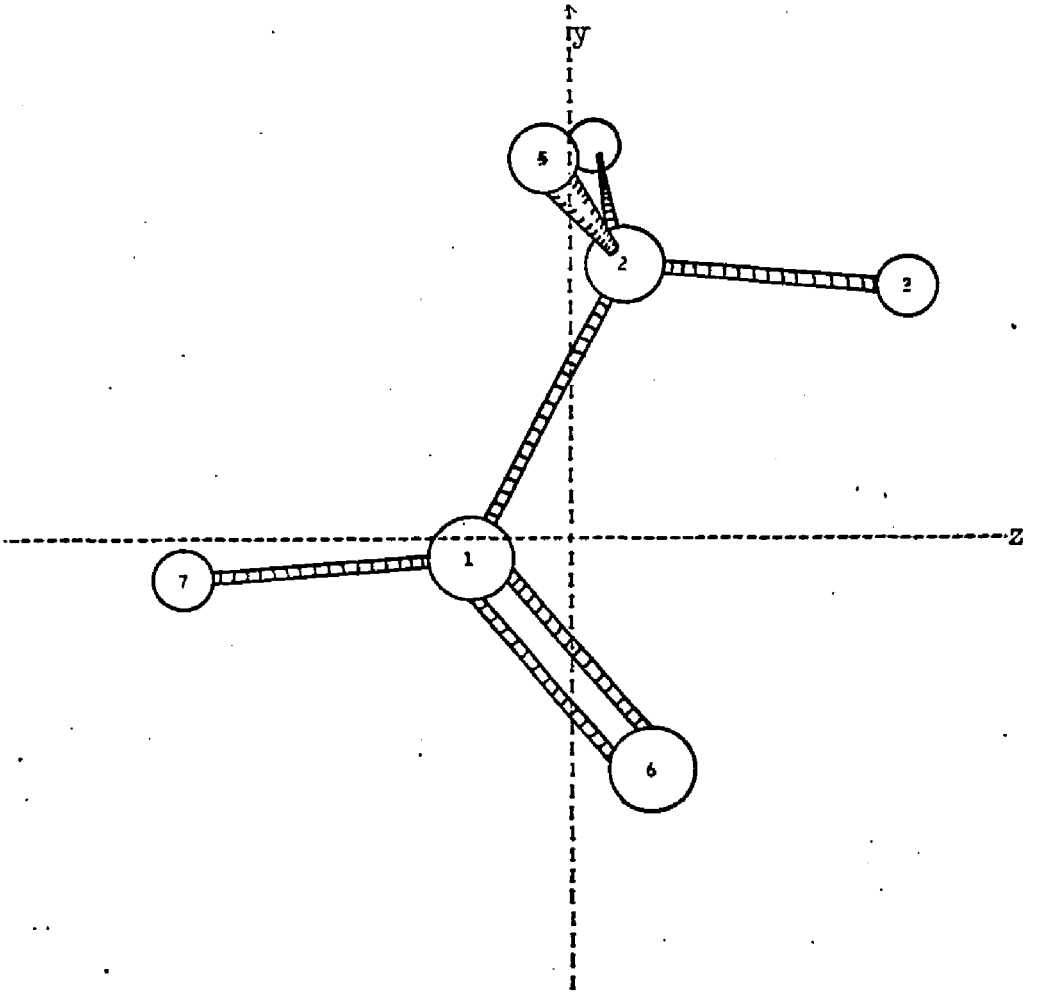
PRINCIPAL CARTESIAN COORDINATES ---- CO3-CCH

ATOM NO.	X	Y	Z
1 ---	0.0	-0.44155	-0.23393
2 ---	0.0	0.12087	1.15717
3 ---	0.0	1.20640	1.12537
4 ---	-0.88189	-0.20972	1.69790
5 ---	0.88189	-0.20972	1.69790
6 ---	0.0	0.23936	-1.24080
7 ---	0.0	-1.55049	-0.33994



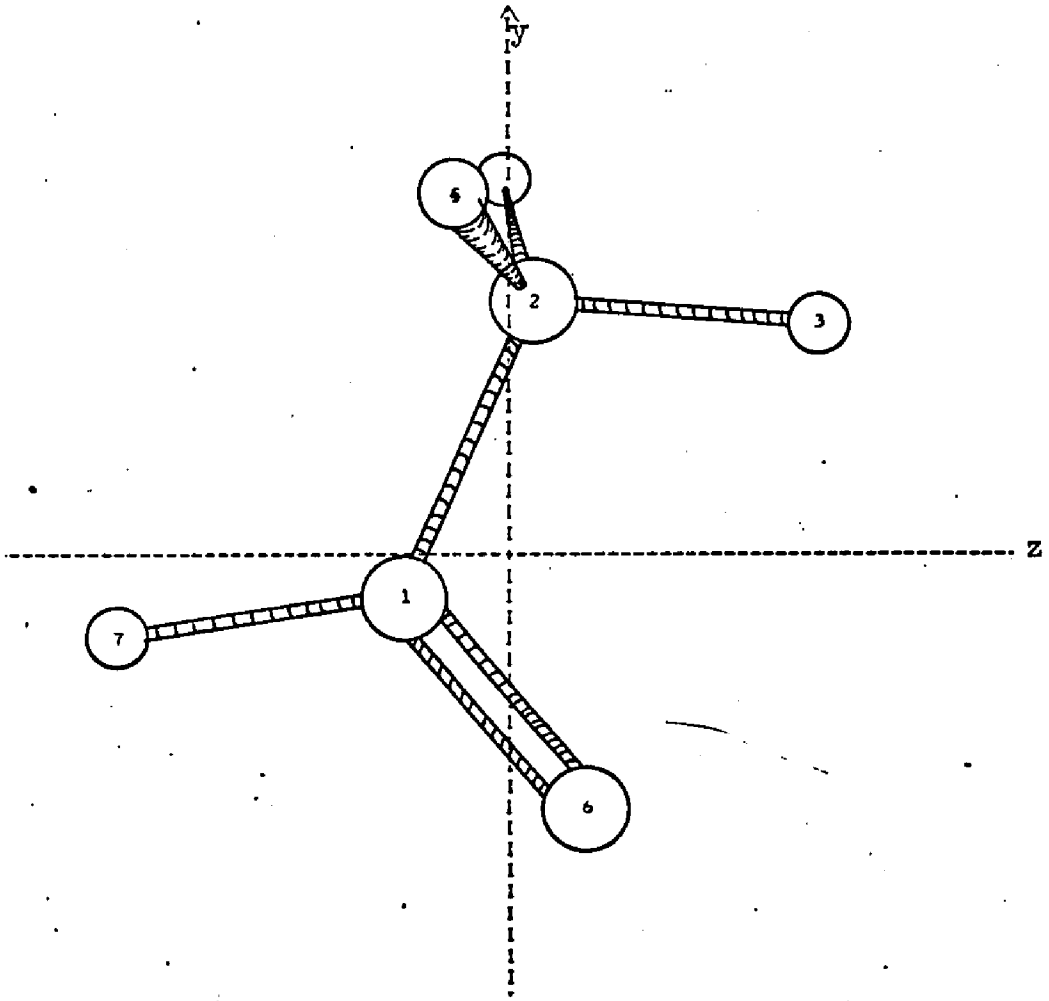
PRINCIPAL CARTESIAN COORDINATES ---- CH3-COD

ATOM NO.	X	Y	Z
1 ---	0.0	-0.39057	-0.12161
2 ---	0.0	0.18537	1.26396
3 ---	0.0	1.27054	1.22159
4 ---	-0.88189	-0.13994	1.80788
5 ---	0.88189	-0.13994	1.80788
6 ---	0.0	0.28052	-1.13506
7 ---	0.0	-1.50049	-0.21682



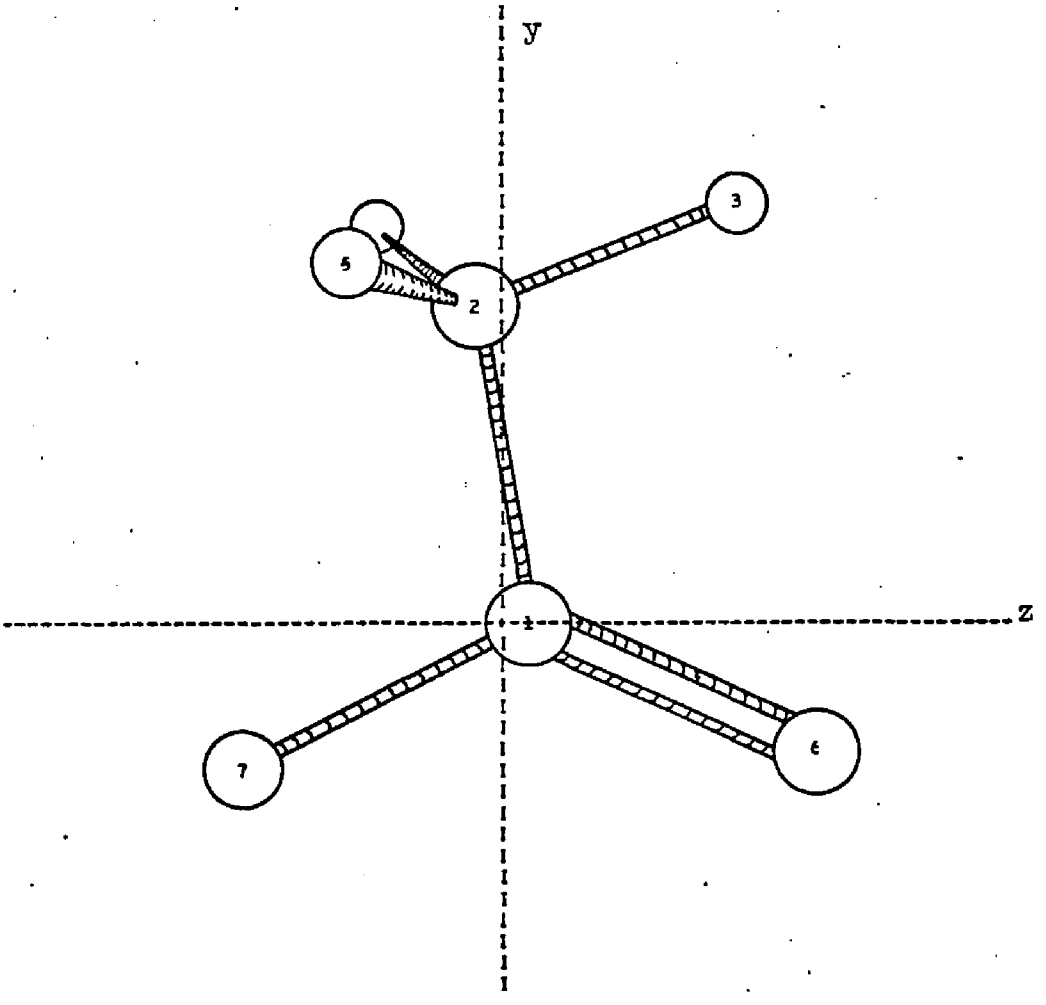
PRINCIPAL CARTESIAN COORDINATES ---- CD3-COD

ATOM NO.	X	Y	Z
1 ---	0.0	-0.40643	-0.23158
2 ---	0.0	0.13570	1.16600
3 ---	0.0	1.22553	1.14687
4 ---	-0.88189	-0.19718	1.70282
5 ---	0.88189	-0.19718	1.70282
6 ---	0.0	0.28620	-1.23043
7 ---	0.0	-1.51406	-0.35054



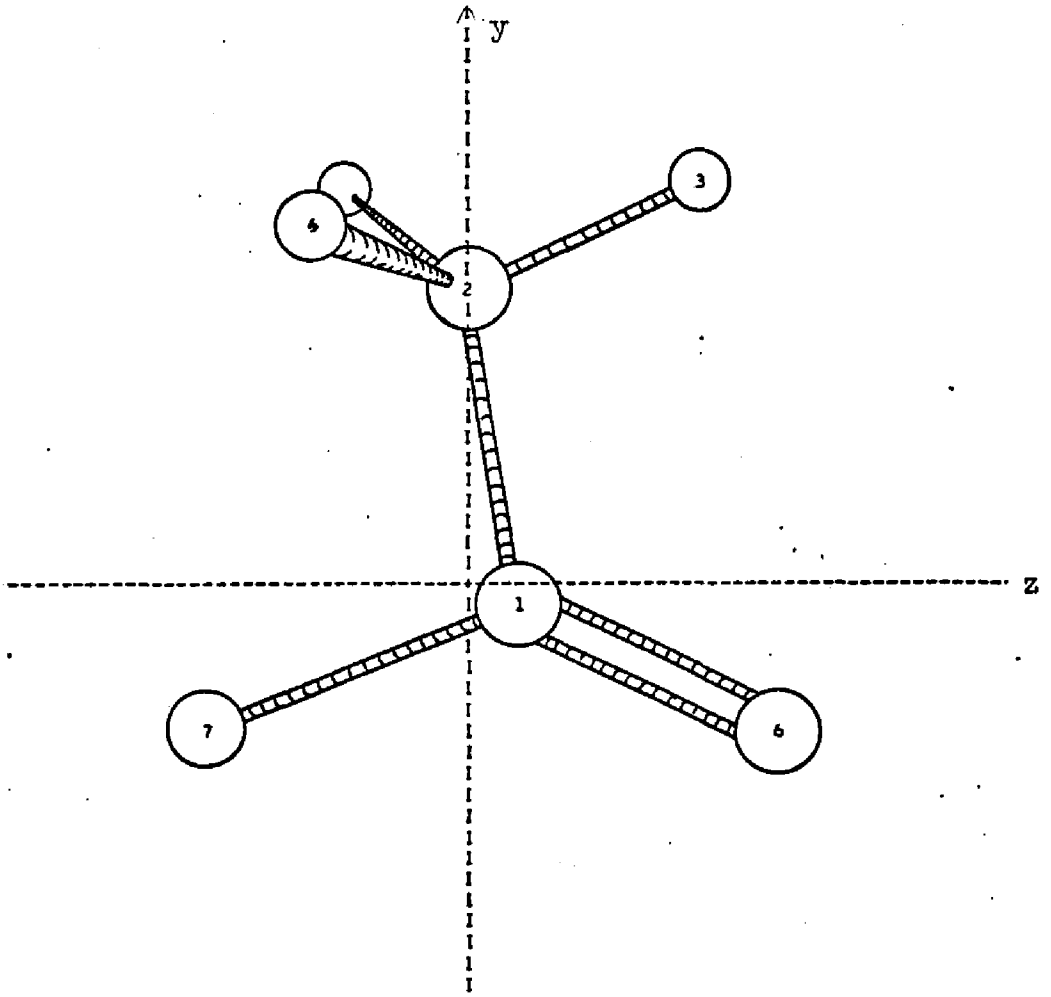
PRINCIPAL CARTESIAN COORDINATES ---- CH3-COF

ATOM NO.	X	Y	Z
1 ---	0.0	0.14922	-0.02752
2 ---	0.0	-0.06249	1.45948
3 ---	0.0	0.88836	1.97582
4 ---	-0.89852	-0.62586	1.73603
5 ---	0.89852	-0.62586	1.73603
6 ---	0.0	1.17756	-0.61638
7 ---	0.0	-1.02723	-0.67528



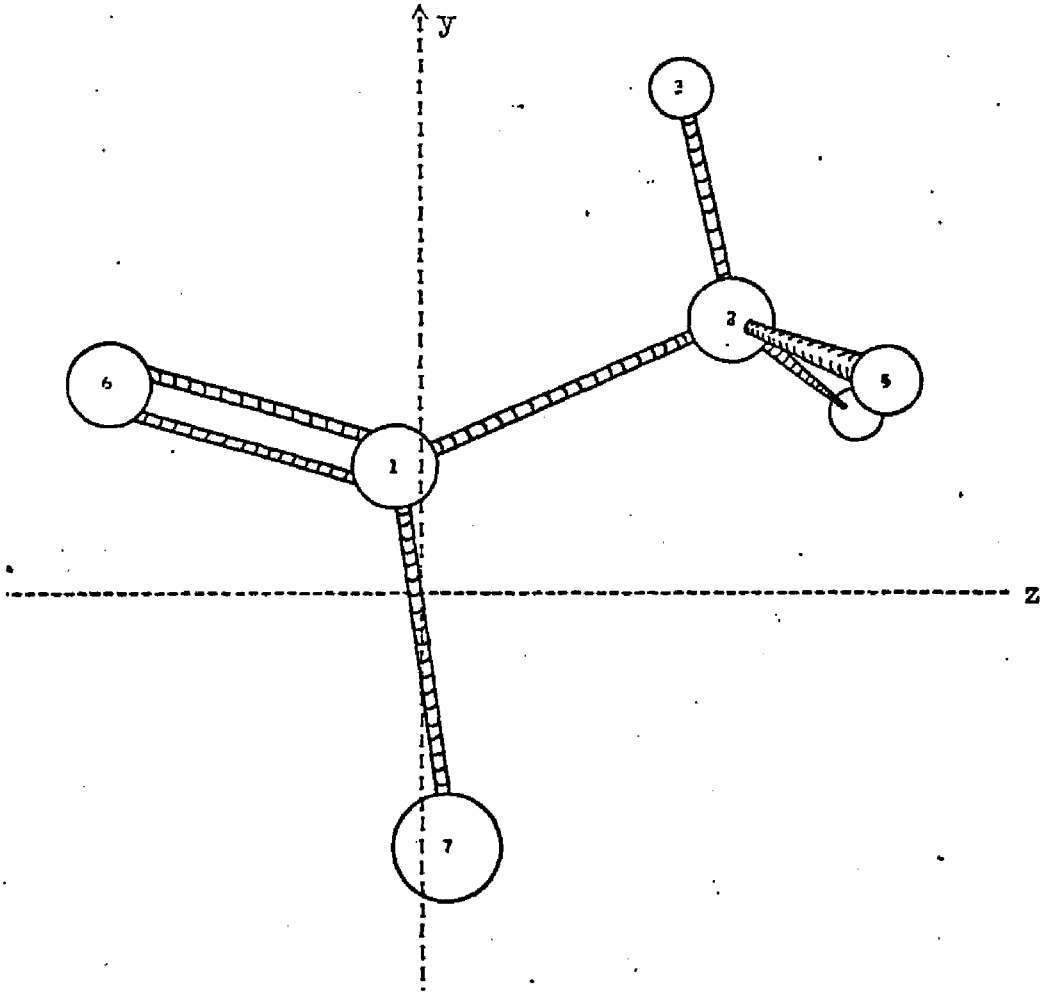
PRINCIPAL CARTESIAN COORDINATES ---- CD3-COF

ATOM NO.		X	Y	Z
1	---	0.0	0.15172	-0.11598
2	---	0.0	-0.01907	1.37628
3	---	0.0	0.94560	1.86630
4	---	-0.89852	-0.57463	1.66820
5	---	0.89852	-0.57463	1.66820
6	---	0.0	1.16348	-0.73286
7	---	0.0	-1.04209	-0.73117



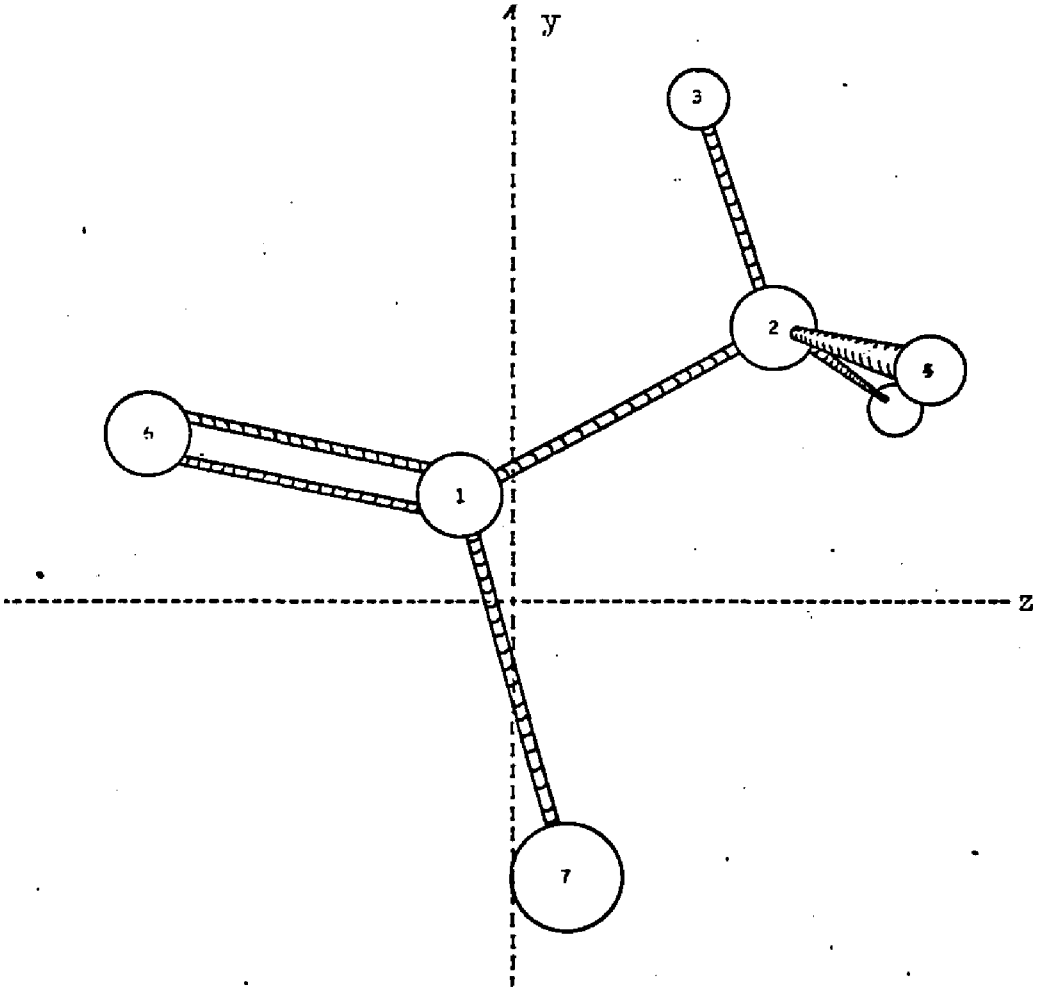
PRINCIPAL CARTESIAN COORDINATES ---- CH3-COCL (CL=35)

ATOM NO.	X	Y	Z
1 ---	0.0	-0.13255	0.55028
2 ---	0.0	1.17600	1.28151
3 ---	0.0	1.00944	2.35162
4 ---	-0.87937	1.75243	1.02203
5 ---	0.87937	1.75243	1.02202
6 ---	0.0	-1.22385	1.02978
7 ---	0.0	0.07142	-1.22705



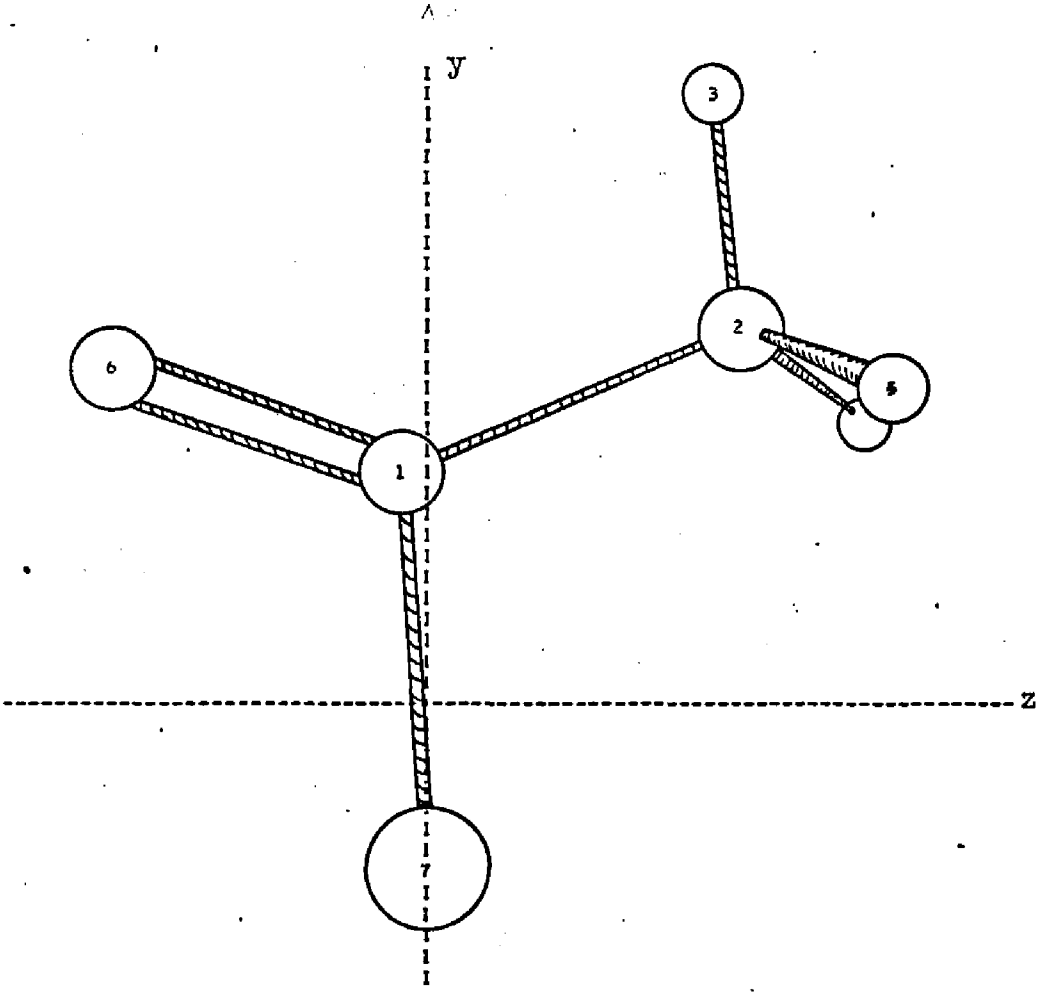
PRINCIPAL CARTESIAN COORDINATES ---- CO3-COCL (CL=35)

ATOM NO.	X	Y	Z
1 ---	0.0	-0.24038	0.47277
2 ---	0.0	0.98274	1.33935
3 ---	0.0	0.70303	2.38561
4 ---	-0.87937	1.58355	1.14281
5 ---	0.87937	1.58355	1.14281
6 ---	0.0	-1.37659	0.83317
7 ---	0.0	0.15194	-1.27268



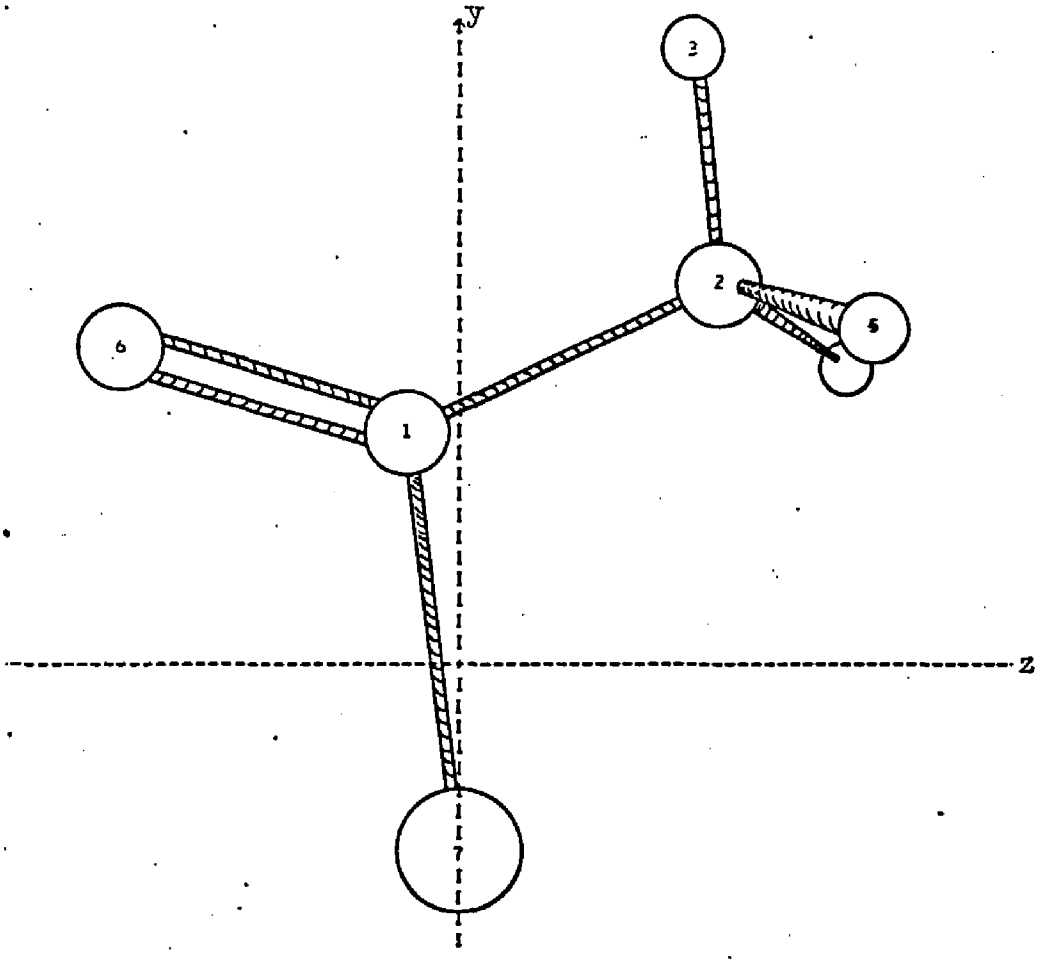
PRINCIPAL CARTESIAN COORDINATES ---- CH3-COUR

ATOM NO.	X	Y	Z
1 ---	0.0	-0.12980	1.11472
2 ---	0.0	1.20601	1.79687
3 ---	0.0	1.07961	2.87247
4 ---	-0.87937	1.77232	1.51600
5 ---	0.87937	1.77232	1.51600
6 ---	0.0	-1.20236	1.63479
7 ---	0.0	0.02064	-0.83949



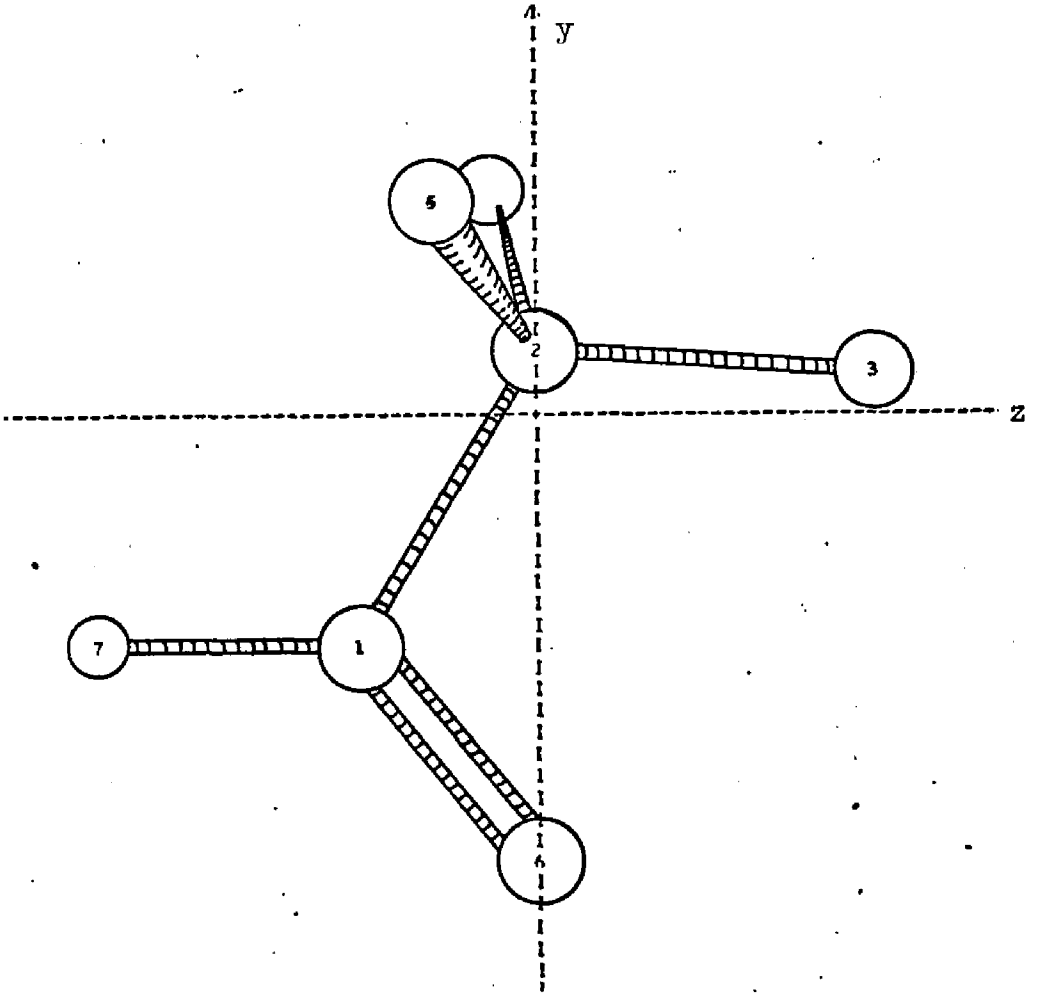
PRINCIPAL CARTESIAN COORDINATES ---- CD3-COBR

ATOM NO.	X	Y	Z
1 ---	0.0	-0.23813	1.05394
2 ---	0.0	1.04879	1.82436
3 ---	0.0	0.85037	2.88903
4 ---	-0.87937	1.63271	1.58220
5 ---	0.87937	1.63271	1.58220
6 ---	0.0	-1.34322	1.50072
7 ---	0.0	0.04336	-0.88574



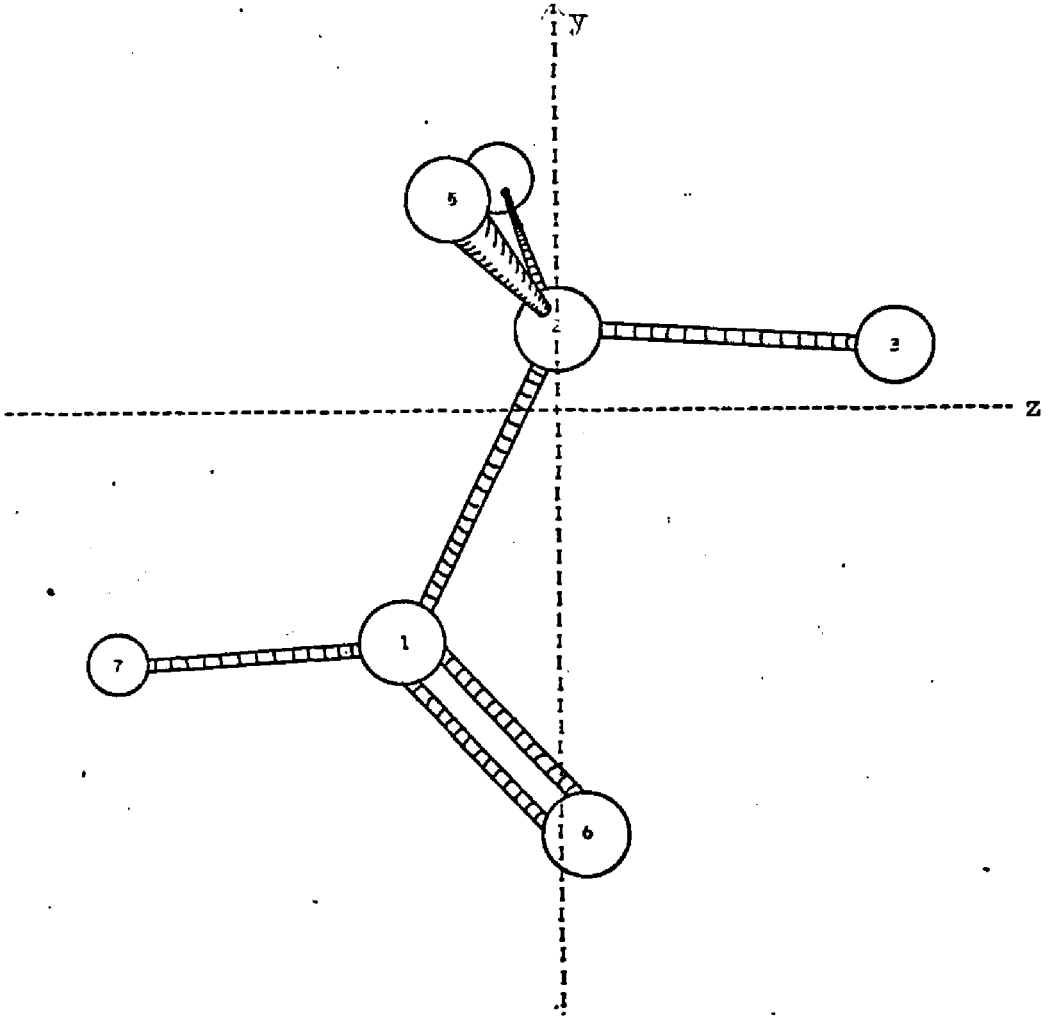
PRINCIPAL CARTESIAN COORDINATES ---- CF3-COH

ATOM NO.	X	Y	Z
1 ---	0.0	-0.65273	-1.06318
2 ---	0.0	-0.01871	0.34025
3 ---	0.0	1.30916	0.23547
4 ---	-1.08535	-0.40401	1.00942
5 ---	1.08535	-0.40401	1.00942
6 ---	0.0	0.01859	-2.06265
7 ---	0.0	-1.74022	-1.13709



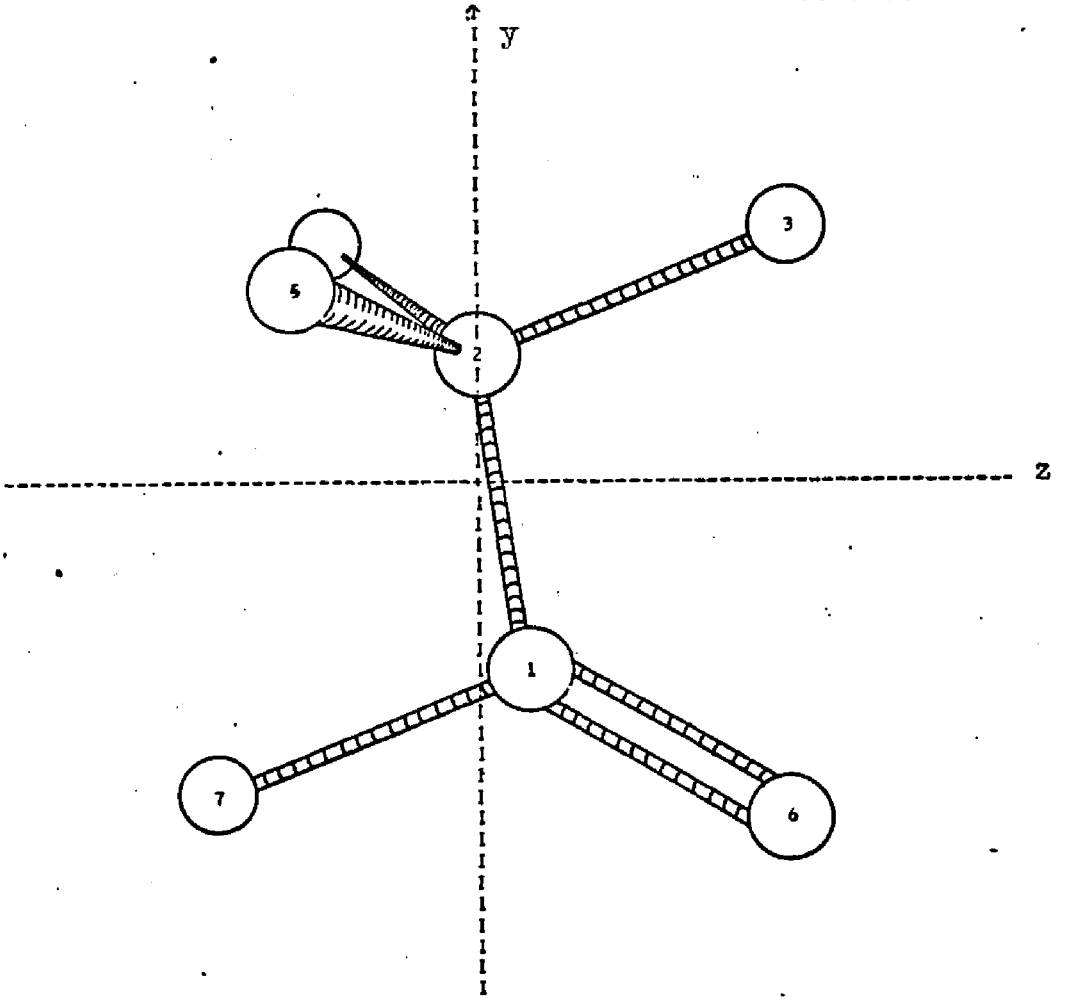
PRINCIPAL CARTESIAN COORDINATES ---- CF3-COD

ATOM NO.	X	Y	Z
1 ---	0.0	-0.60740	-1.06784
2 ---	0.0	-0.01022	0.35165
3 ---	0.0	1.31994	0.28156
4 ---	-1.08535	-0.41284	1.01054
5 ---	1.08535	-0.41284	1.01054
6 ---	0.0	0.08977	-2.04945
7 ---	0.0	-1.69259	-1.17011



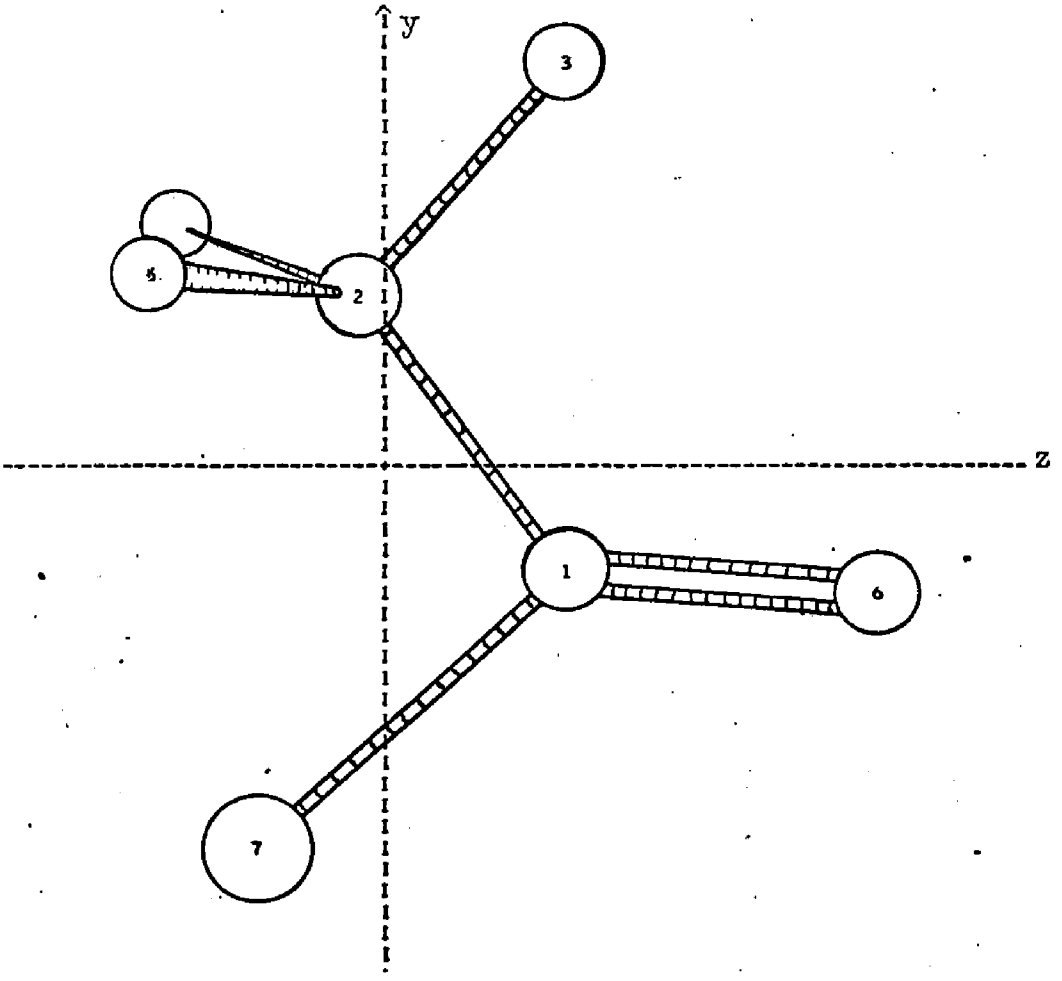
PRINCIPAL CARTESIAN COORDINATES ---- CF3-COF

ATOM NO.	X	Y	Z
1 ---	0.0	0.56859	-0.47450
2 ---	0.0	-0.09678	0.89213
3 ---	0.0	0.81120	1.87760
4 ---	-1.08059	-0.87158	1.05830
5 ---	1.08059	-0.87158	1.05830
6 ---	0.0	1.71285	-0.71856
7 ---	0.0	-0.43340	-1.95778



PRINCIPAL CARTESIAN COORDINATES ---- CF3-COCL

ATOM NO.	X	Y	Z
1 ---	0.0	0.67932	-0.51914
2 ---	0.0	-0.10727	0.83844
3 ---	0.0	0.72119	1.87890
4 ---	-1.07252	-0.88617	0.94759
5 ---	1.07252	-0.88617	0.94759
6 ---	0.0	1.85304	-0.64088
7 ---	0.0	-0.46675	-1.84165



B. GMATRIX

1. B Matrix

The following matrices are the Cartesian coordinate to internal coordinate transformations for each molecule of this study. See page I-41 for definition of the B matrix.

1	2	-0.39140	1	3	-0.92022	1	5	0.39140	1	6	0.92022
2	5	-0.99888	2	6	0.04723	2	8	0.99888	2	9	-0.04723
3	4	0.81205	3	5	0.29542	3	6	-0.50329	3	10	-0.81205
3	11	-0.29542	3	12	0.50329	4	4	-0.81205	4	5	0.29542
4	6	-0.50329	4	13	0.81205	4	14	-0.29542	4	15	0.50329
5	2	-0.54523	5	3	0.83828	5	17	0.54523	5	18	-0.83828
6	2	0.99701	6	3	0.07728	6	20	-0.99701	6	21	-0.07728
7	5	-0.75704	7	6	1.28973	7	10	-0.53737	7	11	0.37852
7	12	-0.64486	7	13	0.53737	7	14	0.37852	7	15	-0.64486
8	4	1.04048	8	5	0.90135	8	6	0.58435	8	7	-0.78893
8	8	-0.02243	8	9	-0.47433	8	13	-0.25156	8	14	-0.87893
8	15	-0.11002	9	4	-1.04048	9	5	0.90135	9	6	0.58435
9	7	0.78893	9	8	-0.02243	9	9	-0.47433	9	10	0.25156
9	11	-0.87893	9	12	-0.11002	10	1	-0.57716	10	2	0.30664
10	3	-0.13042	10	4	0.85428	10	5	-0.79181	10	6	-0.60149
10	13	-0.27712	10	14	0.48518	10	15	0.73192	11	2	-0.61328
11	3	0.26085	11	5	0.56979	11	6	-1.18063	11	8	0.04349
11	9	0.91979	12	1	0.57716	12	2	0.30664	12	3	-0.13042
12	4	-0.85428	12	5	-0.79181	12	6	-0.60149	12	10	0.27712
12	11	0.48518	12	12	0.73192	13	2	-0.62029	13	3	-1.34355
13	17	0.68966	13	18	0.44857	13	20	-0.06937	13	21	0.89498
14	2	1.30294	14	3	0.18772	14	5	-0.61328	14	6	0.26085
14	17	-0.68966	14	18	-0.44857	15	2	-0.68265	15	3	1.15583
15	5	0.61328	15	6	-0.26085	15	20	0.06937	15	21	-0.89498
16	1	-1.23239	16	4	0.35003	16	16	0.43669	16	19	0.44566
17	1	-0.04060	17	4	0.05079	17	7	-0.32734	17	10	0.16367
17	11	-0.26087	17	12	0.11096	17	13	0.16367	17	14	0.26087
17	15	-0.11096	17	16	0.49570	17	19	-0.50589			

B MATRIX FOR THE MOLECULE CH3-COH

1	2	-0.37482	1	3	-0.92710	1	5	0.37482	1	6	0.92710
2	5	-0.99957	2	6	0.02929	2	8	0.99957	2	9	-0.02929
3	4	0.81205	3	5	0.30440	3	6	-0.49790	3	10	-0.81205
3	11	-0.30440	3	12	0.49790	4	4	-0.81205	4	5	0.30440
4	6	-0.49790	4	13	0.81205	4	14	-0.30440	4	15	0.49790
5	2	-0.56020	5	3	0.82836	5	17	0.56020	5	18	-0.82836
6	2	0.99546	6	3	0.09516	6	20	-0.99546	6	21	-0.09516
7	5	-0.78007	7	6	1.27593	7	10	-0.53737	7	11	0.39004
7	12	-0.63796	7	13	0.53737	7	14	0.39004	7	15	-0.63796
8	4	1.04048	8	5	0.89072	8	6	0.60044	8	7	-0.78893
8	8	-0.01391	8	9	-0.47465	8	13	-0.25156	8	14	-0.87681
8	15	-0.12578	9	4	-1.04048	9	5	0.89072	9	6	0.60044
9	7	0.78893	9	8	-0.01391	9	9	-0.47465	9	10	0.25156
9	11	-0.87681	9	12	-0.12578	10	1	-0.57716	10	2	0.30893
10	3	-0.12490	10	4	0.85428	10	5	-0.78089	10	6	-0.61561
10	13	-0.27712	10	14	0.47196	10	15	0.74051	11	2	-0.61786
11	3	0.24980	11	5	0.59089	11	6	-1.17022	11	8	0.02697
11	9	0.92042	12	1	0.57716	12	2	0.30893	12	3	-0.12490
12	4	-0.85428	12	5	-0.78089	12	6	-0.61561	12	10	0.27712
12	11	0.47196	12	12	0.74051	13	2	-0.59607	13	3	-1.35447
13	17	0.68150	13	18	0.46088	13	20	-0.08542	13	21	0.89360
14	2	1.29936	14	3	0.21108	14	5	-0.61786	14	6	0.24980
14	17	-0.68150	14	18	-0.46088	15	2	-0.70329	15	3	1.14339
15	5	0.61786	15	6	-0.24980	15	20	0.08543	15	21	-0.89360
16	1	-1.23239	16	4	0.35004	16	16	0.43669	16	19	0.44567
17	1	-0.04060	17	4	0.05079	17	7	-0.32734	17	10	0.16367
17	11	-0.26282	17	12	0.10626	17	13	0.16367	17	14	0.26282
17	15	-0.10626	17	16	0.49570	17	19	-0.50589			

B MATRIX FOR THE MOLECULE CO3-COH

1	2	-0.38383	1	3	-0.92340	1	5	0.38383	1	6	0.92340
2	5	-0.99924	2	6	0.03902	2	8	0.99924	2	9	-0.03902
3	4	0.81205	3	5	0.29954	3	6	-0.50084	3	10	-0.81205
3	11	-0.29954	3	12	0.50084	4	4	-0.81205	4	5	0.29954
4	6	-0.50084	4	13	0.81205	4	14	-0.29954	4	15	0.50084
5	2	-0.55211	5	3	0.83377	5	17	0.55211	5	18	-0.83377
6	2	0.99634	6	3	0.08547	6	20	-0.99634	6	21	-0.08547
7	5	-0.76762	7	6	1.28346	7	10	-0.53737	7	11	0.38381
7	12	-0.64173	7	13	0.53737	7	14	0.38381	7	15	-0.64173
8	4	1.04049	8	5	0.89652	8	6	0.59174	8	7	-0.78893
8	8	-0.01853	8	9	-0.47449	8	13	-0.25156	8	14	-0.87799
8	15	-0.11724	9	4	-1.04049	9	5	0.89652	9	6	0.59174
9	7	0.78893	9	8	-0.01853	9	9	-0.47449	9	10	0.25156
9	11	-0.87799	9	12	-0.11724	10	1	-0.57716	10	2	0.30770
10	3	-0.12790	10	4	0.85428	10	5	-0.78684	10	6	-0.60798
10	13	-0.27712	10	14	0.47914	10	15	0.73588	11	2	-0.61540
11	3	0.25580	11	5	0.57947	11	6	-1.17591	11	8	0.03593
11	9	0.92011	12	1	0.57716	12	2	0.30770	12	3	-0.12790
12	4	-0.85428	12	5	-0.78684	12	6	-0.60798	12	10	0.27712
12	11	0.47914	12	12	0.73588	13	2	-0.60923	13	3	-1.34861
13	17	0.68595	13	18	0.45422	13	20	-0.07672	13	21	0.89438
14	2	1.30135	14	3	0.19842	14	5	-0.61540	14	6	0.25580
14	17	-0.68595	14	18	-0.45422	15	2	-0.69212	15	3	1.15018
15	5	0.61540	15	6	-0.25580	15	20	0.07672	15	21	-0.89438
16	1	-1.23239	16	4	0.35003	16	16	0.43669	16	19	0.44566
17	1	-0.04060	17	4	0.05079	17	7	-0.32734	17	10	0.16367
17	11	-0.26177	17	12	0.10881	17	13	0.16367	17	14	0.26177
17	15	-0.10881	17	16	0.49570	17	19	-0.50589			

B MATRIX FOR THE MOLECULE CH3-COD

1	2	-0.36397	1	3	-0.93141	1	5	0.36397	1	6	0.93141
2	5	-0.99984	2	6	0.01761	2	8	0.99984	2	9	-0.01761
3	4	0.81205	3	5	0.31020	3	6	-0.49431	3	10	-0.81205
3	11	-0.31020	3	12	0.49431	4	4	-0.81205	4	5	0.31020
4	6	-0.49431	4	13	0.81205	4	14	-0.31020	4	15	0.49431
5	2	-0.56983	5	3	0.82176	5	17	0.56983	5	18	-0.82176
6	2	0.99428	6	3	0.10679	6	20	-0.99428	6	21	-0.10679
7	5	-0.79492	7	6	1.26673	7	10	-0.53737	7	11	0.39746
7	12	-0.63337	7	13	0.53737	7	14	0.39746	7	15	-0.63337
8	4	1.04048	8	5	0.88364	8	6	0.61080	8	7	-0.78893
8	8	-0.00836	8	9	-0.47478	8	13	-0.25155	8	14	-0.87528
8	15	-0.13602	9	4	-1.04048	9	5	0.88364	9	6	0.61080
9	7	0.78893	9	8	-0.00836	9	9	-0.47478	9	10	0.25155
9	11	-0.87528	9	12	-0.13602	10	1	-0.57716	10	2	0.31037
10	3	-0.12128	10	4	0.85428	10	5	-0.77365	10	6	-0.62469
10	13	-0.27712	10	14	0.46328	10	15	0.74597	11	2	-0.62074
11	3	0.24256	11	5	0.60452	11	6	-1.16323	11	8	0.01621
11	9	0.92067	12	1	0.57716	12	2	0.31037	12	3	-0.12128
12	4	-0.85428	12	5	-0.77365	12	6	-0.62469	12	10	0.27712
12	11	0.46328	12	12	0.74597	13	2	-0.58021	13	3	-1.36134
13	17	0.07607	13	18	0.46881	13	20	-0.09586	13	21	0.89254
14	2	1.29680	14	3	0.22624	14	5	-0.62074	14	6	0.24256
14	17	-0.67607	14	18	-0.46881	15	2	-0.71659	15	3	1.13510
15	5	0.62074	15	6	-0.24256	15	20	0.09586	15	21	-0.89254
16	1	-1.23239	16	4	0.35004	16	16	0.43669	16	19	0.44566
17	1	-0.04060	17	4	0.05079	17	7	-0.32734	17	10	0.16367
17	11	-0.26404	17	12	0.10318	17	13	0.16367	17	14	0.26404
17	15	-0.10318	17	16	0.49570	17	19	-0.50589			

B MATRIX FOR THE MOLECULE CD3-COD

1	2	0.14095	1	3	-0.99002	1	5	-0.14095	1	6	0.99002
2	5	-0.87879	2	6	-0.47721	2	8	0.87879	2	9	0.47721
3	4	0.81982	3	5	0.51402	3	6	-0.25233	3	10	-0.81982
3	11	-0.51402	3	12	0.25233	4	4	-0.81982	4	5	0.51402
4	6	-0.25233	4	13	0.81982	4	14	-0.51402	4	15	0.25233
5	2	-0.86779	5	3	0.49692	5	17	0.86779	5	18	-0.49692
6	2	0.87599	6	3	0.48232	6	20	-0.87599	6	21	-0.48232
7	5	-1.34295	7	6	0.65924	7	10	-0.52246	7	11	0.67148
7	12	-0.32962	7	13	0.52246	7	14	0.67148	7	15	-0.32962
8	4	1.06571	8	5	0.46682	8	6	0.94434	8	7	-0.80305
8	8	0.21831	8	9	-0.40203	8	13	-0.26266	8	14	-0.68513
8	15	-0.54231	9	4	-1.06570	9	5	0.46682	9	6	0.94434
9	7	0.80305	9	8	0.21831	9	9	-0.40203	9	10	0.26266
9	11	-0.68513	9	12	-0.54231	10	1	-0.57658	10	2	0.32957
10	3	0.04692	10	4	0.83123	10	5	-0.35337	10	6	-0.92276
10	13	-0.25464	10	14	0.02380	10	15	0.87583	11	2	-0.65913
11	3	-0.09384	11	5	1.10018	11	6	-0.71835	11	8	-0.44104
11	9	0.81219	12	1	0.57658	12	2	0.32957	12	3	0.04692
12	4	-0.83123	12	5	-0.35337	12	6	-0.92275	12	10	0.25464
12	11	0.02380	12	12	0.87583	13	2	-0.06021	13	3	-1.38458
13	17	0.41935	13	18	0.73232	13	20	-0.35914	13	21	0.65227
14	2	1.07848	14	3	0.82616	14	5	-0.65913	14	6	-0.09384
14	17	-0.41935	14	18	-0.73232	15	2	-1.01827	15	3	0.55842
15	5	0.65913	15	6	0.09384	15	20	0.35914	15	21	-0.65227
16	1	-2.07998	16	4	0.60785	16	16	0.84388	16	19	0.62824
17	1	-0.27675	17	4	0.14752	17	7	-0.32869	17	10	0.16064
17	11	-0.27546	17	12	-0.03922	17	13	0.16064	17	14	0.27546
17	15	0.03922	17	16	0.53472	17	19	-0.39808			

B MATRIX FOR THE MOLECULE CH3-COF

1	2	0.11371	1	3	-0.99351	1	5	-0.11371	1	6	0.99351
2	5	-0.89157	2	6	-0.45288	2	8	0.89157	2	9	0.45288
3	4	0.81982	3	5	0.50690	3	6	-0.26635	3	10	-0.81982
3	11	-0.50690	3	12	0.26635	4	4	-0.81982	4	5	0.50690
4	6	-0.26635	4	13	0.81982	4	14	-0.50690	4	15	0.26635
5	2	-0.85381	5	3	0.52058	5	17	0.85381	5	18	-0.52058
6	2	0.88891	6	3	0.45808	6	20	-0.88891	6	21	-0.45808
7	5	-1.32433	7	6	0.69588	7	10	-0.52246	7	11	0.66217
7	12	-0.34794	7	13	0.52246	7	14	0.66217	7	15	-0.34794
8	4	1.06571	8	5	0.49258	8	6	0.93116	8	7	-0.80305
8	8	0.20719	8	9	-0.40788	8	13	-0.26266	8	14	-0.69977
8	15	-0.52329	9	4	-1.06570	9	5	0.49258	9	6	0.93116
9	7	0.80305	9	8	0.20719	9	9	-0.40788	9	10	0.26266
9	11	-0.69977	9	12	-0.52329	10	1	-0.57658	10	2	0.33073
10	3	0.03785	10	4	0.83123	10	5	-0.37858	10	6	-0.91270
10	13	-0.25464	10	14	0.04785	10	15	0.87485	11	2	-0.66146
11	3	-0.07570	11	5	1.08003	11	6	-0.74830	11	8	-0.41856
11	9	0.82400	12	1	0.57658	12	2	0.33073	12	3	0.03785
12	4	-0.83123	12	5	-0.37858	12	6	-0.91270	12	10	0.25464
12	11	0.04785	12	12	0.87485	13	2	-0.09822	13	3	-1.38241
13	17	0.43931	13	18	0.72052	13	20	-0.34108	13	21	0.66189
14	2	1.10077	14	3	0.79622	14	5	-0.66146	14	6	-0.07570
14	17	-0.43931	14	18	-0.72052	15	2	-1.00255	15	3	0.58618
15	5	0.66146	15	6	0.07570	15	20	0.34109	15	21	-0.66189
16	1	-2.07998	16	4	0.60785	16	16	0.84388	16	19	0.62824
17	1	-0.27676	17	4	0.14753	17	7	-0.32869	17	10	0.16064
17	11	-0.27643	17	12	-0.03164	17	13	0.16064	17	14	0.27643
17	15	0.03164	17	16	0.53472	17	19	-0.39808			

B MATRIX FOR THE MOLECULE CO3-COF

1	2	-0.87295	1	3	-0.48781	1	5	0.87295	1	6	0.48781
2	5	0.15379	2	6	-0.98810	2	8	-0.15379	2	9	0.98810
3	4	0.81197	3	5	-0.53225	3	6	0.23960	3	10	-0.81197
3	11	0.53225	3	12	-0.23960	4	4	-0.81197	4	5	-0.53225
4	6	0.23960	4	13	0.81197	4	14	0.53225	4	15	-0.23960
5	2	0.91552	5	3	-0.40227	5	17	-0.91552	5	18	0.40227
6	2	-0.11401	6	3	0.99348	6	20	0.11401	6	21	-0.99348
7	5	1.36734	7	6	-0.61552	7	10	-0.53896	7	11	-0.68367
7	12	0.30776	7	13	0.53896	7	14	-0.68367	7	15	0.30776
8	4	1.04297	8	5	0.48612	8	6	0.96145	8	7	-0.79097
8	8	-0.47075	8	9	-0.07327	8	13	-0.25200	8	14	-0.01537
8	15	-0.88818	9	4	-1.04297	9	5	0.48612	9	6	0.96145
9	7	0.79097	9	8	-0.47075	9	9	-0.07327	9	10	0.25200
9	11	-0.01537	9	12	-0.88818	10	1	-0.57774	10	2	-0.16271
10	3	0.29118	10	4	0.85582	10	5	-0.51471	10	6	-0.85364
10	13	-0.27808	10	14	0.67742	10	15	0.56247	11	2	0.32542
11	3	-0.58236	11	5	-1.23780	11	6	0.44035	11	8	0.91238
11	9	0.14201	12	1	0.57774	12	2	-0.16271	12	3	0.29118
12	4	-0.85582	12	5	-0.51471	12	6	-0.85364	12	10	0.27808
12	11	0.67742	12	12	0.56247	13	2	-0.89280	13	3	-0.83179
13	17	0.33747	13	18	0.76806	13	20	0.55533	13	21	0.06373
14	2	0.01205	14	3	1.35042	14	5	0.32542	14	6	-0.58236
14	17	-0.33747	14	18	-0.76806	15	2	0.88075	15	3	-0.51863
15	5	-0.32542	15	6	0.58236	15	20	-0.55533	15	21	-0.06373
16	1	1.94645	16	4	-0.62433	16	16	-0.83893	16	19	-0.48319
17	1	0.33589	17	4	-0.11293	17	7	0.32828	17	10	-0.16414
17	11	-0.13868	17	12	0.24818	17	13	-0.16414	17	14	0.13868
17	15	-0.24818	17	16	-0.52580	17	19	0.30284			

B MATRIX FOR THE MOLECULE CH3-COCL

1	2	-0.81596	1	3	-0.57811	1	5	0.81596	1	6	0.57811
2	5	0.25827	2	6	-0.96607	2	8	-0.25827	2	9	0.96607
3	4	0.81197	3	5	-0.55476	3	6	0.18148	3	10	-0.81197
3	11	0.55476	3	12	-0.18148	4	4	-0.81197	4	5	-0.55476
4	6	0.18148	4	13	0.81197	4	14	0.55476	4	15	-0.18148
5	2	0.95319	5	3	-0.30235	5	17	-0.95319	5	18	0.30235
6	2	-0.21930	6	3	0.97566	6	20	0.21930	6	21	-0.97566
7	5	1.42518	7	6	-0.46621	7	10	-0.53896	7	11	-0.71259
7	12	0.23311	7	13	0.53896	7	14	-0.71259	7	15	0.23311
8	4	1.04297	8	5	0.38084	8	6	1.00780	8	7	-0.79097
8	8	-0.46025	8	9	-0.12305	8	13	-0.25200	8	14	0.07942
8	15	-0.88475	9	4	-1.04297	9	5	0.38084	9	6	1.00780
9	7	0.79097	9	8	-0.46025	9	9	-0.12305	9	10	0.25200
9	11	0.07942	9	12	-0.88475	10	1	-0.57774	10	2	-0.19283
10	3	0.27217	10	4	0.85582	10	5	-0.42075	10	6	-0.90366
10	13	-0.27808	10	14	0.61359	10	15	0.63149	11	2	0.38566
11	3	-0.54434	11	5	-1.27770	11	6	0.30586	11	8	0.89204
11	9	0.23848	12	1	0.57774	12	2	-0.19283	12	3	0.27217
12	4	-0.85582	12	5	-0.42076	12	6	-0.90366	12	10	0.27808
12	11	0.61359	12	12	0.63149	13	2	-0.79902	13	3	-0.92224
13	17	0.25365	13	18	0.79966	13	20	0.54537	13	21	0.12258
14	2	-0.13201	14	3	1.34400	14	5	0.38566	14	6	-0.54434
14	17	-0.25365	14	18	-0.79966	15	2	0.93103	15	3	-0.42176
15	5	-0.38566	15	6	0.54434	15	20	-0.54537	15	21	-0.12258
16	1	1.94645	16	4	-0.62433	16	16	-0.83893	16	19	-0.48319
17	1	0.33588	17	4	-0.11293	17	7	0.32828	17	10	-0.16414
17	11	-0.16435	17	12	0.23197	17	13	-0.16414	17	14	0.16435
17	15	-0.23197	17	16	-0.52580	17	19	0.30284			

B MATRIX FOR THE MOLECULE CD3-COCL

1	2	-0.89059	1	3	-0.45480	1	5	0.89059	1	6	0.45480
2	5	0.11670	2	6	-0.99317	2	8	-0.11670	2	9	0.99317
3	4	0.81197	3	5	-0.52291	3	6	0.25935	3	10	-0.81197
3	11	0.52291	3	12	-0.25935	4	4	-0.81197	4	5	-0.52291
4	6	0.25935	4	13	0.81197	4	14	0.52291	4	15	-0.25935
5	2	0.89980	5	3	-0.43630	5	17	-0.89980	5	18	0.43630
6	2	-0.07675	6	3	0.99705	6	20	0.07675	6	21	-0.99705
7	5	1.34335	7	6	-0.66625	7	10	-0.53896	7	11	-0.67168
7	12	0.33313	7	13	0.53896	7	14	-0.67167	7	15	0.33313
8	4	1.04297	8	5	0.52177	8	6	0.94258	8	7	-0.79096
8	8	-0.47316	8	9	-0.05560	8	13	-0.25200	8	14	-0.04860
8	15	-0.88698	9	4	-1.04297	9	5	0.52177	9	6	0.94258
9	7	0.79096	9	8	-0.47316	9	9	-0.05560	9	10	0.25200
9	11	-0.04860	9	12	-0.88698	10	1	-0.57739	10	2	-0.15161
10	3	0.29688	10	4	0.85547	10	5	-0.54639	10	6	-0.83361
10	13	-0.27808	10	14	0.69800	10	15	0.53672	11	2	0.30322
11	3	-0.59377	11	5	-1.22027	11	6	0.48601	11	8	0.91705
11	9	0.10776	12	1	0.57739	12	2	-0.15161	12	3	0.29688
12	4	-0.85547	12	5	-0.54639	12	6	-0.83361	12	10	0.27808
12	11	0.69800	12	12	0.53672	13	2	-0.87472	13	3	-0.79403
13	17	0.36602	13	18	0.75487	13	20	0.50870	13	21	0.03916
14	2	0.06280	14	3	1.34864	14	5	0.30322	14	6	-0.59377
14	17	-0.36602	14	18	-0.75487	15	2	0.81192	15	3	-0.55461
15	5	-0.30322	15	6	0.59377	15	20	-0.50870	15	21	-0.03916
16	1	1.90391	16	4	-0.62393	16	16	-0.83893	16	19	-0.44106
17	1	0.36218	17	4	-0.11283	17	7	0.32828	17	10	-0.16414
17	11	-0.12930	17	12	0.25319	17	13	-0.16414	17	14	0.12930
17	15	-0.25319	17	16	-0.52578	17	19	0.27642			

B MATRIX FOR THE MOLECULE CH3-COBR

1	2	-0.85800	1	3	-0.51365	1	5	0.85800	1	6	0.51365
2	5	0.18321	2	6	-0.98307	2	8	-0.18321	2	9	0.98307
3	4	0.81197	3	5	-0.53917	3	6	0.22360	3	10	-0.81197
3	11	0.53917	3	12	-0.22360	4	4	-0.81197	4	5	-0.53917
4	6	0.22360	4	13	0.81197	4	14	0.53917	4	15	-0.22360
5	2	0.92710	5	3	-0.37482	5	17	-0.92710	5	18	0.37482
6	2	-0.14361	6	3	0.98963	6	20	0.14361	6	21	-0.98963
7	5	1.38510	7	6	-0.57443	7	10	-0.53896	7	11	-0.69255
7	12	0.28722	7	13	0.53896	7	14	-0.69255	7	15	0.28722
8	4	1.04297	8	5	0.45721	8	6	0.97553	8	7	-0.79097
8	8	-0.46835	8	9	-0.08729	8	13	-0.25200	8	14	0.01114
8	15	-0.88824	9	4	-1.04297	9	5	0.45721	9	6	0.97553
9	7	0.79097	9	8	-0.46835	9	9	-0.08729	9	10	0.25200
9	11	0.01114	9	12	-0.88824	10	1	-0.57739	10	2	-0.17123
10	3	0.28602	10	4	0.85547	10	5	-0.48911	10	6	-0.86845
10	13	-0.27808	10	14	0.66033	10	15	0.58243	11	2	0.34245
11	3	-0.57204	11	5	-1.25019	11	6	0.40287	11	8	0.90773
11	9	0.16917	12	1	0.57739	12	2	-0.17123	12	3	0.28602
12	4	-0.85547	12	5	-0.48911	12	6	-0.86845	12	10	0.27808
12	11	0.66033	12	12	0.58243	13	2	-0.81936	13	3	-0.85104
13	17	0.31445	13	18	0.77777	13	20	0.50492	13	21	0.07327
14	2	-0.02801	14	3	1.34981	14	5	0.34245	14	6	-0.57204
14	17	-0.31444	14	18	-0.77777	15	2	0.84737	15	3	-0.49877
15	5	-0.34245	15	6	0.57204	15	20	-0.50492	15	21	-0.07327
16	1	1.90391	16	4	-0.62393	16	16	-0.83893	16	19	-0.44105
17	1	0.36219	17	4	-0.11283	17	7	0.32828	17	10	-0.16414
17	11	-0.14603	17	12	0.24393	17	13	-0.16414	17	14	0.14603
17	15	-0.24393	17	16	-0.52578	17	19	0.27642			

B MATRIX FOR THE MOLECULE CD3-COBR

1	2	-0.41170	1	3	-0.91132	1	5	0.41170	1	6	0.91132
2	5	-0.99690	2	6	0.07866	2	8	0.99690	2	9	-0.07866
3	4	0.81483	3	5	0.28926	3	6	-0.50238	3	10	-0.81483
3	11	-0.28926	3	12	0.50238	4	4	-0.81483	4	5	0.28926
4	6	-0.50238	4	13	0.81483	4	14	-0.28926	4	15	0.50238
5	2	-0.55758	5	3	0.83012	5	17	0.55758	5	18	-0.83012
6	2	0.99770	6	3	0.06781	6	20	-0.99770	6	21	-0.06781
7	5	-0.61049	7	6	1.06027	7	10	-0.43521	7	11	0.30525
7	12	-0.53013	7	13	0.43521	7	14	0.30525	7	15	-0.53013
8	4	0.85985	8	5	0.74673	8	6	0.44712	8	7	-0.64753
8	8	-0.02988	8	9	-0.37873	8	13	-0.21232	8	14	-0.71685
8	15	-0.06839	9	4	-0.85985	9	5	0.74673	9	6	0.44712
9	7	0.64753	9	8	-0.02988	9	9	-0.37873	9	10	0.21232
9	11	-0.71685	9	12	-0.06839	10	1	-0.56235	10	2	0.29588
10	3	-0.13367	10	4	0.78259	10	5	-0.70257	10	6	-0.45771
10	13	-0.22024	10	14	0.40669	10	15	0.59138	11	2	-0.59177
11	3	0.26734	11	5	0.53271	11	6	-1.01576	11	8	0.05906
11	9	0.74843	12	1	0.56235	12	2	0.29588	12	3	-0.13367
12	4	-0.78259	12	5	-0.70257	12	6	-0.45771	12	10	0.22024
12	11	0.40669	12	12	0.59138	13	2	-0.62726	13	3	-1.37843
13	17	0.68947	13	18	0.46310	13	20	-0.06221	13	21	0.91532
14	2	1.28124	14	3	0.19577	14	5	-0.59177	14	6	0.26734
14	17	-0.68947	14	18	-0.46310	15	2	-0.65398	15	3	1.18266
15	5	0.59177	15	6	-0.26734	15	20	0.06221	15	21	-0.91532
16	1	-1.17257	16	4	0.31793	16	16	0.41383	16	19	0.44082
17	1	0.00465	17	4	0.02722	17	7	-0.26597	17	10	0.13299
17	11	-0.20991	17	12	0.09483	17	13	0.13299	17	14	0.20991
17	15	-0.09483	17	16	0.48863	17	19	-0.52050			

B MATRIX FOR THE MOLECULE CF3-COH

1	2	-0.38778	1	3	-0.92175	1	5	0.38778	1	6	0.92175
2	5	-0.99861	2	6	0.05262	2	8	0.99861	2	9	-0.05262
3	4	0.81483	3	5	0.30227	3	6	-0.49466	3	10	-0.81483
3	11	-0.30227	3	12	0.49466	4	4	-0.81483	4	5	0.30227
4	6	-0.49466	4	13	0.81483	4	14	-0.30227	4	15	0.49466
5	2	-0.57905	5	3	0.81529	5	17	0.57905	5	18	-0.81529
6	2	0.99559	6	3	0.09382	6	20	-0.99559	6	21	-0.09382
7	5	-0.63795	7	6	1.04398	7	10	-0.43521	7	11	0.31898
7	12	-0.52199	7	13	0.43521	7	14	0.31898	7	15	-0.52199
8	4	0.85985	8	5	0.73481	8	6	0.46645	8	7	-0.64753
8	8	-0.01999	8	9	-0.37938	8	13	-0.21232	8	14	-0.71482
8	15	-0.08707	9	4	-0.85985	9	5	0.73481	9	6	0.46645
9	7	0.64753	9	8	-0.01999	9	9	-0.37938	9	10	0.21232
9	11	-0.71482	9	12	-0.08707	10	1	-0.56235	10	2	0.29927
10	3	-0.12590	10	4	0.78259	10	5	-0.69039	10	6	-0.47589
10	13	-0.22024	10	14	0.39112	10	15	0.60179	11	2	-0.59854
11	3	0.25181	11	5	0.55903	11	6	-1.00152	11	8	0.03951
11	9	0.74971	12	1	0.56235	12	2	0.29927	12	3	-0.12590
12	4	-0.78259	12	5	-0.69039	12	6	-0.47589	12	10	0.22024
12	11	0.39112	12	12	0.60179	13	2	-0.59108	13	3	-1.39432
13	17	0.67716	13	18	0.48094	13	20	-0.08607	13	21	0.91339
14	2	1.27570	14	3	0.22913	14	5	-0.59854	14	6	0.25181
14	17	-0.67716	14	18	-0.48094	15	2	-0.68462	15	3	1.16519
15	5	0.59854	15	6	-0.25181	15	20	0.08607	15	21	-0.91339
16	1	-1.17257	16	4	0.31793	16	16	0.41383	16	19	0.44082
17	1	0.00465	17	4	0.02722	17	7	-0.26597	17	10	0.13299
17	11	-0.21232	17	12	0.08932	17	13	0.13299	17	14	0.21232
17	15	-0.08932	17	16	0.48863	17	19	-0.52050			

B MATRIX FOR THE MOLECULE CF3-COO

1	2	0.43774	1	3	-0.89910	1	5	-0.43774	1	6	0.89910
2	5	-0.67760	2	6	-0.73543	2	8	0.67760	2	9	0.73543
3	4	0.80641	3	5	0.57821	3	6	-0.12401	3	10	-0.80641
3	11	-0.57821	3	12	0.12401	4	4	-0.80641	4	5	0.57821
4	6	-0.12401	4	13	0.80641	4	14	-0.57821	4	15	0.12401
5	2	-0.97800	5	3	0.20859	5	17	0.97800	5	18	-0.20859
6	2	0.55977	6	3	0.82865	6	20	-0.55977	6	21	-0.82865
7	5	-1.17684	7	6	0.25240	7	10	-0.44131	7	11	0.58842
7	12	-0.12620	7	13	0.44131	7	14	0.58842	7	15	-0.12620
8	4	0.82065	8	5	0.10115	8	6	0.87462	8	7	-0.63098
8	8	0.29305	8	9	-0.27001	8	13	-0.18967	8	14	-0.39420
8	15	-0.60461	9	4	-0.82065	9	5	0.10115	9	6	0.87462
9	7	0.63098	9	8	0.29305	9	9	-0.27001	9	10	0.18967
9	11	-0.39420	9	12	-0.60461	10	1	-0.56975	10	2	0.29576
10	3	0.14400	10	4	0.80540	10	5	-0.11389	10	6	-0.82833
10	13	-0.23564	10	14	-0.18187	10	15	0.68434	11	2	-0.59151
11	3	-0.28799	11	5	1.14034	11	6	-0.21768	11	8	-0.54883
11	9	0.50567	12	1	0.56975	12	2	0.29576	12	3	0.14400
12	4	-0.80540	12	5	-0.11389	12	6	-0.82833	12	10	0.23564
12	11	-0.18187	12	12	0.68434	13	2	0.28465	13	3	-1.14862
13	17	0.17828	13	18	0.83590	13	20	-0.46293	13	21	0.31272
14	2	0.76980	14	3	1.12389	14	5	-0.59151	14	6	-0.28799
14	17	-0.17829	14	18	-0.83590	15	2	-1.05445	15	3	0.02473
15	5	0.59151	15	6	0.28799	15	20	0.46293	15	21	-0.31272
16	1	-2.06739	16	4	0.70435	16	16	0.85470	16	19	0.50833
17	1	-0.28686	17	4	0.06708	17	7	-0.26715	17	10	0.13357
17	11	-0.20801	17	12	-0.10127	17	13	0.13357	17	14	0.20801
17	15	0.10127	17	16	0.54232	17	19	-0.32254			

B MATRIX FOR THE MOLECULE CF3-COF

1	2	0.50133	1	3	-0.86525	1	5	-0.50133	1	6	0.86525
2	5	-0.62290	2	6	-0.78230	2	8	0.62290	2	9	0.78230
3	4	0.80641	3	5	0.58564	3	6	-0.08207	3	10	-0.80641
3	11	-0.58564	3	12	0.08207	4	4	-0.80641	4	5	0.58564
4	6	-0.08207	4	13	0.80641	4	14	-0.58564	4	15	0.08207
5	2	-0.99468	5	3	0.10300	5	17	0.99468	5	18	-0.10300
6	2	0.65490	6	3	0.75572	6	20	-0.65490	6	21	-0.75572
7	5	-1.20091	7	6	0.16829	7	10	-0.44463	7	11	0.60046
7	12	-0.08414	7	13	0.44463	7	14	0.60046	7	15	-0.08414
8	4	0.82682	8	5	0.03821	8	6	0.88624	8	7	-0.63572
8	8	0.31407	8	9	-0.25008	8	13	-0.19109	8	14	-0.35228
8	15	-0.63616	9	4	-0.82682	9	5	0.03821	9	6	0.88624
9	7	0.63572	9	8	0.31407	9	9	-0.25008	9	10	0.19109
9	11	-0.35228	9	12	-0.63617	10	1	-0.55196	10	2	0.27573
10	3	0.15976	10	4	0.78937	10	5	-0.04334	10	6	-0.83426
10	13	-0.23741	10	14	-0.23239	10	15	0.67450	11	2	-0.55147
11	3	-0.31952	11	5	1.13967	11	6	-0.14883	11	8	-0.58820
11	9	0.46835	12	1	0.55196	12	2	0.27573	12	3	0.15976
12	4	-0.78937	12	5	-0.04334	12	6	-0.83426	12	10	0.23741
12	11	-0.23239	12	12	0.67450	13	2	0.34455	13	3	-1.21718
13	17	0.08728	13	18	0.84295	13	20	-0.43184	13	21	0.37423
14	2	0.63876	14	3	1.16248	14	5	-0.55147	14	6	-0.31952
14	17	-0.08729	14	18	-0.84295	15	2	-0.98331	15	3	0.05470
15	5	0.55147	15	6	0.31952	15	20	0.43184	15	21	-0.37423
16	1	-1.88856	16	4	0.55217	16	16	0.84746	16	19	0.48893
17	1	-0.34338	17	4	0.12180	17	7	-0.26916	17	10	0.13458
17	11	-0.20169	17	12	-0.11686	17	13	0.13458	17	14	0.20169
17	15	0.11686	17	16	0.52376	17	19	-0.30218			

B MATRIX FOR THE MOLECULE CF3-COCL

2. Symmetrized G Matrix

The symmetrized G matrices on the next pages are broken down into their a' and a" symmetry blocks. Above each block are listed the symmetry coordinates associated with each row and its corresponding column.

1 THE ASYM. HCH2 STRETCH ---
2 THE SYMMETRIC CH3 STRETCH
3 THE C-Z STRETCH ----------
4 THE C=C STRETCH ----------
5 THE HCH2 DEFORMATION -----
6 THE CH3 UMBRELLA BEND ----
7 THE SCISSORS BEND -------
8 THE IN-PLANE CH3 ROCK ----
9 THE C-C STRETCH ----------
10 THE O=C-Z ROCK ----------

1	1.1021	0.0	0.0	0.0	0.1408	0.0	0.0	-0.1156	0.0	-0.0902
2	0.0	1.0224	0.0	0.0	0.0	-0.1077	0.0	0.0	-0.0502	0.0
3	0.0	0.0	1.0756	-0.0399	0.0	0.0	-0.0737	-0.0603	-0.0384	-0.1122
4	0.0	0.0	-0.0399	0.1459	0.0	0.0	-0.0804	0.0564	-0.0465	0.1116
5	0.1408	0.0	0.0	0.0	2.2569	0.0	0.0	0.2857	0.0	-0.1156
6	0.0	-0.1077	0.0	0.0	0.0	2.1204	0.0	0.0	0.1790	0.0
7	0.0	0.0	-0.0737	-0.0804	0.0	0.0	1.5365	0.0037	0.1510	-0.6608
8	-0.1156	0.0	-0.0603	0.0564	0.2857	0.0	0.0037	1.0185	0.0	0.2010
9	0.0	-0.0502	-0.0384	-0.0465	0.0	0.1790	0.1510	0.0	0.1667	-0.0067
10	-0.0902	0.0	-0.1122	0.1116	-0.1156	0.0	-0.6608	0.2010	-0.0067	0.6983

11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION -------------

11	1.1021	0.1408	0.1156	0.0335	0.0049
12	0.1408	2.2569	-0.2857	0.0429	0.0062
13	0.1156	-0.2857	1.0185	0.1191	0.0079
14	0.0335	0.0429	0.1191	0.3458	-0.2045
15	0.0049	0.0062	0.0079	-0.2045	0.5886

G MATRIX FOR THE MOLECULE CH3-COH

1 THE C-Z STRETCH ----------
2 THE ASYM. DCD2 STRETCH ---
3 THE SYMMETRIC CD3 STRETCH
4 THE C=C STRETCH ----------
5 THE SCISSORS BEND -------
6 THE C-C STRETCH ----------
7 THE DCD2 DEFORMATION -----
8 THE CD3 UMBRELLA BEND ----
9 THE IN-PLANE CD3 ROCK ----
10 THE O=C-Z ROCK ----------

1	1.0756	0.0	0.0	-0.0399	-0.0737	-0.0384	0.0	0.0	-0.0603	-0.1122
2	0.0	0.6064	0.0	0.0	0.0	0.0	0.1408	0.0	-0.1156	-0.0902
3	0.0	0.0	0.5267	0.0	0.0	-0.0502	0.0	-0.1077	0.0	0.0
4	-0.0399	0.0	0.0	0.1459	-0.0804	-0.0465	0.0	0.0	0.0564	0.1116
5	-0.0737	0.0	0.0	-0.0804	1.5365	0.1510	0.0	0.0	0.0037	-0.6608
6	-0.0384	0.0	-0.0502	-0.0465	0.1510	0.1667	0.0	0.1790	0.0	-0.0067
7	0.0	0.1408	0.0	0.0	0.0	0.0	1.2195	0.0	0.0690	-0.1156
8	0.0	0.0	-0.1077	0.0	0.0	0.1790	0.0	1.2532	0.0	0.0
9	-0.0603	-0.1156	0.0	0.0564	0.0037	0.0	0.0690	0.0	0.5982	0.2010
10	-0.1122	-0.0902	0.0	0.1116	-0.6608	-0.0067	-0.1156	0.0	0.2010	0.6983

11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CD3 WAG
15 THE TORSION --------------

11	0.6064	C.1408	0.0335	0.1156	0.0049
12	0.1408	1.2195	0.0429	-0.0690	0.0062
13	0.0335	0.0429	0.3458	0.1191	-0.2045
14	0.1156	-0.0690	0.1191	0.5982	0.0079
15	0.0049	0.0062	-0.2045	0.0079	0.4293

G MATRIX FOR THE MOLECULE CD3-COH

```
 1 THE ASYM. HCH2 STRETCH ---
 2 THE SYMMETRIC CH3 STRETCH
 3 THE C-Z STRETCH ----------
 4 THE C=O STRETCH ----------
 5 THE HCH2 DEFORMATION -----
 6 THE CH3 UMBRELLA BEND ----
 7 THE C-C STRETCH ----------
 8 THE IN-PLANE CH3 ROCK ----
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK -----------
-----------------------------
```

1	1.1021	0.0	0.0	0.0	0.1408	0.0	0.0	-0.1156	0.0	-0.0902
2	0.0	1.0224	0.0	0.0	0.0	-0.1077	-0.0502	0.0	0.0	0.0
3	0.0	0.0	0.5799	-0.0399	0.0	0.0	-0.0384	-0.0603	-0.0737	-0.1122
4	0.0	0.0	-0.0399	0.1459	0.0	0.0	-0.0465	0.0564	-0.0804	0.1116
5	0.1408	0.0	0.0	0.0	2.2569	0.0	0.0	0.2857	0.0	-0.1156
6	0.0	-0.1077	0.0	0.0	0.0	2.1204	0.1790	0.0	0.0	0.0
7	0.0	-0.0502	-0.0384	-0.0465	0.0	0.1790	0.1667	0.0	0.1510	-0.0067
8	-0.1156	0.0	-0.0603	0.0564	0.2857	0.0	0.0	1.0185	0.0037	0.2010
9	0.0	0.0	-0.0737	-0.0804	0.0	0.0	0.1510	0.0037	0.9374	-0.3148
10	-0.0902	0.0	-0.1122	0.1116	-0.1156	0.0	-0.0067	0.2010	-0.3148	0.4986

```
11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

11	1.1021	0.1408	0.1156	0.0335	0.0049
12	0.1408	2.2569	-0.2857	0.0429	0.0062
13	0.1156	-0.2857	1.0185	0.1191	0.0079
14	0.0335	0.0429	0.1191	0.2473	-0.0928
15	0.0049	0.0062	0.0079	-0.0928	0.4617

G MATRIX FOR THE MOLECULE CH3-COO

```
 1 THE ASYM. DCD2 STRETCH ---
 2 THE SYMMETRIC CD3 STRETCH
 3 THE C-Z STRETCH ----------
 4 THE C=O STRETCH ----------
 5 THE C-C STRETCH ----------
 6 THE DCD2 DEFORMATION -----
 7 THE CD3 UMBRELLA BEND ----
 8 THE SCISSORS BEND -------
 9 THE IN-PLANE CD3 ROCK ----
10 THE O=C-Z ROCK -----------
-----------------------------
```

1	0.6064	0.0	0.0	0.0	0.0	0.1408	0.0	0.0	-0.1156	-0.0902
2	0.0	0.5267	0.0	0.0	-0.0502	0.0	-0.1077	0.0	0.0	0.0
3	0.0	0.0	0.5799	-0.0399	-0.0384	0.0	0.0	-0.0737	-0.0603	-0.1122
4	0.0	0.0	-0.0399	0.1459	-0.0465	0.0	0.0	-0.0804	0.0564	0.1116
5	0.0	-0.0502	-0.0384	-0.0465	0.1667	0.0	0.1790	0.1510	0.0	-0.0067
6	0.1408	0.0	0.0	0.0	0.0	1.2195	0.0	0.0	0.0690	-0.1156
7	0.0	-0.1077	0.0	0.0	0.1790	0.0	1.2532	0.0	0.0	0.0
8	0.0	0.0	-0.0737	-0.0804	0.1510	0.0	0.0	0.9374	0.0037	-0.3148
9	-0.1156	0.0	-0.0603	0.0564	0.0	0.0690	0.0	0.0037	0.5982	0.2010
10	-0.0902	0.0	-0.1122	0.1116	-0.0067	-0.1156	0.0	-0.3148	0.2010	0.4986

```
11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CD3 WAG
15 THE TORSION --------------.
-----------------------------
```

11	0.6064	0.1408	0.0335	0.1156	0.0049
12	0.1408	1.2195	0.0429	-0.0690	0.0062
13	0.0335	0.0429	0.2473	0.1191	-0.0928
14	0.1156	-0.0690	0.1191	0.5982	0.0079
15	0.0049	0.0062	-0.0928	0.0079	0.3024

G MATRIX FOR THE MOLECULE CD3-COD

1 THE ASYM. HCH2 STRETCH ---
2 THE SYMMETRIC CH3 STRETCH
3 THE C=O STRETCH ----------
4 THE HCH2 DEFORMATION -----
5 THE CH3 UMBRELLA BEND ----
6 THE C-Z STRETCH ----------
7 THE IN-PLANE CH3 ROCK ----
8 THE C-C STRETCH ----------
9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------

1	1.1028	0.0005	0.0	0.1436	-0.0009	0.0	-0.1150	-0.0018	0.0	-0.0904
2	0.0005	1.0196	0.0	0.0004	-0.1009	0.0	0.0006	-0.0478	0.0	0.0004
3	0.0	0.0	0.1459	0.0	0.0	-0.0434	0.0536	-0.0512	-0.0649	0.0994
4	0.1436	0.0004	0.0	2.2553	-0.0135	0.0	0.2583	-0.0018	0.0	-0.1174
5	-0.0009	-0.1009	0.0	-0.0135	2.0296	0.0	-0.0157	0.1760	0.0	-0.0024
6	0.0	0.0	-0.0434	0.0	0.0	0.1360	-0.0635	-0.0295	-0.0735	-0.1158
7	-0.1150	0.0006	0.0536	0.2583	-0.0157	-0.0635	1.0155	-0.0002	0.0212	0.1956
8	-0.0018	-0.0478	-0.0512	-0.0018	0.1760	-0.0295	-0.0002	0.1667	0.1390	-0.0018
9	0.0	0.0	-0.0649	0.0	0.0	-0.0735	0.0212	0.1390	0.3506	0.0491
10	-0.0904	0.0004	0.0994	-0.1174	-0.0024	-0.1158	0.1956	-0.0018	0.0491	0.2969

11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION ---------------

11	1.1043	0.1456	0.1136	0.0587	0.0143
12	0.1456	2.2951	-0.2735	0.0763	0.0350
13	0.1136	-0.2735	0.9966	0.2009	0.0333
14	0.0587	0.0763	0.2009	0.4566	0.0705
15	0.0143	0.0350	0.0333	0.0705	0.3464

G MATRIX FOR THE MOLECULE CH3-COF

```
 1 THE ASYM. DCD2 STRETCH ---
 2 THE SYMMETRIC CD3 STRETCH
 3 THE C=O STRETCH ----------
 4 THE C-Z STRETCH ----------
 5 THE CD3 UMBRELLA BEND ----
 6 THE DCD2 DEFORMATION -----
 7 THE IN-PLANE CD3 ROCK ----
 8 THE C-C STRETCH ----------
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------
-----------------------------
```

1	0.6071	0.0005	0.0	0.0	-0.0009	0.1436	-0.1150	-0.0018	0.0	-0.0904
2	0.0005	0.5239	0.0	0.0	-0.1009	0.0004	0.0006	-0.0478	0.0	0.0004
3	0.0	0.0	0.1459	-0.0434	0.0	0.0	0.0536	-0.0512	-0.0649	0.0994
4	0.0	0.0	-0.0434	0.1360	0.0	0.0	-0.0635	-0.0295	-0.0735	-0.1158
5	-0.0009	-0.1009	0.0	0.0	1.2014	-0.0068	-0.0095	0.1760	0.0	-0.0024
6	0.1436	0.0004	0.0	0.0	-0.0068	1.2217	0.0546	-0.0018	0.0	-0.1174
7	-0.1150	0.0006	0.0536	-0.0635	-0.0095	0.0546	0.5956	-0.0002	0.0212	0.1956
8	-0.0018	-0.0478	-0.0512	-0.0295	0.1760	-0.0018	-0.0002	0.1667	0.1390	-0.0018
9	0.0	0.0	-0.0649	-0.0735	0.0	0.0	0.0212	0.1390	0.3506	0.0491
10	-0.0904	0.0004	0.0994	-0.1158	-0.0024	-0.1174	0.1956	-0.0018	0.0491	0.2969

```
11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE CD3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

11	0.6085	0.1456	0.1136	0.0587	0.0143
12	0.1456	1.2430	-0.0631	0.0763	0.0268
13	0.1136	-0.0631	0.5839	0.2009	0.0333
14	0.0587	0.0763	0.2009	0.4566	0.0705
15	0.0143	0.0268	0.0333	0.0705	0.1906

G MATRIX FOR THE MOLECULE CD3-COF

1 THE ASYM. HCH2 STRETCH ---
2 THE SYMMETRIC CH3 STRETCH
3 THE C=C STRETCH ----------
4 THE HCH2 DEFORMATION -----
5 THE CH3 UMBRELLA BEND ----
6 THE IN-PLANE CH3 ROCK ----
7 THE C-C STRETCH ----------
8 THE C-Z STRETCH ----------
9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------

1	1.1021	0.0	0.0	0.1411	0.0	-0.1158	0.0	0.0	0.0	-0.0903
2	0.0	1.0225	0.0	0.0	-0.1081	0.0	-0.0502	0.0	0.0	0.0
3	0.0	0.0	0.1459	0.0	0.0	0.0543	-0.0502	-0.0420	-0.0493	0.0912
4	0.1411	0.0	0.0	2.2688	0.0	0.2877	0.0	0.0	0.0	-0.1160
5	0.0	-0.1081	0.0	0.0	2.1332	0.0	0.1795	0.0	0.0	0.0
6	-0.1158	0.0	0.0543	0.2877	0.0	1.0237	0.0	-0.0628	0.0242	0.1941
7	0.0	-0.0502	-0.0502	0.0	0.1795	0.0	0.1667	-0.0321	0.1210	0.0090
8	0.0	0.0	-0.0420	0.0	0.0	-0.0628	-0.0321	0.1115	-0.0740	-0.1153
9	0.0	0.0	-0.0493	0.0	0.0	0.0242	0.1210	-0.0740	0.2653	0.0867
10	-0.0903	0.0	0.0912	-0.1160	0.0	0.1941	0.0090	-0.1153	0.0867	0.2776

11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION ------------

11	1.1021	0.1411	0.1158	-0.0597	-0.0108
12	0.1411	2.2688	-0.2877	-0.0767	-0.0139
13	0.1158	-0.2877	1.0237	-0.1955	-0.0343
14	-0.0597	-0.0767	-0.1955	0.3988	0.0838
15	-0.0108	-0.0139	-0.0343	0.0838	0.3511

G MATRIX FOR THE MOLECULE CH3-COCL

1 THE ASYM. DCD2 STRETCH ---
2 THE SYMMETRIC CD3 STRETCH
3 THE C=O STRETCH ----------
4 THE DCD2 DEFORMATION -----
5 THE CD3 UMBRELLA BEND ----
6 THE C-C STRETCH ----------
7 THE IN-PLANE CD3 ROCK ----
8 THE C-Z STRETCH ----------
9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------

1	0.6064	0.0	0.0	0.1411	0.0	0.0	-0.1158	0.0	0.0	-0.0903
2	0.0	0.5268	0.0	0.0	-0.1081	-0.0502	0.0	0.0	0.0	0.0
3	0.0	0.0	0.1459	0.0	0.0	-0.0502	0.0543	-0.0420	-0.0493	0.0912
4	0.1411	0.0	0.0	1.2259	0.0	0.0	0.0697	0.0	0.0	-0.1160
5	0.0	-0.1081	0.0	0.0	1.2607	0.1795	0.0	0.0	0.0	0.0
6	0.0	-0.0502	-0.0502	0.0	0.1795	0.1667	0.0	-0.0321	0.1210	0.0090
7	-0.1158	0.0	0.0543	0.0697	0.0	0.0	0.6010	-0.0628	0.0242	0.1941
8	0.0	0.0	-0.0420	0.0	0.0	-0.0321	-0.0628	0.1115	-0.0740	-0.1153
9	0.0	0.0	-0.0493	0.0	0.0	0.1210	0.0242	-0.0740	0.2653	0.0867
10	-0.0903	0.0	0.0912	-0.1160	0.0	0.0090	0.1941	-0.1153	0.0867	0.2776

11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE CD3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------

11	0.6064	0.1411	0.1158	-0.0597	-0.0108
12	0.1411	1.2259	-0.0697	-0.0767	-0.0139
13	0.1158	-0.0697	0.6010	-0.1955	-0.0343
14	-0.0597	-0.0767	-0.1955	0.3988	0.0838
15	-0.0108	-0.0139	-0.0343	0.0838	0.1909

G MATRIX FOR THE MOLECULE CD3-COCL

1 THE ASYM. HCH2 STRETCH ---
2 THE SYMMETRIC CH3 STRETCH
3 THE C=O STRETCH ----------
4 THE HCH2 DEFORMATION -----
5 THE CH3 UMBRELLA BEND ----
6 THE IN-PLANE CH3 ROCK ----
7 THE C-C STRETCH ----------
8 THE C-Z STRETCH ----------
9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------

1	1.1021	0.0	0.0	0.1411	0.0	-0.1158	0.0	0.0	0.0	-0.0902
2	0.0	1.0225	0.0	0.0	-0.1081	0.0	-0.0502	0.0	0.0	0.0
3	0.0	0.0	0.1459	0.0	0.0	0.0543	-0.0502	-0.0420	-0.0450	0.0887
4	0.1411	0.0	0.0	2.2688	0.0	0.2878	0.0	0.0	0.0	-0.1159
5	0.0	-0.1081	0.0	0.0	2.1332	0.0	0.1795	0.0	0.0	0.0
6	-0.1158	0.0	0.0543	0.2878	0.0	1.0235	0.0	-0.0628	0.0258	0.1930
7	0.0	-0.0502	-0.0502	0.0	0.1795	0.0	0.1667	-0.0321	0.1164	0.0117
8	0.0	0.0	-0.0420	0.0	0.0	-0.0628	-0.0321	0.0958	-0.0739	-0.1152
9	0.0	0.0	-0.0450	0.0	0.0	0.0258	0.1164	-0.0739	0.2453	0.0971
10	-0.0902	0.0	0.0887	-0.1159	0.0	0.1930	0.0117	-0.1152	0.0971	0.2720

11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------

11	1.1021	0.1411	0.1158	-0.0597	-0.0108
12	0.1411	2.2688	-0.2878	-0.0767	-0.0139
13	0.1158	-0.2878	1.0235	-0.1925	-0.0360
14	-0.0597	-0.0767	-0.1925	0.3810	0.0894
15	-0.0108	-0.0139	-0.0360	0.0894	0.3510

G MATRIX FOR THE MOLECULE CH3-COBR

```
 1 THE ASYM. DCD2 STRETCH ---
 2 THE SYMMETRIC CD3 STRETCH
 3 THE C=O STRETCH ----------
 4 THE DCD2 DEFORMATION -----
 5 THE CD3 UMBRELLA BEND ----
 6 THE IN-PLANE CD3 ROCK ----
 7 THE C-C STRETCH ----------
 8 THE C-Z STRETCH ----------
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK -----------
-----------------------------
```

1	0.6064	0.0	0.0	0.1411	0.0	-0.1158	0.0	0.0	0.0	-0.0902
2	0.0	0.5268	0.0	0.0	-0.1081	0.0	-0.0502	0.0	0.0	0.0
3	0.0	0.0	0.1459	0.0	0.0	0.0543	-0.0502	-0.0420	-0.0450	0.0886
4	0.1411	0.0	0.0	1.2259	0.0	0.0697	0.0	0.0	0.0	-0.1159
5	0.0	-0.1081	0.0	0.0	1.2607	0.0	0.1795	0.0	0.0	0.0
6	-0.1158	0.0	0.0543	0.0697	0.0	0.6009	0.0	-0.0628	0.0258	0.1930
7	0.0	-0.0502	-0.0502	0.0	0.1795	0.0	0.1667	-0.0321	0.1164	0.0117
8	0.0	0.0	-0.0420	0.0	0.0	-0.0628	-0.0321	0.0958	-0.0739	-0.1152
9	0.0	0.0	-0.0450	0.0	0.0	0.0258	0.1164	-0.0739	0.2453	0.0971
10	-0.0902	0.0	0.0886	-0.1159	0.0	0.1930	0.0117	-0.1152	0.0971	0.2720

```
11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE CD3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

11	0.6064	0.1411	0.1158	-0.0597	-0.0108
12	0.1411	1.2259	-0.0697	-0.0767	-0.0139
13	0.1158	-0.0697	0.6009	-0.1925	-0.0360
14	-0.0597	-0.0767	-0.1925	0.3810	0.0894
15	-0.0108	-0.0139	-0.0360	0.0894	0.1908

G MATRIX FOR THE MOLECULE CD3-COBR

1 THE C-Z STRETCH ----------
2 THE C=C STRETCH ----------
3 THE SCISSORS BEND -------
4 THE SYMMETRIC CF3 STRETCH
5 THE ASYM. FCF2 STRETCH ---
6 THE C-C STRETCH ----------
7 THE CF3 UMBRELLA BEND ----
8 THE FCF2 DEFORMATION -----
9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----

1	1.0756	-0.0417	-0.0734	0.0	0.0	-0.0394	0.0	0.0	-0.1098	-0.0584
2	-0.0417	0.1459	-0.0811	0.0	0.0	-0.0439	0.0	0.0	0.1119	0.0563
3	-0.0734	-0.0811	1.6041	0.0	0.0	0.1546	0.0	0.0	-0.6965	0.0003
4	0.0	0.0	0.0	0.0813	0.0	-0.0489	-0.0851	0.0	0.0	0.0
5	0.0	0.0	0.0	0.0	0.1633	0.0	0.0	0.1168	-0.0882	-0.1063
6	-0.0394	-0.0439	0.1546	-0.0489	0.0	0.1667	0.1451	0.0	-0.0060	0.0
7	0.0	0.0	0.0	-0.0851	0.0	0.1451	0.3126	0.0	0.0	0.0
8	0.0	0.0	0.0	0.0	0.1168	0.0	0.0	0.1970	-0.0931	-0.0971
9	-0.1098	0.1119	-0.6965	0.0	-0.0882	-0.0060	0.0	-0.0931	0.7060	0.1864
10	-0.0584	0.0563	0.0003	0.0	-0.1063	0.0	0.0	-0.0971	0.1864	0.1844

11 THE A'' FCF2 STRETCH -----
12 THE OUT-OF-PLANE WAG -----
13 THE A'' FCF2 DEFORMATION -
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION --------------

11	0.1633	0.0305	0.1168	0.1063	0.0026
12	0.0305	0.3265	0.0322	0.1070	-0.2148
13	0.1168	0.0322	0.1970	0.0971	0.0028
14	0.1063	0.1070	0.0971	0.1844	0.0022
15	0.0026	-0.2148	0.0028	0.0022	0.2950

G MATRIX FOR THE MOLECULE CF3-COH

1 THE C-Z STRETCH ----------
2 THE C=C STRETCH ----------
3 THE SYMMETRIC CF3 STRETCH
4 THE ASYM. FCF2 STRETCH ---
5 THE SCISSORS BEND -------
6 THE C-C STRETCH ----------
7 THE CF3 UMBRELLA BEND ----
8 THE FCF2 DEFORMATION -----
9 THE O=C-Z ROCK ----------
10 THE IN-PLANE CF3 ROCK ----

1	0.5799	-0.0417	0.0	0.0	-0.0734	-0.0394	0.0	0.0	-0.1098	-0.0584
2	-0.0417	0.1459	0.0	0.0	-0.0811	-0.0439	0.0	0.0	0.1119	0.0563
3	0.0	0.0	0.0813	0.0	0.0	-0.0489	-0.0851	0.0	0.0	0.0
4	0.0	0.0	0.0	0.1633	0.0	0.0	0.0	0.1168	-0.0882	-0.1063
5	-0.0734	-0.0811	0.0	0.0	0.9783	0.1546	0.0	0.0	-0.3351	0.0003
6	-0.0394	-0.0439	-0.0489	0.0	0.1546	0.1667	0.1451	0.0	-0.0060	0.0
7	0.0	0.0	-0.0851	0.0	0.0	0.1451	0.3126	0.0	0.0	0.0
8	0.0	0.0	0.0	0.1168	0.0	0.0	0.0	0.1970	-0.0931	-0.0971
9	-0.1098	0.1119	0.0	-0.0882	-0.3351	-0.0060	0.0	-0.0931	0.4974	0.1864
10	-0.0584	0.0563	0.0	-0.1063	0.0003	0.0	0.0	-0.0971	0.1864	0.1844

11 THE A'' FCF2 STRETCH -----
12 THE OUT-OF-PLANE WAG -----
13 THE A'' FCF2 DEFORMATION -
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION -------------

11	0.1633	0.0305	0.1168	0.1063	0.0026
12	0.0305	0.2302	0.0322	0.1070	-0.1010
13	0.1168	0.0322	0.1970	0.0971	0.0028
14	0.1063	0.1070	0.0971	0.1844	0.0022
15	0.0026	-0.1010	0.0028	0.0022	0.1607

G MATRIX FOR THE MOLECULE CF3-COD

1 THE C=O STRETCH ----------
2 THE SYMMETRIC CF3 STRETCH
3 THE ASYM. FCF2 STRETCH ---
4 THE C-Z STRETCH ----------
5 THE C-C STRETCH ----------
6 THE SCISSORS BEND -------
7 THE CF3 UMBRELLA BEND ----
8 THE FCF2 DEFORMATION -----
9 THE C=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----

1	0.1459	0.0	0.0	-0.0312	-0.0513	-0.0529	0.0	0.0	0.0916	0.0529
2	0.0	0.0859	0.0	0.0	-0.0526	0.0	-0.0926	0.0	0.0	0.0
3	0.0	0.0	0.1610	0.0	0.0	0.0	0.0	0.1103	-0.0884	-0.1082
4	-0.0312	0.0	0.0	0.1360	-0.0417	-0.0809	0.0	0.0	-0.1138	-0.0582
5	-0.0513	-0.0526	0.0	-0.0417	0.1667	0.1181	0.1467	0.0	0.0112	0.0
6	-0.0529	0.0	0.0	-0.0809	0.1181	0.2682	0.0	0.0	0.0790	0.0203
7	0.0	-0.0926	0.0	0.0	0.1467	0.0	0.3208	0.0	0.0	0.0
8	0.0	0.0	0.1103	0.0	0.0	0.0	0.0	0.1835	-0.0900	-0.0945
9	0.0916	0.0	-0.0884	-0.1138	0.0112	0.0790	0.0	-0.0900	0.2922	0.1890
10	0.0529	0.0	-0.1082	-0.0582	0.0	0.0203	0.0	-0.0945	0.1890	0.1915

11 THE A'' FCF2 STRETCH -----
12 THE A'' FCF2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION --------------

11	0.1610	0.1103	0.0669	-0.1082	0.0064
12	0.1103	0.1835	0.0681	-0.0945	0.0065
13	0.0669	0.0681	0.4568	-0.2057	0.0737
14	-0.1082	-0.0945	-0.2057	0.1915	-0.0256
15	0.0064	0.0065	0.0737	-0.0256	0.0424

G MATRIX FOR THE MOLECULE CF3-COF

1 THE C=O STRETCH ----------
2 THE SYMMETRIC CF3 STRETCH
3 THE ASYM. FCF2 STRETCH ---
4 THE C-C STRETCH ----------
5 THE C-Z STRETCH ----------
6 THE FCF2 DEFORMATION -----
7 THE CF3 UMBRELLA BEND ----
8 THE SCISSORS BEND -------
9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----

1	0.1459	0.0	0.0	-0.0490	-0.0478	0.0	0.0	-0.0478	-0.0883	0.0526
2	0.0	0.0859	0.0	-0.0526	0.0	0.0	-0.0933	0.0	0.0	0.0
3	0.0	0.0	0.1610	0.0	0.0	0.1111	0.0	0.0	0.0857	-0.1061
4	-0.0490	-0.0526	0.0	0.1667	-0.0271	0.0	0.1478	0.1251	-0.0086	0.0
5	-0.0478	0.0	0.0	-0.0271	0.1115	0.0	0.0	-0.0709	0.1119	-0.0615
6	0.0	0.0	0.1111	0.0	0.0	0.1862	0.0	0.0	0.0878	-0.0929
7	0.0	-0.0933	0.0	0.1478	0.0	0.0	0.3256	0.0	0.0	0.0
8	-0.0478	0.0	0.0	0.1251	-0.0709	0.0	0.0	0.2812	-0.0879	0.0249
9	-0.0883	0.0	0.0857	-0.0086	0.1119	0.0878	0.0	-0.0879	0.2555	-0.1740
10	0.0526	0.0	-0.1061	0.0	-0.0615	-0.0929	0.0	0.0249	-0.1740	0.1844

11 THE A'' FCF2 STRETCH -----
12 THE A'' FCF2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION -------------

11	0.1610	0.1111	0.0525	0.1061	0.0116
12	0.1111	0.1862	0.0538	0.0929	0.0119
13	0.0525	0.0538	0.3743	0.1742	0.0832
14	0.1061	0.0929	0.1742	0.1844	0.0337
15	0.0116	0.0119	0.0832	0.0337	0.0422

G MATRIX FOR THE MOLECULE CF3-COCL

C. ZSYM

1. Symmetrized Z Matrix

The Z matrices listed on the next pages are the symmetrized forms of the Urey-Bradley Z matrices as output from the program UBZM. Each symmetrized Z matrix requires two pages to complete. See page I-25 for definition of the Z matrix.

4	4	1	1.0000	3	3	2	1.0000	9	9	3	1.0000	1	1	4	0.3333
1	2	4	-0.4714	2	2	4	0.6667	11	11	4	1.0000	1	1	5	0.6667
1	2	5	0.4714	2	2	5	0.3333	7	7	6	0.1667	7	10	6	0.2887
10	10	6	0.5000	7	7	7	0.6667	7	7	8	0.1667	7	10	8	-0.2887
10	10	8	0.5000	5	5	9	0.3333	5	6	9	-0.3333	6	6	9	0.3333
12	12	9	1.0000	5	5	10	0.6667	5	6	10	0.3333	6	6	10	0.1667
6	6	11	0.3333	6	8	11	0.3333	8	8	11	0.3333	13	13	11	1.0000
6	6	12	0.1667	6	8	12	-0.3333	8	8	12	0.6667	14	14	13	1.0000
15	15	14	1.0000	1	1	15	0.1176	1	2	15	0.6217	1	5	15	-0.1544
1	6	15	0.1544	2	2	15	1.7585	2	5	15	-0.4367	2	6	15	0.4367
5	5	15	0.1598	5	6	15	-0.1598	6	6	15	0.1598	11	11	15	0.6254
11	12	15	-0.4632	12	12	15	0.4794	1	1	16	0.4396	1	2	16	-0.6217
1	5	16	-0.3088	1	6	16	-0.1544	2	2	16	0.8792	2	5	16	0.4367
2	6	16	0.2183	5	5	16	0.3196	5	6	16	0.1598	6	6	16	0.0799
11	11	16	-0.0681	1	1	17	0.5228	1	8	17	0.4513	2	2	17	0.5228
2	6	17	-0.3191	2	9	17	1.2001	6	6	17	0.3097	6	9	17	-0.7224
8	8	17	0.6194	9	9	17	2.2501	11	11	17	0.5228	11	13	17	-0.4513
13	13	17	0.6194	4	4	18	0.7041	4	7	18	-0.1912	4	9	18	0.7977
4	10	18	-0.3312	7	7	18	0.0898	7	9	18	-0.2157	7	10	18	0.1556
9	9	18	0.8058	9	10	18	-0.3736	10	10	18	0.2694	3	3	19	0.6128
3	7	19	-0.1846	3	9	19	0.7488	3	10	19	0.3197	7	7	19	0.0929
7	9	19	-0.2261	7	10	19	-0.1610	9	9	19	0.7866	9	10	19	0.3916
10	10	19	0.2788	3	3	20	0.6880	3	4	20	0.7647	3	7	20	0.3639
4	4	20	0.7380	4	7	20	0.3852	7	7	20	0.3013	1	1	21	0.1949
1	2	21	-0.2254	1	4	21	-0.3108	1	6	21	0.0658	1	7	21	0.0384
1	8	21	0.2191	1	9	21	-0.2377	1	10	21	0.0666	2	2	21	0.3543
2	4	21	0.9118	2	6	21	-0.2014	2	7	21	-0.2607	2	8	21	-0.0930
2	9	21	0.9448	2	10	21	-0.4516	4	4	21	1.6892	4	6	21	-0.6927
4	7	21	-0.4497	4	8	21	-0.0405	4	9	21	2.0138	4	10	21	-0.7789
6	6	21	0.3876	6	7	21	0.2570	6	8	21	-0.1709	6	9	21	-0.8162
6	10	21	0.4451	7	7	21	0.3426	7	8	21	-0.2700	7	9	21	-0.7004
7	10	21	0.5935	8	8	21	0.9460	8	9	21	0.4290	8	10	21	-0.4677
9	9	21	2.2949	9	10	21	-1.2131	10	10	21	1.0279	11	11	21	0.5136
11	13	21	-0.3506	11	15	21	0.2175	13	13	21	0.6042	13	15	21	-0.3385
15	15	21	0.1810	1	1	22	0.0620	1	2	22	-0.0877	1	3	22	-0.2908
1	6	22	0.0926	1	7	22	0.1332	1	8	22	0.0926	1	9	22	-0.3939
1	10	22	-0.2306	2	2	22	0.1240	2	3	22	0.4112	2	6	22	-0.1310
2	7	22	-0.1883	2	8	22	-0.1310	2	9	22	0.5571	2	10	22	0.3262
3	3	22	0.5641	3	6	22	-0.4046	3	7	22	-0.2769	3	8	22	-0.4046
3	9	22	1.1032	3	10	22	0.4796	6	6	22	0.2815	6	7	22	0.2279
6	8	22	0.2815	6	9	22	-0.6314	6	10	22	-0.3948	7	7	22	0.2598
7	8	22	0.2279	7	9	22	-0.5955	7	10	22	-0.4500	8	8	22	0.2815
8	9	22	-0.6314	8	10	22	-0.3548	9	9	22	1.6706	9	10	22	1.0314
10	10	22	0.7794	11	11	22	0.1860	11	13	22	-0.2778	11	15	22	-0.1530
13	13	22	0.0444	13	15	22	0.4967	15	15	22	0.1478	5	5	23	-0.2100
5	8	23	0.4073	6	6	23	-0.5424	8	8	23	-0.2100	12	12	23	-0.2100
12	13	23	-0.4073	13	13	23	-0.2100	1	9	24	0.8165	2	9	24	0.5773
1	9	25	-0.8165	2	9	25	1.1547	4	9	26	1.0000	3	9	27	1.0000
5	9	28	0.8165	6	9	28	0.4082	5	9	29	-0.8165	6	9	29	0.8165
6	9	30	-0.8165	8	9	30	-0.8165	6	9	31	-0.4082	8	9	31	0.8165
7	9	32	0.8165	7	9	33	-0.4082	9	10	33	-0.7071	7	9	34	-0.4082
9	10	34	0.7071	1	1	35	-1.3333	1	2	35	0.4714	2	2	35	1.3333

SYMMETRIZED Z MATRIX ----------CH3-COH

1	5	36	0.6667	1	6	36	0.3333	2	5	36	0.4714	2	6	36	0.2357
1	5	37	-0.6667	1	6	37	0.6667	2	5	37	-0.4714	2	6	37	0.4714
1	6	38	-0.6667	1	8	38	-0.6667	2	6	38	-0.4714	2	8	38	-0.4714
1	6	39	-0.3333	1	8	39	0.6667	2	6	39	-0.2357	2	8	39	0.4714
1	1	40	0.3333	1	2	40	-0.4714	2	2	40	0.6667	11	11	40	-1.0000
1	5	41	-0.6667	1	6	41	-0.3333	2	5	41	0.9428	2	6	41	0.4714
1	5	42	0.3333	1	6	42	-0.3333	2	5	42	-0.4714	2	6	42	0.4714
11	12	42	1.0000	1	5	43	0.3333	1	6	43	-0.3333	2	5	43	-0.4714
2	6	43	0.4714	11	12	43	-1.0000	1	6	44	0.3333	1	8	44	0.3333
2	6	44	-0.4714	2	8	44	-0.4714	11	13	44	1.0000	1	6	45	0.3333
1	8	45	-0.6667	2	6	45	-0.4714	2	8	45	0.9428	1	6	46	0.3333
1	8	46	0.3333	2	6	46	-0.4714	2	8	46	-0.4714	11	13	46	-1.0000
3	4	47	1.0000	4	7	48	0.8165	4	7	49	-0.4082	4	10	49	-0.7071
4	7	50	-0.4082	4	10	50	0.7071	3	7	51	0.8165	3	7	52	-0.4082
3	10	52	-0.7071	3	7	53	-0.4082	3	10	53	0.7071	5	5	54	-1.3333
5	6	54	0.3333	6	6	54	0.6667	5	6	55	-0.6667	5	8	55	-0.6667
6	6	55	-0.6667	6	8	55	-0.3333	5	6	56	-0.3333	5	8	56	0.6667
6	6	56	-0.3333	6	8	56	0.3333	5	5	57	0.3333	5	6	57	-0.3333
6	6	57	0.3333	12	12	57	-1.0000	5	6	58	0.3333	5	8	58	0.3333
6	6	58	-0.6667	6	8	58	-0.3333	12	13	58	1.0000	5	6	59	0.3333
5	8	59	-0.6667	6	6	59	-0.6667	6	8	59	0.6667	5	6	60	0.3333
5	8	60	0.3333	6	6	60	-0.6667	6	8	60	-0.3333	12	13	60	-1.0000
6	6	61	0.6667	6	8	61	-0.3333	8	8	61	-1.3333	6	6	62	0.3333
6	8	62	0.3333	8	8	62	0.3333	13	13	62	-1.0000	6	7	63	-0.3333
7	8	63	0.6667	6	7	64	0.1667	6	10	64	0.2887	7	8	64	-0.3333
8	10	64	-0.5773	6	7	65	0.1667	6	10	65	-0.2887	7	8	65	-0.3333
8	10	65	0.5773	7	7	66	-0.6667	7	10	66	-0.5773	7	7	67	-0.6667
7	10	67	0.5773	7	7	68	0.3333	10	10	68	-1.0000	14	15	69	1.0000
13	14	70	-1.4142	12	14	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CH3-COH

4	4	1	1.0000	1	1	2	1.0000	6	6	3	1.0000	2	2	4	0.3333
2	3	4	-0.4714	3	3	4	0.6667	11	11	4	1.0000	2	2	5	0.6667
2	3	5	0.4714	3	3	5	0.3333	5	5	6	0.1667	5	10	6	0.2887
10	10	6	0.5000	5	5	7	0.6667	5	5	8	0.1667	5	10	8	-0.2887
10	10	8	0.5000	7	7	9	0.3333	7	8	9	-0.3333	8	8	9	0.3333
12	12	9	1.0000	7	7	10	0.6667	7	8	10	0.3333	8	8	10	0.1667
8	8	11	0.3333	8	9	11	0.3333	9	9	11	0.3333	14	14	11	1.0000
8	8	12	0.1667	8	9	12	-0.3333	9	9	12	0.6667	13	13	13	1.0000
15	15	14	1.0000	2	2	15	0.1176	2	3	15	0.6217	2	7	15	-0.1544
2	8	15	0.1544	3	3	15	1.7585	3	7	15	-0.4367	3	8	15	0.4367
7	7	15	0.1598	7	8	15	-0.1598	8	8	15	0.1598	11	11	15	0.6254
11	12	15	-0.4632	12	12	15	0.4794	2	2	16	0.4396	2	3	16	-0.6217
2	7	16	-0.3038	2	8	16	-0.1544	3	3	16	0.8792	3	7	16	0.4367
3	8	16	0.2183	7	7	16	0.3196	7	8	16	0.1598	8	8	16	0.0799
11	11	16	-0.0681	2	2	17	0.5228	2	9	17	0.4513	3	3	17	0.5228
3	6	17	1.2001	3	8	17	-0.3191	6	6	17	2.2501	6	8	17	-0.7224
6	8	17	0.3097	9	9	17	0.6194	11	11	17	0.5228	11	14	17	-0.4513
14	14	17	0.6194	4	4	18	0.7041	4	5	18	-0.1912	4	6	18	0.7977
4	10	18	-0.3312	5	5	18	0.0898	5	6	18	-0.2157	5	10	18	0.1556
6	6	18	0.8058	6	10	18	-0.3736	10	10	18	0.2694	1	1	19	0.6128
1	5	19	-0.1846	1	6	19	0.7488	1	10	19	0.3197	5	5	19	0.0929
5	6	19	-0.2261	5	10	19	-0.1610	6	6	19	0.7866	6	10	19	0.3916
10	10	19	0.2788	1	1	20	0.6880	1	4	20	0.7647	1	5	20	0.3639
4	4	20	0.7380	4	5	20	0.3852	5	5	20	0.3013	2	2	21	0.1949
2	3	21	-0.2254	2	4	21	-0.3108	2	5	21	0.0384	2	6	21	-0.2377
2	8	21	0.0658	2	9	21	0.2191	2	10	21	0.0666	3	3	21	0.3543
3	4	21	0.9118	3	5	21	-0.2607	3	6	21	0.9448	3	8	21	-0.2014
3	9	21	-0.0930	3	10	21	-0.4516	4	4	21	1.6892	4	5	21	-0.4497
4	6	21	2.0138	4	8	21	-0.6927	4	9	21	-0.0405	4	10	21	-0.7789
5	5	21	0.3426	5	6	21	-0.7004	5	8	21	0.2570	5	9	21	-0.2700
5	10	21	0.5935	6	6	21	2.2949	6	8	21	-0.8162	6	9	21	0.4290
6	10	21	-1.2131	8	8	21	0.3876	8	9	21	-0.1709	8	10	21	0.4451
9	9	21	0.9460	9	10	21	-0.4677	10	10	21	1.0279	11	11	21	0.5136
11	14	21	-0.3506	11	15	21	0.2175	14	14	21	0.6042	14	15	21	-0.3385
15	15	21	0.1810	1	1	22	0.5641	1	2	22	-0.2908	1	3	22	0.4112
1	5	22	-0.2769	1	6	22	1.1032	1	8	22	-0.4046	1	9	22	-0.4046
1	10	22	0.4796	2	2	22	0.0620	2	3	22	-0.0877	2	5	22	0.1332
2	6	22	-0.3939	2	8	22	0.0926	2	9	22	0.0926	2	10	22	-0.2306
3	3	22	0.1240	3	5	22	-0.1883	3	6	22	0.5571	3	8	22	-0.1310
3	9	22	-0.1310	3	10	22	0.3262	5	5	22	0.2598	5	6	22	-0.5955
5	8	22	0.2279	5	9	22	0.2279	5	10	22	-0.4500	6	6	22	1.6706
6	8	22	-0.6314	6	9	22	-0.6314	6	10	22	1.0314	8	8	22	0.2815
8	9	22	0.2815	8	10	22	-0.3948	9	9	22	0.2815	9	10	22	-0.3948
10	10	22	0.7794	11	11	22	0.1860	11	14	22	-0.2778	11	15	22	-0.1530
14	14	22	0.8444	14	15	22	0.4967	15	15	22	0.1478	7	7	23	-0.2100
7	9	23	0.4073	8	8	23	-0.5424	9	9	23	-0.2100	12	12	23	-0.2100
12	14	23	-0.4073	14	14	23	-0.2100	2	6	24	0.8165	3	6	24	0.5773
2	6	25	-0.8165	3	6	25	1.1547	4	6	26	1.0000	1	6	27	1.0000
6	7	28	0.8165	6	8	28	0.4082	6	7	29	-0.8165	6	8	29	0.8165
6	8	30	-0.8165	6	9	30	-0.8165	6	8	31	-0.4082	6	9	31	0.8165
5	6	32	0.8165	5	6	33	-0.4082	6	10	33	-0.7071	5	6	34	-0.4082
6	10	34	0.7071	2	2	35	-1.3333	2	3	35	0.4714	3	3	35	1.3333

SYMMETRIZED Z MATRIX ----------CO3-COH

2	7	36	0.6667	2	8	36	0.3333	3	7	36	0.4714	3	8	36	0.2357
2	7	37	-0.6667	2	8	37	0.6667	3	7	37	-0.4714	3	8	37	0.4714
2	8	38	-0.6667	2	9	38	-0.6667	3	8	38	-0.4714	3	9	38	-0.4714
2	8	39	-0.3333	2	9	39	0.6667	3	8	39	-0.2357	3	9	39	0.4714
2	2	40	0.3333	2	3	40	-0.4714	3	3	40	0.6667	11	11	40	-1.0000
2	7	41	-0.6667	2	8	41	-0.3333	3	7	41	0.9428	3	8	41	0.4714
2	7	42	0.3333	2	8	42	-0.3333	3	7	42	-0.4714	3	8	42	0.4714
11	12	42	1.0000	2	7	43	0.3333	2	8	43	-0.3333	3	7	43	-0.4714
3	8	43	0.4714	11	12	43	-1.0000	2	8	44	0.3333	2	9	44	0.3333
3	8	44	-0.4714	3	9	44	-0.4714	11	14	44	1.0000	2	8	45	0.3333
2	9	45	-0.6667	3	8	45	-0.4714	3	9	45	0.9428	2	8	46	0.3333
2	9	46	0.3333	3	8	46	-0.4714	3	9	46	-0.4714	11	14	46	-1.0000
1	4	47	1.0000	4	5	48	0.8165	4	5	49	-0.4082	4	10	49	-0.7071
4	5	50	-0.4082	4	10	50	0.7071	1	5	51	0.8165	1	5	52	-0.4082
1	10	52	-0.7071	1	5	53	-0.4082	1	10	53	0.7071	7	7	54	-1.3333
7	8	54	0.3333	8	8	54	0.6667	7	8	55	-0.6667	7	9	55	-0.6667
8	8	55	-0.6667	8	9	55	-0.3333	7	8	56	-0.3333	7	9	56	0.6667
8	8	56	-0.3333	8	9	56	0.3333	7	7	57	0.3333	7	8	57	-0.3333
8	8	57	0.3333	12	12	57	-1.0000	7	8	58	0.3333	7	9	58	0.3333
8	8	58	-0.6667	8	9	58	-0.3333	12	14	58	1.0000	7	8	59	0.3333
7	9	59	-0.6667	8	8	59	-0.6667	8	9	59	0.6667	7	8	60	0.3333
7	9	60	0.3333	8	8	60	-0.6667	8	9	60	-0.3333	12	14	60	-1.0000
8	8	61	0.6667	8	9	61	-0.3333	9	9	61	-1.3333	8	8	62	0.3333
8	9	62	0.3333	9	9	62	0.3333	14	14	62	-1.0000	5	8	63	-0.3333
5	9	63	0.6667	5	8	64	0.1667	5	9	64	-0.3333	8	10	64	0.2887
9	10	64	-0.5773	5	8	65	0.1667	5	9	65	-0.3333	8	10	65	-0.2887
9	10	65	0.5773	5	5	66	-0.6667	5	10	66	-0.5773	5	5	67	-0.6667
5	10	67	0.5773	5	5	68	0.3333	10	10	68	-1.0000	13	15	69	1.0000
13	14	70	-1.4142	12	13	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CD3-COH

4	4	1	1.0000	3	3	2	1.0000	7	7	3	1.0000	1	1	4	0.3333
1	2	4	-0.4714	2	2	4	0.6667	11	11	4	1.0000	1	1	5	0.6667
1	2	5	0.4714	2	2	5	0.3333	9	9	6	0.1667	9	10	6	0.2887
10	10	6	0.5000	9	9	7	0.6667	9	9	8	0.1667	9	10	8	-0.2887
10	10	8	0.5000	5	5	9	0.3333	5	6	9	-0.3333	6	6	9	0.3333
12	12	9	1.0000	5	5	10	0.6667	5	6	10	0.3333	6	6	10	0.1667
6	6	11	0.3333	6	8	11	0.3333	8	8	11	0.3333	13	13	11	1.0000
6	6	12	0.1667	6	8	12	-0.3333	8	8	12	0.6667	14	14	13	1.0000
15	15	14	1.0000	1	1	15	0.1176	1	2	15	0.6217	1	5	15	-0.1544
1	6	15	0.1544	2	2	15	1.7585	2	5	15	-0.4367	2	6	15	0.4367
5	5	15	0.1598	5	6	15	-0.1598	6	6	15	0.1598	11	11	15	0.6254
11	12	15	-0.4632	12	12	15	0.4794	1	1	16	0.4396	1	2	16	-0.6217
1	5	16	-0.3088	1	6	16	-0.1544	2	2	16	0.8792	2	5	16	0.4367
2	6	16	0.2183	5	5	16	0.3196	5	6	16	0.1598	6	6	16	0.0799
11	11	16	-0.0681	1	1	17	0.5228	1	8	17	0.4513	2	2	17	0.5228
2	6	17	-0.3191	2	7	17	1.2001	6	6	17	0.3097	6	7	17	-0.7224
7	7	17	2.2501	8	8	17	0.6194	11	11	17	0.5228	11	13	17	-0.4513
13	13	17	0.6194	4	4	18	0.7041	4	7	18	0.7977	4	9	18	-0.1912
4	10	18	-0.3312	7	7	18	0.8058	7	9	18	-0.2157	7	10	18	-0.3736
9	9	18	0.0898	9	10	18	0.1556	10	10	18	0.2694	3	3	19	0.6128
3	7	19	0.7488	3	9	19	-0.1846	3	10	19	0.3197	7	7	19	0.7866
7	9	19	-0.2261	7	10	19	0.3916	9	9	19	0.0929	9	10	19	-0.1610
10	10	19	0.2788	3	3	20	0.6880	3	4	20	0.7647	3	9	20	0.3639
4	4	20	0.7380	4	9	20	0.3852	9	9	20	0.3013	1	1	21	0.1949
1	2	21	-0.2254	1	4	21	-0.3108	1	6	21	0.0658	1	7	21	-0.2377
1	8	21	0.2191	1	9	21	0.0384	1	10	21	0.0666	2	2	21	0.3543
2	4	21	0.9118	2	6	21	-0.2014	2	7	21	0.9448	2	8	21	-0.0930
2	9	21	-0.2607	2	10	21	-0.4516	4	4	21	1.6892	4	6	21	-0.6927
4	7	21	2.0138	4	8	21	-0.0405	4	9	21	-0.4497	4	10	21	-0.7789
6	6	21	0.3876	6	7	21	-0.8162	6	8	21	-0.1709	6	9	21	0.2570
6	10	21	0.4451	7	7	21	2.2949	7	8	21	0.4290	7	9	21	-0.7004
7	10	21	-1.2131	8	8	21	0.9460	8	9	21	-0.2700	8	10	21	-0.4677
9	9	21	0.3426	9	10	21	0.5935	10	10	21	1.0279	11	11	21	0.5136
11	13	21	-0.3506	11	15	21	0.2175	13	13	21	0.6042	13	15	21	-0.3385
15	15	21	0.1810	1	1	22	0.0620	1	2	22	-0.0877	1	3	22	-0.2908
1	6	22	0.0926	1	7	22	-0.3939	1	8	22	0.0926	1	9	22	0.1332
1	10	22	-0.2306	2	2	22	0.1240	2	3	22	0.4112	2	6	22	-0.1310
2	7	22	0.5571	2	8	22	-0.1310	2	9	22	-0.1883	2	10	22	0.3262
3	3	22	0.5641	3	6	22	-0.4046	3	7	22	1.1032	3	8	22	-0.4046
3	9	22	-0.2769	3	10	22	0.4796	6	6	22	0.2815	6	7	22	-0.6314
6	8	22	0.2815	6	9	22	0.2279	6	10	22	-0.3948	7	7	22	1.6706
7	8	22	-0.6314	7	9	22	-0.5955	7	10	22	1.0314	8	8	22	0.2815
8	9	22	0.2279	8	10	22	-0.3948	9	9	22	0.2598	9	10	22	-0.4500
10	10	22	0.7794	11	11	22	0.1860	11	13	22	-0.2778	11	15	22	-0.1530
13	13	22	0.8444	13	15	22	0.4967	15	15	22	0.1478	5	5	23	-0.2100
5	8	23	0.4073	6	6	23	-0.5424	8	8	23	-0.2100	12	12	23	-0.2100
12	13	23	-0.4073	13	13	23	-0.2100	1	7	24	0.8165	2	7	24	0.5773
1	7	25	-0.8165	2	7	25	1.1547	4	7	26	1.0000	3	7	27	1.0000
5	7	28	0.8165	6	7	28	0.4082	5	7	29	-0.8165	6	7	29	0.8165
6	7	30	-0.8165	7	8	30	-0.8165	6	7	31	-0.4082	7	8	31	0.8165
7	9	32	0.8165	7	9	33	-0.4082	7	10	33	-0.7071	7	9	34	-0.4082
7	10	34	0.7071	1	1	35	-1.3333	1	2	35	0.4714	2	2	35	1.3333

SYMMETRIZED Z MATRIX ----------CH3-COD

1	5	36	0.6667	1	6	36	0.3333	2	5	36	0.4714	2	6	36	0.2357
1	5	37	-0.6667	1	6	37	0.6667	2	5	37	-0.4714	2	6	37	0.4714
1	6	38	-0.6667	1	8	38	-0.6667	2	6	38	-0.4714	2	8	38	-0.4714
1	6	39	-0.3333	1	8	39	0.6667	2	6	39	-0.2357	2	8	39	0.4714
1	1	40	0.3333	1	2	40	-0.4714	2	2	40	0.6667	11	11	40	-1.0000
1	5	41	-0.6667	1	6	41	-0.3333	2	5	41	0.9428	2	6	41	0.4714
1	5	42	0.3333	1	6	42	-0.3333	2	5	42	-0.4714	2	6	42	0.4714
11	12	42	1.0000	1	5	43	0.3333	1	6	43	-0.3333	2	5	43	-0.4714
2	6	43	0.4714	11	12	43	-1.0000	1	6	44	0.3333	1	8	44	0.3333
2	6	44	-0.4714	2	8	44	-0.4714	11	13	44	1.0000	1	6	45	0.3333
1	8	45	-0.6667	2	6	45	-0.4714	2	8	45	0.9428	1	6	46	0.3333
1	8	46	0.3333	2	6	46	-0.4714	2	8	46	-0.4714	11	13	46	-1.0000
3	4	47	1.0000	4	9	48	0.8165	4	9	49	-0.4082	4	10	49	-0.7071
4	9	50	-0.4082	4	10	50	0.7071	3	9	51	0.8165	3	9	52	-0.4082
3	10	52	-0.7071	3	9	53	-0.4082	3	10	53	0.7071	5	5	54	-1.3333
5	6	54	0.3333	6	6	54	0.6667	5	6	55	-0.6667	5	8	55	-0.6667
6	6	55	-0.6667	6	8	55	-0.3333	5	6	56	-0.3333	5	8	56	0.6667
6	6	56	-0.3333	6	8	56	0.3333	5	5	57	0.3333	5	6	57	-0.3333
6	6	57	0.3333	12	12	57	-1.0000	5	6	58	0.3333	5	8	58	0.3333
6	6	58	-0.6667	6	8	58	-0.3333	12	13	58	1.0000	5	6	59	0.3333
5	8	59	-0.6667	6	6	59	-0.6667	6	8	59	0.6667	5	6	60	0.3333
5	8	60	0.3333	6	6	60	-0.6667	6	8	60	-0.3333	12	13	60	-1.0000
6	6	61	0.6667	6	8	61	-0.3333	8	8	61	-1.3333	6	6	62	0.3333
6	8	62	0.3333	8	8	62	0.3333	13	13	62	-1.0000	6	9	63	-0.3333
6	9	63	0.6667	6	9	64	0.1667	6	10	64	0.2887	8	9	64	-0.3333
8	10	64	-0.5773	6	9	65	0.1667	6	10	65	-0.2887	8	9	65	-0.3333
8	10	65	0.5773	9	9	66	-0.6667	9	10	66	-0.5773	9	9	67	-0.6667
9	10	67	0.5773	9	9	68	0.3333	10	10	68	-1.0000	14	15	69	1.0000
13	14	70	-1.4142	12	14	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CH3-COD

4	4	1	1.0000	3	3	2	1.0000	5	5	3	1.0000	1	1	4	0.3333
1	2	4	-0.4714	2	2	4	0.6667	11	11	4	1.0000	1	1	5	0.6667
1	2	5	0.4714	2	2	5	0.3333	8	8	6	0.1667	8	10	6	0.2887
10	10	6	0.5000	8	8	7	0.6667	8	8	8	0.1667	8	10	8	-0.2887
10	10	8	0.5000	6	6	9	0.3333	6	7	9	-0.3333	7	7	9	0.3333
12	12	9	1.0000	6	6	10	0.6667	6	7	10	0.3333	7	7	10	0.1667
7	7	11	0.3333	7	9	11	0.3333	9	9	11	0.3333	14	14	11	1.0000
7	7	12	0.1667	7	9	12	-0.3333	9	9	12	0.6667	13	13	13	1.0000
15	15	14	1.0000	1	1	15	0.1176	1	2	15	0.6217	1	6	15	-0.1544
1	7	15	0.1544	2	2	15	1.7585	2	6	15	-0.4367	2	7	15	0.4367
6	6	15	0.1598	6	7	15	-0.1598	7	7	15	0.1598	11	11	15	0.6254
11	12	15	-0.4632	12	12	15	0.4794	1	1	16	0.4396	1	2	16	-0.6217
1	6	16	-0.3088	1	7	16	-0.1544	2	2	16	0.8792	2	6	16	0.4367
2	7	16	0.2183	6	6	16	0.3196	6	7	16	0.1598	7	7	16	0.0799
11	11	16	-0.0681	1	1	17	0.5228	1	9	17	0.4513	2	2	17	0.5228
2	5	17	1.2001	2	7	17	-0.3191	5	5	17	2.2501	5	7	17	-0.7224
7	7	17	0.3097	9	9	17	0.6194	11	11	17	0.5228	11	14	17	-0.4513
14	14	17	0.6194	4	4	18	0.7041	4	5	18	0.7977	4	8	18	-0.1912
4	10	18	-0.3312	5	5	18	0.8058	5	8	18	-0.2157	5	10	18	-0.3736
8	8	18	0.0898	8	10	18	0.1556	10	10	18	0.2694	3	3	19	0.6128
3	5	19	0.7488	3	8	19	-0.1846	3	10	19	0.3197	5	5	19	0.7866
5	8	19	-0.2261	5	10	19	0.3916	8	8	19	0.0929	8	10	19	-0.1610
10	10	19	0.2738	3	3	20	0.6880	3	4	20	0.7647	3	8	20	0.3639
4	4	20	0.7380	4	8	20	0.3852	8	8	20	0.3013	1	1	21	0.1949
1	2	21	-0.2254	1	4	21	-0.3108	1	5	21	-0.2377	1	7	21	0.0658
1	8	21	0.0384	1	9	21	0.2191	1	10	21	0.0666	2	2	21	0.3543
2	4	21	0.9118	2	5	21	0.9448	2	7	21	-0.2014	2	8	21	-0.2607
2	9	21	-0.0930	2	10	21	-0.4516	4	4	21	1.6892	4	5	21	2.0138
4	7	21	-0.6927	4	8	21	-0.4497	4	9	21	-0.0405	4	10	21	-0.7789
5	5	21	2.2949	5	7	21	-0.8162	5	8	21	-0.7004	5	9	21	0.4290
5	10	21	-1.2131	7	7	21	0.3876	7	8	21	0.2570	7	9	21	-0.1709
7	10	21	0.4451	8	8	21	0.3426	8	9	21	-0.2700	8	10	21	0.5935
9	9	21	0.9460	9	10	21	-0.4677	10	10	21	1.0279	11	11	21	0.5136
11	14	21	-0.3506	11	15	21	0.2175	14	14	21	0.6042	14	15	21	-0.3385
15	15	21	0.1810	1	1	22	0.0620	1	2	22	-0.0877	1	3	22	-0.2908
1	5	22	-0.3939	1	7	22	0.0926	1	8	22	0.1332	1	9	22	0.0926
1	10	22	-0.2306	2	2	22	0.1240	2	3	22	0.4112	2	5	22	0.5571
2	7	22	-0.1310	2	8	22	-0.1883	2	9	22	-0.1310	2	10	22	0.3262
3	3	22	0.5641	3	5	22	1.1032	3	7	22	-0.4046	3	8	22	-0.2769
3	9	22	-0.4046	3	10	22	0.4796	5	5	22	1.6706	5	7	22	-0.6314
5	8	22	-0.5955	5	9	22	-0.6314	5	10	22	1.0314	7	7	22	0.2815
7	8	22	0.2279	7	9	22	0.2915	7	10	22	-0.3948	8	8	22	0.2598
8	9	22	0.2279	8	10	22	-0.4500	9	9	22	0.2815	9	10	22	-0.3948
10	10	22	0.7794	11	11	22	0.1860	11	14	22	-0.2778	11	15	22	-0.1530
14	14	22	0.8444	14	15	22	0.4967	15	15	22	0.1478	6	6	23	-0.2100
6	9	23	0.4073	7	7	23	-0.5424	9	9	23	-0.2100	12	12	23	-0.2100
12	14	23	-0.4073	14	14	23	-0.2100	1	5	24	0.8165	2	5	24	0.5773
1	5	25	-0.8165	2	5	25	1.1547	4	5	26	1.0000	3	5	27	1.0000
5	6	28	0.8165	5	7	28	0.4082	5	6	29	-0.8165	5	7	29	0.8165
5	7	30	-0.8165	5	9	30	-0.8165	5	7	31	-0.4082	5	9	31	0.8165
5	8	32	0.8165	5	8	33	-0.4082	5	10	33	-0.7071	5	8	34	-0.4082
5	10	34	0.7071	1	1	35	-1.3333	1	2	35	0.4714	2	2	35	1.3333

SYMMETRIZED Z MATRIX ----------CO3-COD

1	6	36	0.6667	1	7	36	0.3333	2	6	36	0.4714	2	7	36	0.2357
1	6	37	-0.6667	1	7	37	0.6667	2	6	37	-0.4714	2	7	37	0.4714
1	7	38	-0.6667	1	9	38	-0.6667	2	7	38	-0.4714	2	9	38	-0.4714
1	7	39	-0.3333	1	9	39	0.6667	2	7	39	-0.2357	2	9	39	0.4714
1	1	40	0.3333	1	2	40	-0.4714	2	2	40	0.6667	11	11	40	-1.0000
1	6	41	-0.6667	1	7	41	-0.3333	2	6	41	0.9428	2	7	41	0.4714
1	6	42	0.3333	1	7	42	-0.3333	2	6	42	-0.4714	2	7	42	0.4714
11	12	42	1.0000	1	6	43	0.3333	1	7	43	-0.3333	2	6	43	-0.4714
2	7	43	0.4714	11	12	43	-1.0000	1	7	44	0.3333	1	9	44	0.3333
2	7	44	-0.4714	2	9	44	-0.4714	11	14	44	1.0000	1	7	45	0.3333
1	9	45	-0.6667	2	7	45	-0.4714	2	9	45	0.9428	1	7	46	0.3333
1	9	46	0.3333	2	7	46	-0.4714	2	9	46	-0.4714	11	14	46	-1.0000
3	4	47	1.0000	4	8	48	0.8165	4	8	49	-0.4082	4	10	49	-0.7071
4	8	50	-0.4082	4	10	50	0.7071	3	8	51	0.8165	3	8	52	-0.4082
3	10	52	-0.7071	3	8	53	-0.4082	3	10	53	0.7071	6	6	54	-1.3333
6	7	54	0.3333	7	7	54	0.6667	6	7	55	-0.6667	6	9	55	-0.6667
7	7	55	-0.6667	7	9	55	-0.3333	6	7	56	-0.3333	6	9	56	0.6667
7	7	56	-0.3333	7	9	56	0.3333	6	6	57	0.3333	6	7	57	-0.3333
7	7	57	0.3333	12	12	57	-1.0000	6	7	58	0.3333	6	9	58	0.3333
7	7	58	-0.6667	7	9	58	-0.3333	12	14	58	1.0000	6	7	59	0.3333
6	9	59	-0.6667	7	7	59	-0.6667	7	9	59	0.6667	6	7	60	0.3333
6	9	60	0.3333	7	7	60	-0.6667	7	9	60	-0.3333	12	14	60	-1.0000
7	7	61	0.6667	7	9	61	-0.3333	9	9	61	-1.3333	7	7	62	0.3333
7	9	62	0.3333	9	9	62	0.3333	14	14	62	-1.0000	7	8	63	-0.3333
8	9	63	0.6667	7	8	64	0.1667	7	10	64	0.2887	8	9	64	-0.3333
9	10	64	-0.5773	7	8	65	0.1667	7	10	65	-0.2887	8	9	65	-0.3333
9	10	65	0.5773	8	8	66	-0.6667	8	10	66	-0.5773	8	8	67	-0.6667
8	10	67	0.5773	8	8	68	0.3333	10	10	68	-1.0000	13	15	69	1.0000
13	14	70	-1.4142	12	13	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CD3-COD

3	3	1	1.0000	6	6	2	1.0000	8	8	3	1.0000	1	1	4	0.3333
1	2	4	-0.4714	2	2	4	0.6667	11	11	4	1.0000	1	1	5	0.6667
1	2	5	0.4714	2	2	5	0.3333	9	9	6	0.1667	9	10	6	0.2887
10	10	6	0.5000	9	9	7	0.6667	9	9	8	0.1667	9	10	8	-0.2887
10	10	8	0.5000	4	4	9	0.3333	4	5	9	-0.3333	5	5	9	0.3333
12	12	9	1.0000	4	4	10	0.6667	4	5	10	0.3333	5	5	10	0.1667
5	5	11	0.3333	5	7	11	0.3333	7	7	11	0.3333	13	13	11	1.0000
5	5	12	0.1667	5	7	12	-0.3333	7	7	12	0.6667	14	14	13	1.0000
15	15	14	1.0000	1	1	15	0.1169	1	2	15	0.6209	1	4	15	-0.1516
1	5	15	0.1516	2	2	15	1.7750	2	4	15	-0.4359	2	5	15	0.4359
4	4	15	0.1585	4	5	15	-0.1585	5	5	15	0.1585	11	11	15	0.6369
11	12	15	-0.4648	12	12	15	0.4754	1	1	16	0.4481	1	2	16	-0.6337
1	4	16	-0.3087	1	5	16	-0.1544	2	2	16	0.8961	2	4	16	0.4366
2	5	16	0.2183	4	4	16	0.3164	4	5	16	0.1582	5	5	16	0.0791
11	11	16	-0.0656	1	1	17	0.5172	1	2	17	0.0066	1	5	17	0.0027
1	7	17	0.4519	1	8	17	0.0095	2	2	17	0.5125	2	5	17	-0.3214
2	7	17	-0.0038	2	8	17	1.1869	5	5	17	0.3175	5	7	17	0.0093
5	8	17	-0.7305	7	7	17	0.6257	7	8	17	-0.0090	8	8	17	2.2277
11	11	17	0.5078	11	13	17	-0.4573	13	13	17	0.6443	3	3	18	0.7357
3	8	18	0.8228	3	9	18	-0.1790	3	10	18	-0.3100	8	8	18	0.8355
8	9	18	-0.2024	8	10	18	-0.3505	9	9	18	0.0801	9	10	18	0.1387
10	10	18	0.2402	6	6	19	0.6045	6	8	19	0.7077	6	9	19	-0.2321
6	10	19	0.4019	8	8	19	0.6838	8	9	19	-0.2540	8	10	19	0.4399
9	9	19	0.1308	9	10	19	-0.2265	10	10	19	0.3924	3	3	20	0.7026
3	6	20	0.7829	3	9	20	0.3790	6	6	20	0.7685	6	9	20	0.4091
9	9	20	0.3336	1	1	21	0.1989	1	2	21	-0.2018	1	3	21	-0.2885
1	5	21	0.0621	1	7	21	0.2359	1	8	21	-0.2097	1	9	21	0.0199
1	10	21	0.0345	2	2	21	0.3415	2	3	21	0.9226	2	5	21	-0.2107
2	7	21	-0.0878	2	8	21	0.9538	2	9	21	-0.2373	2	10	21	-0.4110
3	3	21	1.7971	3	5	21	-0.7372	3	7	21	-0.0533	3	8	21	2.0840
3	9	21	-0.4214	3	10	21	-0.7299	5	5	21	0.4012	5	7	21	-0.1459
5	8	21	-0.8433	5	9	21	0.2394	5	10	21	0.4146	7	7	21	0.9483
7	8	21	0.3821	7	9	21	-0.2543	7	10	21	-0.4405	8	8	21	2.3291
8	9	21	-0.6431	8	10	21	-1.1139	9	9	21	0.3064	9	10	21	0.5306
10	10	21	0.9191	11	11	21	0.4842	11	13	21	-0.3600	11	15	21	0.1991
13	13	21	0.6565	13	15	21	-0.3332	15	15	21	0.1641	1	1	22	0.0368
1	2	22	-0.0520	1	5	22	0.0708	1	6	22	-0.2552	1	7	22	0.0708
1	8	22	-0.3251	1	9	22	0.1376	1	10	22	-0.2384	2	2	22	0.0735
2	5	22	-0.1001	2	6	22	0.3609	2	7	22	-0.1001	2	8	22	0.4598
2	9	22	-0.1946	2	10	22	0.3371	5	5	22	0.2810	5	6	22	-0.4125
5	7	22	0.2810	5	8	22	-0.6169	5	9	22	0.2760	5	10	22	-0.4781
6	6	22	0.5441	6	7	22	-0.4125	6	8	22	1.0742	6	9	22	-0.3601
6	10	22	0.6238	7	7	22	0.2810	7	8	22	-0.6169	7	9	22	0.2760
7	10	22	-0.4781	8	8	22	1.5618	8	9	22	-0.6927	8	10	22	1.1998
9	9	22	0.3666	9	10	22	-0.6350	10	10	22	1.0999	11	11	22	0.1103
11	13	22	-0.2124	11	15	22	-0.1491	13	13	22	0.8429	13	15	22	0.6428
15	15	22	0.2828	4	4	23	-0.1898	4	5	23	-0.0039	4	7	23	0.3908
5	5	23	-0.6005	5	7	23	0.0040	7	7	23	-0.1896	12	12	23	-0.2013
12	13	23	-0.3949	13	13	23	-0.2013	1	8	24	0.8165	2	8	24	0.5773
1	8	25	-0.8165	2	8	25	1.1547	3	8	26	1.0000	6	8	27	1.0000
4	8	28	0.8165	5	8	28	0.4082	4	8	29	-0.8165	5	8	29	0.8165
5	8	30	-0.8165	7	8	30	-0.8165	5	8	31	-0.4082	7	8	31	0.8165

SYMMETRIZED Z MATRIX ----------CH3-COF

8	9	32	0.8165	8	9	33	-0.4082	8	10	33	-0.7071	8	9	34	-0.4082
8	10	34	0.7071	1	1	35	-1.3333	1	2	35	0.4714	2	2	35	1.3333
1	4	36	0.6667	1	5	36	0.3333	2	4	36	0.4714	2	5	36	0.2357
1	4	37	-0.6667	1	5	37	0.6667	2	4	37	-0.4714	2	5	37	0.4714
1	5	38	-0.6667	1	7	38	-0.6667	2	5	38	-0.4714	2	7	38	-0.4714
1	5	39	-0.3333	1	7	39	0.6667	2	5	39	-0.2357	2	7	39	0.4714
1	1	40	0.3333	1	2	40	-0.4714	2	2	40	0.6667	11	11	40	-1.0000
1	4	41	-0.6667	1	5	41	-0.3333	2	4	41	0.9428	2	5	41	0.4714
1	4	42	0.3333	1	5	42	-0.3333	2	4	42	-0.4714	2	5	42	0.4714
11	12	42	1.0000	1	4	43	0.3333	1	5	43	-0.3333	2	4	43	-0.4714
2	5	43	0.4714	11	12	43	-1.0000	1	5	44	0.3333	1	7	44	0.3333
2	5	44	-0.4714	2	7	44	-0.4714	11	13	44	1.0000	1	5	45	0.3333
1	7	45	-0.6667	2	5	45	-0.4714	2	7	45	0.9428	1	5	46	0.3333
1	7	46	0.3333	2	5	46	-0.4714	2	7	46	-0.4714	11	13	46	-1.0000
3	6	47	1.0000	3	9	48	0.8165	3	9	49	-0.4082	3	10	49	-0.7071
3	9	50	-0.4082	3	10	50	0.7071	6	9	51	0.8165	6	9	52	-0.4082
6	10	52	-0.7071	6	9	53	-0.4082	6	10	53	0.7071	4	4	54	-1.3333
4	5	54	0.3333	5	5	54	0.6667	4	5	55	-0.6667	4	7	55	-0.6667
5	5	55	-0.6667	5	7	55	-0.3333	4	5	56	-0.3333	4	7	56	0.6667
5	5	56	-0.3333	5	7	56	0.3333	4	4	57	0.3333	4	5	57	-0.3333
5	5	57	0.3333	12	12	57	-1.0000	4	5	58	0.3333	4	7	58	0.3333
5	5	58	-0.6667	5	7	58	-0.3333	12	13	58	1.0000	4	5	59	0.3333
4	7	59	-0.6667	5	5	59	-0.6667	5	7	59	0.6667	4	5	60	0.3333
4	7	60	0.3333	5	5	60	-0.6667	5	7	60	-0.3333	12	13	60	-1.0000
5	5	61	0.6667	5	7	61	-0.3333	7	7	61	-1.3333	5	5	62	0.3333
5	7	62	0.3333	7	7	62	0.3333	13	13	62	-1.0000	5	9	63	-0.3333
7	9	63	0.6667	5	9	64	0.1667	5	10	64	0.2887	7	9	64	-0.3333
7	10	64	-0.5773	5	9	65	0.1667	5	10	65	-0.2887	7	9	65	-0.3333
7	10	65	0.5773	9	9	66	-0.6667	9	10	66	-0.5773	9	9	67	-0.6667
9	10	67	0.5773	9	9	68	0.3333	10	10	68	-1.0000	14	15	69	1.0000
13	14	70	-1.4142	12	14	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CH3-COF

3	3	1	1.0000	4	4	2	1.0000	8	8	3	1.0000	1	1	4	0.3333
1	2	4	-0.4714	2	2	4	0.6667	11	11	4	1.0000	1	1	5	0.6667
1	2	5	0.4714	2	2	5	0.3333	9	9	6	0.1667	9	10	6	0.2887
10	10	6	0.5000	9	9	7	0.6667	9	9	8	0.1667	9	10	8	-0.2887
10	10	8	0.5000	5	5	9	0.3333	5	6	9	-0.3333	6	6	9	0.3333
12	12	9	1.0000	5	5	10	0.1667	5	6	10	0.3333	6	6	10	0.6667
5	5	11	0.3333	5	7	11	0.3333	7	7	11	0.3333	13	13	11	1.0000
5	5	12	0.1667	5	7	12	-0.3333	7	7	12	0.6667	14	14	13	1.0000
15	15	14	1.0000	1	1	15	0.1169	1	2	15	0.6209	1	5	15	0.1516
1	6	15	-0.1516	2	2	15	1.7750	2	5	15	0.4359	2	6	15	-0.4359
5	5	15	0.1585	5	6	15	-0.1585	6	6	15	0.1585	11	11	15	0.6369
11	12	15	-0.4648	12	12	15	0.4754	1	1	16	0.4481	1	2	16	-0.6337
1	5	16	-0.1544	1	6	16	-0.3087	2	2	16	0.8961	2	5	16	0.2183
2	6	16	0.4366	5	5	16	0.0791	5	6	16	0.1582	6	6	16	0.3164
11	11	16	-0.0656	1	1	17	0.5172	1	2	17	0.0066	1	5	17	0.0027
1	7	17	0.4519	1	8	17	0.0095	2	2	17	0.5125	2	5	17	-0.3214
2	7	17	-0.0038	2	8	17	1.1869	5	5	17	0.3175	5	7	17	0.0093
5	8	17	-0.7305	7	7	17	0.6257	7	8	17	-0.0090	8	8	17	2.2277
11	11	17	0.5078	11	13	17	-0.4573	13	13	17	0.6443	3	3	18	0.7357
3	8	18	0.8228	3	9	18	-0.1790	3	10	18	-0.3100	8	8	18	0.8355
8	9	18	-0.2024	8	10	18	-0.3505	9	9	18	0.0801	9	10	18	0.1387
10	10	18	0.2402	4	4	19	0.6045	4	8	19	0.7077	4	9	19	-0.2321
4	10	19	0.4019	8	8	19	0.6838	8	9	19	-0.2540	8	10	19	0.4399
9	9	19	0.1308	9	10	19	-0.2265	10	10	19	0.3924	3	3	20	0.7026
3	4	20	0.7829	3	9	20	0.3790	4	4	20	0.7685	4	9	20	0.4091
9	9	20	0.3330	1	1	21	0.1989	1	2	21	-0.2018	1	3	21	-0.2885
1	5	21	0.0621	1	7	21	0.2359	1	8	21	-0.2097	1	9	21	0.0199
1	10	21	0.0345	2	2	21	0.3415	2	3	21	0.9226	2	5	21	-0.2107
2	7	21	-0.0878	2	8	21	0.9538	2	9	21	-0.2373	2	10	21	-0.4110
3	3	21	1.7971	3	5	21	-0.7372	3	7	21	-0.0533	3	8	21	2.0840
3	9	21	-0.4214	3	10	21	-0.7299	5	5	21	0.4012	5	7	21	-0.1459
5	8	21	-0.8433	5	9	21	0.2394	5	10	21	0.4146	7	7	21	0.9483
7	8	21	0.3821	7	9	21	-0.2543	7	10	21	-0.4405	8	8	21	2.3291
8	9	21	-0.6431	8	10	21	-1.1139	9	9	21	0.3064	9	10	21	0.5306
10	10	21	0.9191	11	11	21	0.4842	11	13	21	-0.3600	11	15	21	0.1991
13	13	21	0.6565	13	15	21	-0.3332	15	15	21	0.1641	1	1	22	0.0968
1	2	22	-0.0520	1	4	22	-0.2552	1	5	22	0.0708	1	7	22	0.0708
1	8	22	-0.3251	1	9	22	0.1376	1	10	22	-0.2384	2	2	22	0.0735
2	4	22	0.3609	2	5	22	-0.1001	2	7	22	-0.1001	2	8	22	0.4598
2	9	22	-0.1946	2	10	22	0.3371	4	4	22	0.5441	4	5	22	-0.4125
4	7	22	-0.4125	4	8	22	1.0742	4	9	22	-0.3601	4	10	22	0.6238
5	5	22	0.2810	5	7	22	0.2810	5	8	22	-0.6169	5	9	22	0.2760
5	10	22	-0.4781	7	7	22	0.2810	7	8	22	-0.6169	7	9	22	0.2760
7	10	22	-0.4781	8	8	22	1.5618	8	9	22	-0.6927	8	10	22	1.1998
9	9	22	0.3600	9	10	22	-0.6350	10	10	22	1.0999	11	11	22	0.1103
11	13	22	-0.2124	11	15	22	-0.1491	13	13	22	0.8429	13	15	22	0.6428
13	15	22	0.2828	5	5	23	-0.6005	5	6	23	-0.0039	5	7	23	0.0040
6	6	23	-0.1898	6	7	23	0.3908	7	7	23	-0.1896	12	12	23	-0.2013
12	13	23	-0.3949	13	13	23	-0.2013	1	8	24	0.8165	2	8	24	0.5773
1	8	25	-0.8165	2	8	25	1.1547	3	8	26	1.0000	4	8	27	1.0000
5	8	28	0.4082	6	8	28	0.8165	5	8	29	-0.8165	6	8	29	-0.8165
5	8	30	-0.8165	7	8	30	-0.8165	5	8	31	-0.4082	7	8	31	0.8165

SYMMETRIZED Z MATRIX ----------CO3-COF

8	9	32	0.8165	8	9	33	-0.4082	8	10	33	-0.7071	8	9	34	-0.4082
8	10	34	0.7071	1	1	35	-1.3333	1	2	35	0.4714	2	2	35	1.3333
1	5	36	0.3333	1	6	36	0.6667	2	5	36	0.2357	2	6	36	0.4714
1	5	37	0.6667	1	6	37	-0.6667	2	5	37	0.4714	2	6	37	-0.4714
1	5	38	-0.6667	1	7	38	-0.6667	2	5	38	-0.4714	2	7	38	-0.4714
1	5	39	-0.3333	1	7	39	0.6667	2	5	39	-0.2357	2	7	39	0.4714
1	1	40	0.3333	1	2	40	-0.4714	2	2	40	0.6667	11	11	40	-1.0000
1	5	41	-0.3333	1	6	41	-0.6667	2	5	41	0.4714	2	6	41	0.9428
1	5	42	-0.3333	1	6	42	0.3333	2	5	42	0.4714	2	6	42	-0.4714
11	12	42	1.0000	1	5	43	-0.3333	1	6	43	0.3333	2	5	43	0.4714
2	6	43	-0.4714	11	12	43	-1.0000	1	5	44	0.3333	1	7	44	0.3333
2	5	44	-0.4714	2	7	44	-0.4714	11	13	44	1.0000	1	5	45	0.3333
1	7	45	-0.6667	2	5	45	-0.4714	2	7	45	0.9428	1	5	46	0.3333
1	7	46	0.3333	2	5	46	-0.4714	2	7	46	-0.4714	11	13	46	-1.0000
3	4	47	1.0000	3	9	48	0.8165	3	9	49	-0.4082	3	10	49	-0.7071
3	9	50	-0.4082	3	10	50	0.7071	4	9	51	0.8165	4	9	52	-0.4082
4	10	52	-0.7071	4	9	53	-0.4082	4	10	53	0.7071	5	5	54	0.6667
5	6	54	0.3333	6	6	54	-1.3333	5	5	55	-0.6667	5	6	55	-0.6667
5	7	55	-0.3333	6	7	55	-0.6667	5	5	56	-0.3333	5	6	56	-0.3333
5	7	56	0.3333	6	7	56	0.6667	5	5	57	0.3333	5	6	57	-0.3333
6	6	57	0.3333	12	12	57	-1.0000	5	5	58	-0.6667	5	6	58	0.3333
5	7	58	-0.3333	6	7	58	0.3333	12	13	58	1.0000	5	5	59	-0.6667
5	6	59	0.3333	5	7	59	0.6667	6	7	59	-0.6667	5	5	60	-0.6667
5	6	60	0.3333	5	7	60	-0.3333	6	7	60	0.3333	12	13	60	-1.0000
5	5	61	0.6667	5	7	61	-0.3333	7	7	61	-1.3333	5	5	62	0.3333
5	7	62	0.3333	7	7	62	0.3333	13	13	62	-1.0000	5	9	63	-0.3333
7	9	63	0.6667	5	9	64	0.1667	5	10	64	0.2887	7	9	64	-0.3333
7	10	64	-0.5773	5	9	65	0.1667	5	10	65	-0.2887	7	9	65	-0.3333
7	10	65	0.5773	9	9	66	-0.6667	9	10	66	-0.5773	9	9	67	-0.6667
9	10	67	0.5773	9	9	68	0.3333	10	10	68	-1.0000	14	15	69	1.0000
13	14	70	-1.4142	12	14	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CD3-COF

3	3	1	1.0000	8	8	2	1.0000	7	7	3	1.0000	1	1	4	0.3333
1	2	4	-0.4714	2	2	4	0.6667	11	11	4	1.0000	1	1	5	0.6667
1	2	5	0.4714	2	2	5	0.3333	9	9	6	0.1667	9	10	6	0.2887
10	10	6	0.5000	9	9	7	0.6667	9	9	8	0.1667	9	10	8	-0.2887
10	10	8	0.5000	4	4	9	0.3333	4	5	9	-0.3333	5	5	9	0.3333
12	12	9	1.0000	4	4	10	0.6667	4	5	10	0.3333	5	5	10	0.1667
5	5	11	0.3333	5	6	11	0.3333	6	6	11	0.3333	13	13	11	1.0000
5	5	12	0.1667	5	6	12	-0.3333	6	6	12	0.6667	14	14	13	1.0000
15	15	14	1.0000	1	1	15	0.1176	1	2	15	0.0216	1	4	15	-0.1540
1	5	15	0.1540	2	2	15	1.7581	2	4	15	-0.4355	2	5	15	0.4355
4	4	15	0.1590	4	5	15	-0.1590	5	5	15	0.1590	11	11	15	0.6252
11	12	15	-0.4619	12	12	15	0.4769	1	1	16	0.4395	1	2	16	-0.6216
1	4	16	-0.3080	1	5	16	-0.1540	2	2	16	0.8791	2	4	16	0.4355
2	5	16	0.2178	4	4	16	0.3180	4	5	16	0.1590	5	5	16	0.0795
11	11	16	-0.0631	1	1	17	0.5224	1	6	17	0.4499	2	2	17	0.5224
2	5	17	-0.3181	2	7	17	1.2000	5	5	17	0.3083	5	7	17	-0.7211
6	6	17	0.6167	7	7	17	2.2520	11	11	17	0.5224	11	13	17	-0.4499
13	13	17	0.6167	3	3	18	0.7299	3	7	18	0.8178	3	9	18	-0.1816
3	10	18	-0.3145	7	7	18	0.8292	7	9	18	-0.2050	7	10	18	-0.3551
9	9	18	0.0819	9	10	18	0.1419	10	10	18	0.2458	7	7	19	0.6009
7	8	19	0.7195	7	9	19	-0.2563	7	10	19	0.4439	8	8	19	0.7198
8	9	19	-0.2936	8	10	19	0.5085	9	9	19	0.1667	9	10	19	-0.2887
10	10	19	0.5000	3	3	20	0.6121	3	8	20	0.7624	3	9	20	0.3853
8	8	20	0.8278	8	9	20	0.4998	9	9	20	0.4390	1	1	21	0.2023
1	2	21	-0.2135	1	3	21	-0.2993	1	5	21	0.0612	1	6	21	0.2306
1	7	21	-0.2234	1	9	21	0.0262	1	10	21	0.0454	2	2	21	0.3532
2	3	21	0.9284	2	5	21	-0.2064	2	6	21	-0.0866	2	7	21	0.9622
2	9	21	-0.2454	2	10	21	-0.4251	3	3	21	1.7737	3	5	21	-0.7156
3	6	21	-0.0375	3	7	21	2.0767	3	9	21	-0.4312	3	10	21	-0.7468
5	5	21	0.3903	5	6	21	-0.1590	5	7	21	-0.8286	5	9	21	0.2422
5	10	21	0.4196	6	6	21	0.9406	6	7	21	0.4015	6	9	21	-0.2587
6	10	21	-0.4431	7	7	21	2.3367	7	9	21	-0.6615	7	10	21	-1.1458
9	9	21	0.3160	9	10	21	0.5473	10	10	21	0.9479	11	11	21	0.5042
11	13	21	-0.3531	11	15	21	-0.2014	13	13	21	0.6225	13	15	21	0.3238
15	15	21	0.1597	1	1	22	0.0151	1	2	22	-0.0214	1	5	22	0.0368
1	6	22	0.0368	1	7	22	-0.2562	1	8	22	-0.2511	1	9	22	0.1263
1	10	22	-0.2187	2	2	22	0.0303	2	5	22	-0.0521	2	6	22	-0.0521
2	7	22	0.3624	2	8	22	0.3551	2	9	22	-0.1786	2	10	22	0.3093
5	5	22	0.2712	5	6	22	0.2712	5	7	22	-0.5909	5	8	22	-0.4906
5	9	22	0.3181	5	10	22	-0.5510	6	6	22	0.2712	6	7	22	-0.5909
6	8	22	-0.4906	6	9	22	0.3181	6	10	22	-0.5510	7	7	22	1.4713
7	8	22	1.2542	7	9	22	-0.7821	7	10	22	1.3547	8	8	22	0.8604
8	9	22	-0.5731	8	10	22	0.9926	9	9	22	0.5162	9	10	22	-0.8975
10	10	22	1.5546	11	11	22	0.0454	11	13	22	-0.1104	11	15	22	0.0895
13	13	22	0.8135	13	15	22	-0.7368	15	15	22	0.3680	4	4	23	-0.2103
4	6	23	0.4075	5	5	23	-0.5416	6	6	23	-0.2103	12	12	23	-0.2103
12	13	23	-0.4075	13	13	23	-0.2103	1	7	24	0.6165	2	7	24	0.5773
1	7	25	-0.8165	2	7	25	1.1547	3	7	26	1.0000	7	8	27	1.0000
4	7	28	0.8165	5	7	28	0.4082	4	7	29	-0.8165	5	7	29	0.8165
5	7	30	-0.8165	6	7	30	-0.8165	5	7	31	-0.4082	6	7	31	0.8165
7	9	32	0.8165	7	9	33	-0.4082	7	10	33	-0.7071	7	9	34	-0.4082
7	10	34	0.7071	1	1	35	-1.3333	1	2	35	0.4714	2	2	35	1.3333

SYMMETRIZED Z MATRIX ----------CH3-COCL

1	4	36	0.6667	1	5	36	0.3333	2	4	36	0.4714	2	5	36	0.2357
1	4	37	-0.6667	1	5	37	0.6667	2	4	37	-0.4714	2	5	37	0.4714
1	5	38	-0.6667	1	6	38	-0.6667	2	5	38	-0.4714	2	6	38	-0.4714
1	5	39	-0.3333	1	6	39	0.6667	2	5	39	-0.2357	2	6	39	0.4714
1	1	40	0.3333	1	2	40	-0.4714	2	2	40	0.6667	11	11	40	-1.0000
1	4	41	-0.6667	1	5	41	-0.3333	2	4	41	0.9428	2	5	41	0.4714
1	4	42	0.3333	1	5	42	-0.3333	2	4	42	-0.4714	2	5	42	0.4714
11	12	42	1.0000	1	4	43	0.3333	1	5	43	-0.3333	2	4	43	-0.4714
2	5	43	0.4714	11	12	43	-1.0000	1	5	44	0.3333	1	6	44	0.3333
2	5	44	-0.4714	2	6	44	-0.4714	11	13	44	1.0000	1	5	45	0.3333
1	6	45	-0.6667	2	5	45	-0.4714	2	6	45	0.9428	1	5	46	0.3333
1	6	46	0.3333	2	5	46	-0.4714	2	6	46	-0.4714	11	13	46	-1.0000
3	8	47	1.0000	3	9	48	0.8165	3	9	49	-0.4082	3	10	49	-0.7071
3	9	50	-0.4082	3	10	50	0.7071	8	9	51	0.8165	8	9	52	-0.4082
8	10	52	-0.7071	8	9	53	-0.4082	8	10	53	0.7071	4	4	54	-1.3333
4	5	54	0.3333	5	5	54	0.6667	4	5	55	-0.6667	4	6	55	-0.6667
5	5	55	-0.6667	5	6	55	-0.3333	4	5	56	-0.3333	4	6	56	0.6667
5	5	56	-0.3333	5	6	56	0.3333	4	4	57	0.3333	4	5	57	-0.3333
5	5	57	0.3333	12	12	57	-1.0000	4	5	58	0.3333	4	6	58	0.3333
5	5	58	-0.6667	5	6	58	-0.3333	12	13	58	1.0000	4	5	59	0.3333
4	6	59	-0.6667	5	5	59	-0.6667	5	6	59	0.6667	4	5	60	0.3333
4	6	60	0.3333	5	5	60	-0.6667	5	6	60	-0.3333	12	13	60	-1.0000
5	5	61	0.6667	5	6	61	-0.3333	6	6	61	-1.3333	5	5	62	0.3333
5	6	62	0.3333	6	6	62	0.3333	13	13	62	-1.0000	5	9	63	-0.3333
6	9	63	0.6667	5	9	64	0.1667	5	10	64	0.2887	6	9	64	-0.3333
6	10	64	-0.5773	5	9	65	0.1667	5	10	65	-0.2887	6	9	65	-0.3333
6	10	65	0.5773	9	9	66	-0.6667	9	10	66	-0.5773	9	9	67	-0.6667
9	10	67	0.5773	9	9	68	0.3333	10	10	68	-1.0000	14	15	69	1.0000
13	14	70	-1.4142	12	14	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CH3-CUCL

5	3	1	1.0000	8	8	2	1.0000	6	6	3	1.0000	1	1	4	0.3333
1	2	4	-0.4714	2	2	4	0.6667	11	11	4	1.0000	1	1	5	0.6667
1	2	5	0.4714	2	2	5	0.3333	9	9	6	0.1667	9	10	6	0.2887
10	10	6	0.5000	9	9	7	0.6667	9	9	8	0.1667	9	10	8	-0.2887
10	10	8	0.5000	4	4	9	0.3333	4	5	9	-0.3333	5	5	9	0.3333
12	12	9	1.0000	4	4	10	0.6667	4	5	10	0.3333	5	5	10	0.1667
5	5	11	0.3333	5	7	11	0.3333	7	7	11	0.3333	13	13	11	1.0000
5	5	12	0.1667	5	7	12	-0.3333	7	7	12	0.6667	14	14	13	1.0000
15	15	14	1.0000	1	1	15	0.1176	1	2	15	0.6216	1	4	15	-0.1540
1	5	15	0.1540	2	2	15	1.7581	2	4	15	-0.4355	2	5	15	0.4355
4	4	15	0.1590	4	5	15	-0.1590	5	5	15	0.1590	11	11	15	0.6252
11	12	15	-0.4619	12	12	15	0.4769	1	1	16	0.4395	1	2	16	-0.6216
1	4	16	-0.3080	1	5	16	-0.1540	2	2	16	0.8791	2	4	16	0.4355
2	5	16	0.2178	4	4	16	0.3180	4	5	16	0.1590	5	5	16	0.0795
11	11	16	-0.0681	1	1	17	0.5224	1	7	17	0.4499	2	2	17	0.5224
2	5	17	-0.3131	2	6	17	1.2000	5	5	17	0.3083	5	6	17	-0.7211
6	6	17	2.2520	7	7	17	0.6167	11	11	17	0.5224	11	13	17	-0.4499
13	13	17	0.6167	3	3	18	0.7298	3	6	18	0.8178	3	9	18	-0.1816
3	10	18	-0.3145	6	6	18	0.8292	6	9	18	-0.2050	6	10	18	-0.3551
9	9	18	0.0819	9	10	18	0.1419	10	10	18	0.2458	6	6	19	0.6009
6	8	19	0.7195	6	9	19	-0.2563	6	10	19	0.4439	8	8	19	0.7198
8	9	19	-0.2936	8	10	19	0.5085	9	9	19	0.1667	9	10	19	-0.2887
10	10	19	0.5000	3	3	20	0.6121	3	8	20	0.7624	3	9	20	0.3853
8	8	20	0.8278	8	9	20	0.4998	9	9	20	0.4390	1	1	21	0.2023
1	2	21	-0.2135	1	3	21	-0.2993	1	5	21	0.0612	1	6	21	-0.2234
1	7	21	0.2306	1	9	21	0.0262	1	10	21	0.0454	2	2	21	0.3532
2	3	21	0.9284	2	5	21	-0.2064	2	6	21	0.9622	2	7	21	-0.0866
2	9	21	-0.2454	2	10	21	-0.4251	3	3	21	1.7737	3	5	21	-0.7156
3	6	21	2.0767	3	7	21	-0.0375	3	9	21	-0.4312	3	10	21	-0.7468
5	5	21	0.3908	5	6	21	-0.8286	5	7	21	-0.1590	5	9	21	0.2422
5	10	21	0.4196	6	6	21	2.3367	6	7	21	0.4015	6	9	21	-0.6615
6	10	21	-1.1458	7	7	21	0.9406	7	9	21	-0.2587	7	10	21	-0.4481
9	9	21	0.3160	9	10	21	0.5473	10	10	21	0.9479	11	11	21	0.5042
11	13	21	-0.3531	11	15	21	-0.2014	13	13	21	0.6225	13	15	21	0.3238
15	15	21	0.1597	1	1	22	0.0151	1	2	22	-0.0214	1	5	22	0.0368
1	6	22	-0.2562	1	7	22	0.0368	1	9	22	-0.2511	1	9	22	0.1263
1	10	22	-0.2187	2	2	22	0.0303	2	5	22	-0.0521	2	6	22	0.3624
2	7	22	-0.0521	2	8	22	0.3551	2	9	22	-0.1786	2	10	22	0.3093
5	5	22	0.2712	5	6	22	-0.5909	5	7	22	0.2712	5	8	22	-0.4906
5	9	22	0.3131	5	10	22	-0.5510	6	6	22	1.4713	6	7	22	-0.5909
6	8	22	1.2542	6	9	22	-0.7821	6	10	22	1.3547	7	7	22	0.2712
7	8	22	-0.4906	7	9	22	0.3161	7	10	22	-0.5510	8	8	22	0.8604
8	9	22	-0.5731	8	10	22	0.9926	9	9	22	0.5182	9	10	22	-0.8975
10	10	22	1.5546	11	11	22	0.0454	11	13	22	-0.1104	11	15	22	0.0995
13	13	22	0.8135	13	15	22	-0.7368	15	15	22	0.3680	4	4	23	-0.2103
4	7	23	0.4075	5	5	23	-0.5416	7	7	23	-0.2103	12	12	23	-0.2103
12	13	23	-0.4075	13	13	23	-0.2103	1	6	24	0.8165	2	6	24	0.5773
1	6	25	-0.8165	2	6	25	1.1547	3	6	26	1.0000	6	8	27	1.0000
4	6	28	0.8165	5	6	28	0.4082	4	6	29	-0.8165	5	6	29	0.8165
5	6	30	-0.8165	6	7	30	-0.8165	5	6	31	-0.4082	6	7	31	0.8165
6	9	32	0.8165	6	9	33	-0.4082	6	10	33	-0.7071	6	9	34	-0.4082
6	10	34	0.7071	1	1	35	-1.3333	1	2	35	0.4714	2	2	35	1.3333

SYMMETRIZED Z MATRIX ----------CD3-COCL

1	4	36	0.6667	1	5	36	0.3333	2	4	36	0.4714	2	5	36	0.2357
1	4	37	-0.6667	1	5	37	0.6667	2	4	37	-0.4714	2	5	37	0.4714
1	5	38	-0.6667	1	7	38	-0.6667	2	5	38	-0.4714	2	7	38	-0.4714
1	5	39	-0.3333	1	7	39	0.6667	2	5	39	-0.2357	2	7	39	0.4714
1	1	40	0.3333	1	2	40	-0.4714	2	2	40	0.6667	11	11	40	-1.0000
1	4	41	-0.6667	1	5	41	-0.3333	2	4	41	0.9428	2	5	41	0.4714
1	4	42	0.3333	1	5	42	-0.3333	2	4	42	-0.4714	2	5	42	0.4714
11	12	42	1.0000	1	4	43	0.3333	1	5	43	-0.3333	2	4	43	-0.4714
2	5	43	0.4714	11	12	43	-1.0000	1	5	44	0.3333	1	7	44	0.3333
2	5	44	-0.4714	2	7	44	-0.4714	11	13	44	1.0000	1	5	45	0.3333
1	7	45	-0.6667	2	5	45	-0.4714	2	7	45	0.9428	1	5	46	0.3333
1	7	46	0.3333	2	5	46	-0.4714	2	7	46	-0.4714	11	13	46	-1.0000
3	8	47	1.0000	3	9	48	0.8165	3	9	49	-0.4082	3	10	49	-0.7071
3	9	50	-0.4082	3	10	50	0.7071	8	9	51	0.8165	8	9	52	-0.4082
8	10	52	-0.7071	8	9	53	-0.4082	8	10	53	0.7071	4	4	54	-1.3333
4	5	54	0.3333	5	5	54	0.6667	4	5	55	-0.6667	4	7	55	-0.6667
5	5	55	-0.6667	5	7	55	-0.3333	4	5	56	-0.3333	4	7	56	0.6667
5	5	56	-0.3333	5	7	56	0.3333	4	4	57	0.3333	4	5	57	-0.3333
5	5	57	0.3333	12	12	57	-1.0000	4	5	58	0.3333	4	7	58	0.3333
5	5	58	-0.6667	5	7	58	-0.3333	12	13	58	1.0000	4	5	59	0.3333
4	7	59	-0.6667	5	5	59	-0.6667	5	7	59	0.6667	4	5	60	0.3333
4	7	60	0.3333	5	5	60	-0.6667	5	7	60	-0.3333	12	13	60	-1.0000
5	5	61	0.6667	5	7	61	-0.3333	7	7	61	-1.3333	5	5	62	0.3333
5	7	62	0.3333	7	7	62	0.3333	13	13	62	-1.0000	5	9	63	-0.3333
7	9	63	0.6667	5	9	64	0.1667	5	10	64	0.2887	7	9	64	-0.3333
7	10	64	-0.5773	5	9	65	0.1667	5	10	65	-0.2887	7	9	65	-0.3333
7	10	65	0.5773	9	9	66	-0.6667	9	10	66	-0.5773	9	9	67	-0.6667
9	10	67	0.5773	9	9	68	0.3333	10	10	68	-1.0000	14	15	69	1.0000
13	14	70	-1.4142	12	14	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CO3-COCL

3	3	1	1.0000	8	8	2	1.0000	7	7	3	1.0000	1	1	4	0.3333
1	2	4	-0.4714	2	2	4	0.6667	11	11	4	1.0000	1	1	5	0.6667
1	2	5	0.4714	2	2	5	0.3333	9	9	6	0.1667	9	10	6	0.2887
10	10	6	0.5000	9	9	7	0.6667	9	9	8	0.1667	9	10	8	-0.2887
10	10	8	0.5000	4	4	9	0.3333	4	5	9	-0.3333	5	5	9	0.3333
12	12	9	1.0000	4	4	10	0.6667	4	5	10	0.3333	5	5	10	0.1667
5	5	11	0.3333	5	6	11	0.3333	6	6	11	0.3333	13	13	11	1.0000
5	5	12	0.1667	5	6	12	-0.3333	6	6	12	0.6667	14	14	13	1.0000
15	15	14	1.0000	1	1	15	0.1176	1	2	15	0.6216	1	4	15	-0.1540
1	5	15	0.1540	2	2	15	1.7581	2	4	15	-0.4355	2	5	15	0.4355
4	4	15	0.1590	4	5	15	-0.1590	5	5	15	0.1590	11	11	15	0.6252
11	12	15	-0.4619	12	12	15	0.4769	1	1	16	0.4395	1	2	16	-0.6216
1	4	16	-0.3090	1	5	16	-0.1540	2	2	16	0.8791	2	4	16	0.4355
2	5	16	0.2178	4	4	16	0.3180	4	5	16	0.1590	5	5	16	0.0795
11	11	16	-0.0681	1	1	17	0.5221	1	6	17	0.4499	2	2	17	0.5221
2	5	17	-0.3181	2	7	17	1.1999	5	5	17	0.3085	5	7	17	-0.7214
6	6	17	0.6170	7	7	17	2.2526	11	11	17	0.5221	11	13	17	-0.4499
13	13	17	0.6170	3	3	18	0.7297	3	7	18	0.8178	3	9	18	-0.1816
3	10	18	-0.3146	7	7	18	0.8293	7	9	18	-0.2051	7	10	18	-0.3552
9	9	18	0.0820	9	10	18	0.1420	10	10	18	0.2459	7	7	19	0.5693
7	8	19	0.7147	7	9	19	-0.2549	7	10	19	0.4415	8	8	19	0.7477
8	9	19	-0.3135	8	10	19	0.5430	9	9	19	0.1804	9	10	19	-0.3124
10	10	19	0.5411	3	3	20	0.5862	3	8	20	0.7557	3	9	20	0.3804
8	8	20	0.8470	8	9	20	0.5252	9	9	20	0.4704	1	1	21	0.2022
1	2	21	-0.2134	1	3	21	-0.2992	1	5	21	0.0613	1	6	21	0.2305
1	7	21	-0.2234	1	9	21	0.0262	1	10	21	0.0454	2	2	21	0.3531
2	3	21	0.9283	2	5	21	-0.2063	2	6	21	-0.0866	2	7	21	0.9622
2	9	21	-0.2455	2	10	21	-0.4252	3	3	21	1.7734	3	5	21	-0.7157
3	6	21	-0.0376	3	7	21	2.0768	3	9	21	-0.4312	3	10	21	-0.7469
5	5	21	0.3908	5	6	21	-0.1590	5	7	21	-0.8287	5	9	21	0.2423
5	10	21	0.4197	6	6	21	0.9407	6	7	21	0.4014	6	9	21	-0.2587
6	10	21	-0.4490	7	7	21	2.3370	7	9	21	-0.6617	7	10	21	-1.1461
9	9	21	0.3161	9	10	21	0.5475	10	10	21	0.9483	11	11	21	0.5040
11	13	21	-0.3531	11	15	21	-0.2014	13	13	21	0.6227	13	15	21	0.3238
15	15	21	0.1597	1	1	22	0.0072	1	2	22	-0.0102	1	5	22	0.0237
1	6	22	0.0237	1	7	22	-0.2281	1	8	22	-0.2402	1	9	22	0.1176
1	10	22	-0.2036	2	2	22	0.0144	2	5	22	-0.0335	2	6	22	-0.0335
2	7	22	0.3226	2	8	22	0.3397	2	9	22	-0.1663	2	10	22	0.2880
5	5	22	0.2673	5	6	22	0.2678	5	7	22	-0.5790	5	8	22	-0.5109
5	9	22	0.3315	5	10	22	-0.5741	6	6	22	0.2678	6	7	22	-0.5790
6	8	22	-0.5109	6	9	22	0.3315	6	10	22	-0.5741	7	7	22	1.4222
7	8	22	1.2880	7	9	22	-0.8030	7	10	22	1.3909	8	8	22	0.9485
8	9	22	-0.6426	8	10	22	1.1131	9	9	22	0.5738	9	10	22	-0.9939
10	10	22	1.7214	11	11	22	0.0217	11	13	22	-0.0711	11	15	22	0.0608
13	13	22	0.8034	13	15	22	-0.7765	15	15	22	0.4091	4	4	23	-0.2103
4	6	23	0.4075	5	5	23	-0.5415	6	6	23	-0.2103	12	12	23	-0.2103
12	13	23	-0.4075	13	13	23	-0.2103	1	7	24	0.8165	2	7	24	0.5773
1	7	25	-0.8165	2	7	25	1.1547	3	7	26	1.0000	7	8	27	1.0000
4	7	28	0.8165	5	7	28	0.4082	4	7	29	-0.8165	5	7	29	0.8165
5	7	30	-0.8165	6	7	30	-0.8165	5	7	31	-0.4082	6	7	31	0.8165
7	9	32	0.8165	7	9	33	-0.4082	7	10	33	-0.7071	7	9	34	-0.4082
7	10	34	0.7071	1	1	35	-1.3333	1	2	35	0.4714	2	2	35	1.3333

SYMMETRIZED Z MATRIX ----------CH3-COBR

1	4	36	0.6667	1	5	36	0.3333	2	4	36	0.4714	2	5	36	0.2357
1	4	37	-0.6667	1	5	37	0.6667	2	4	37	-0.4714	2	5	37	0.4714
1	5	38	-0.6667	1	6	38	-0.6667	2	5	38	-0.4714	2	6	38	-0.4714
1	5	39	-0.3333	1	6	39	0.6667	2	5	39	-0.2357	2	6	39	0.4714
1	1	40	0.3333	1	2	40	-0.4714	2	2	40	0.6667	11	11	40	-1.0000
1	4	41	-0.6667	1	5	41	-0.3333	2	4	41	0.9428	2	5	41	0.4714
1	4	42	0.3333	1	5	42	-0.3333	2	4	42	-0.4714	2	5	42	0.4714
11	12	42	1.0000	1	4	43	0.3333	1	5	43	-0.3333	2	4	43	-0.4714
2	5	43	0.4714	11	12	43	-1.0000	1	5	44	0.3333	1	6	44	0.3333
2	5	44	-0.4714	2	6	44	-0.4714	11	13	44	1.0000	1	5	45	0.3333
1	6	45	-0.6667	2	5	45	-0.4714	2	6	45	0.9428	1	5	46	0.3333
1	6	46	0.3333	2	5	46	-0.4714	2	6	46	-0.4714	11	13	46	-1.0000
3	8	47	1.0000	3	9	48	0.8165	3	9	49	-0.4082	3	10	49	-0.7071
3	9	50	-0.4082	3	10	50	0.7071	8	9	51	0.8165	8	9	52	-0.4082
8	10	52	-0.7071	8	9	53	-0.4082	8	10	53	0.7071	4	4	54	-1.3333
4	5	54	0.3333	5	5	54	0.6667	4	5	55	-0.6667	4	6	55	-0.6667
5	5	55	-0.6667	5	6	55	-0.3333	4	5	56	-0.3333	4	6	56	0.6667
5	5	56	-0.3333	5	6	56	0.3333	4	4	57	0.3333	4	5	57	-0.3333
5	5	57	0.3333	12	12	57	-1.0000	4	5	58	0.3333	4	6	58	0.3333
5	5	58	-0.6667	5	6	58	-0.3333	12	13	58	1.0000	4	5	59	0.3333
4	6	59	-0.6667	5	5	59	-0.6667	5	6	59	0.6667	4	5	60	0.3333
4	6	60	0.3333	5	5	60	-0.6667	5	6	60	-0.3333	12	13	60	-1.0000
5	5	61	0.6667	5	6	61	-0.3333	6	6	61	-1.3333	5	5	62	0.3333
5	6	62	0.3333	6	6	62	0.3333	13	13	62	-1.0000	5	9	63	-0.3333
6	9	63	0.6667	5	9	64	0.1667	5	10	64	0.2887	6	9	64	-0.3333
6	10	64	-0.5773	5	9	65	0.1667	5	10	65	-0.2887	6	9	65	-0.3333
6	10	65	0.5773	9	9	66	-0.6667	9	10	66	-0.5773	9	9	67	-0.6667
9	10	67	0.5773	9	9	68	0.3333	10	10	68	-1.0000	14	15	69	1.0000
13	14	70	-1.4142	12	14	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CH3-COBR

3	3	1	1.0000	8	8	2	1.0000	7	7	3	1.0000	1	1	4	0.3333
1	2	4	-0.4714	2	2	4	0.6667	11	11	4	1.0000	1	1	5	0.6667
1	2	5	0.4714	2	2	5	0.3333	9	9	6	0.1667	9	10	6	0.2887
10	10	6	0.5000	9	9	7	0.6667	9	9	8	0.1667	9	10	8	-0.2887
10	10	8	0.5000	4	4	9	0.3333	4	5	9	-0.3333	5	5	9	0.3333
12	12	9	1.0000	4	4	10	0.6667	4	5	10	0.3333	5	5	10	0.1667
5	5	11	0.3333	5	6	11	0.3333	6	6	11	0.3333	13	13	11	1.0000
5	5	12	0.1667	5	6	12	-0.3333	6	6	12	0.6667	14	14	13	1.0000
15	15	14	1.0000	1	1	15	0.1176	1	2	15	0.6216	1	4	15	-0.1540
1	5	15	0.1540	2	2	15	1.7581	2	4	15	-0.4355	2	5	15	0.4355
4	4	15	0.1590	4	5	15	-0.1590	5	5	15	0.1590	11	11	15	0.6252
11	12	15	-0.4619	12	12	15	0.4769	1	1	16	0.4395	1	2	16	-0.6216
1	4	16	-0.3080	1	5	16	-0.1540	2	2	16	0.8791	2	4	16	0.4355
2	5	16	0.2178	4	4	16	0.3180	4	5	16	0.1590	5	5	16	0.0795
11	11	16	-0.0681	1	1	17	0.5221	1	6	17	0.4499	2	2	17	0.5221
2	5	17	-0.3181	2	7	17	1.1999	5	5	17	0.3085	5	7	17	-0.7214
6	6	17	0.6170	7	7	17	2.2526	11	11	17	0.5221	11	13	17	-0.4499
13	13	17	0.6170	3	3	18	0.7297	3	7	18	0.8178	3	9	18	-0.1816
3	10	18	-0.3146	7	7	18	0.8293	7	9	18	-0.2051	7	10	18	-0.3552
9	9	18	0.0820	9	10	18	0.1420	10	10	18	0.2459	7	7	19	0.5693
7	8	19	0.7147	7	9	19	-0.2549	7	10	19	0.4415	8	8	19	0.7477
8	9	19	-0.3135	8	10	19	0.5430	9	9	19	0.1804	9	10	19	-0.3124
10	10	19	0.5411	3	3	20	0.5862	3	8	20	0.7557	3	9	20	0.3804
6	8	20	0.8470	8	9	20	0.5252	9	9	20	0.4704	1	1	21	0.2022
1	2	21	-0.2134	1	3	21	-0.2992	1	5	21	0.0613	1	6	21	0.2305
1	7	21	-0.2234	1	9	21	0.0262	1	10	21	0.0454	2	2	21	0.3531
2	3	21	0.9233	2	5	21	-0.2063	2	6	21	-0.0866	2	7	21	0.9622
2	9	21	-0.2455	2	10	21	-0.4252	3	3	21	1.7734	3	5	21	-0.7157
3	6	21	-0.0376	3	7	21	2.0768	3	9	21	-0.4312	3	10	21	-0.7469
5	5	21	0.3908	5	6	21	-0.1590	5	7	21	-0.8287	5	9	21	0.2423
5	10	21	0.4197	6	6	21	0.9407	6	7	21	0.4014	6	9	21	-0.2587
6	10	21	-0.4430	7	7	21	2.3370	7	9	21	-0.6617	7	10	21	-1.1461
9	9	21	0.3161	9	10	21	0.5475	10	10	21	0.9483	11	11	21	0.5040
11	13	21	-0.3531	11	15	21	-0.2014	13	13	21	0.6227	13	15	21	0.3238
15	15	21	0.1597	1	1	22	0.0072	1	2	22	-0.0102	1	5	22	0.0237
1	6	22	0.0237	1	7	22	-0.2281	1	8	22	-0.2402	1	9	22	0.1176
1	10	22	-0.2036	2	2	22	0.0144	2	5	22	-0.0335	2	6	22	-0.0335
2	7	22	0.3226	2	8	22	0.3397	2	9	22	-0.1663	2	10	22	0.2880
5	5	22	0.2678	5	6	22	0.2678	5	7	22	-0.5790	5	8	22	-0.5109
5	9	22	0.3315	5	10	22	-0.5741	6	6	22	0.2678	6	7	22	-0.5790
6	8	22	-0.5109	6	9	22	0.3315	6	10	22	-0.5741	7	7	22	1.4222
7	8	22	1.2880	7	9	22	-0.8030	7	10	22	1.3909	8	8	22	0.9485
8	9	22	-0.6426	8	10	22	1.1131	9	9	22	0.5736	9	10	22	-0.9939
10	10	22	1.7214	11	11	22	0.0217	11	13	22	-0.0711	11	15	22	0.0608
13	13	22	0.8034	13	15	22	-0.7765	15	15	22	0.4091	4	4	23	-0.2103
4	6	23	0.4075	5	5	23	-0.5415	6	6	23	-0.2103	12	12	23	-0.2103
12	13	23	-0.4075	13	13	23	-0.2103	1	7	24	0.8165	2	7	24	0.5773
1	7	25	-0.8165	2	7	25	1.1547	3	7	26	1.0000	7	8	27	1.0000
4	7	28	0.8165	5	7	28	0.4082	4	7	29	-0.8165	5	7	29	0.8165
5	7	30	-0.8165	6	7	30	-0.8165	5	7	31	-0.4082	6	7	31	0.8165
7	9	32	0.8165	7	9	33	-0.4082	7	10	33	-0.7071	7	9	34	-0.4082
7	10	34	0.7071	1	1	35	-1.3333	1	2	35	0.4714	2	2	35	1.3333

SYMMETRIZED Z MATRIX ----------CD3-COBR

1	4	36	0.6667	1	5	36	0.3333	2	4	36	0.4714	2	5	36	0.2357
1	4	37	-0.6667	1	5	37	0.6667	2	4	37	-0.4714	2	5	37	0.4714
1	5	38	-0.6667	1	6	38	-0.6667	2	5	38	-0.4714	2	6	38	-0.4714
1	5	39	-0.3333	1	6	39	0.6667	2	5	39	-0.2357	2	6	39	0.4714
1	1	40	0.3333	1	2	40	-0.4714	2	2	40	0.6667	11	11	40	-1.0000
1	4	41	-0.6667	1	5	41	-0.3333	2	4	41	0.9428	2	5	41	0.4714
1	4	42	0.3333	1	5	42	-0.3333	2	4	42	-0.4714	2	5	42	0.4714
11	12	42	1.0000	1	4	43	0.3333	1	5	43	-0.3333	2	4	43	-0.4714
2	5	43	0.4714	11	12	43	-1.0000	1	5	44	0.3333	1	6	44	0.3333
2	5	44	-0.4714	2	6	44	-0.4714	11	13	44	1.0000	1	5	45	0.3333
1	6	45	-0.6667	2	5	45	-0.4714	2	6	45	0.9428	1	5	46	0.3333
1	6	46	0.3333	2	5	46	-0.4714	2	6	46	-0.4714	11	13	46	-1.0000
3	8	47	1.0000	3	9	48	0.8165	3	9	49	-0.4082	3	10	49	-0.7071
3	9	50	-0.4082	3	10	50	0.7071	8	9	51	0.8165	8	9	52	-0.4082
8	10	52	-0.7071	3	9	53	-0.4082	3	10	53	0.7071	4	4	54	-1.3333
4	5	54	0.3333	5	5	54	0.6667	4	5	55	-0.6667	4	6	55	-0.6667
5	5	55	-0.6667	5	6	55	-0.3333	4	5	56	-0.3333	4	6	56	0.6667
5	5	56	-0.3333	5	6	56	0.3333	4	4	57	0.3333	4	5	57	-0.3333
5	5	57	0.3333	12	12	57	-1.0000	4	5	58	0.3333	4	6	58	0.3333
5	5	58	-0.6667	5	6	58	-0.3333	12	13	58	1.0000	4	5	59	0.3333
4	6	59	-0.6667	5	5	59	-0.6667	5	6	59	0.6667	4	5	60	0.3333
4	6	60	0.3333	5	5	60	-0.6667	5	6	60	-0.3333	12	13	60	-1.0000
5	5	61	0.6667	5	6	61	-0.3333	6	6	61	-1.3333	5	5	62	0.3333
5	6	62	0.3333	6	6	62	0.3333	13	13	62	-1.0000	5	9	63	-0.3333
6	9	63	0.6667	5	9	64	0.1667	5	10	64	0.2887	6	9	64	-0.3333
6	10	64	-0.5773	5	9	65	0.1667	5	10	65	-0.2887	6	9	65	-0.3333
6	10	65	0.5773	9	9	66	-0.6667	9	10	66	-0.5773	9	9	67	-0.6667
9	10	67	0.5773	9	9	68	0.3333	10	10	68	-1.0000	14	15	69	1.0000
13	14	70	-1.4142	12	14	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CD3-COBR

2	2	1	1.0000	1	1	2	1.0000	6	6	3	1.0000	4	4	4	0.6667
4	5	4	-0.4714	5	5	4	0.3333	11	11	4	1.0000	4	4	5	0.3333
4	5	5	0.4714	5	5	5	0.6667	3	3	6	0.1667	3	9	6	0.2887
9	9	6	0.5000	3	3	7	0.6667	3	3	8	0.1667	3	9	8	-0.2887
9	9	8	0.5000	7	7	9	0.3333	7	8	9	-0.3333	8	8	9	0.3333
13	13	9	1.0000	7	7	10	0.1667	7	8	10	0.3333	8	8	10	0.6667
7	7	11	0.3333	7	10	11	0.3333	10	10	11	0.3333	14	14	11	1.0000
7	7	12	0.1667	7	10	12	-0.3333	10	10	12	0.6667	12	12	13	1.0000
15	15	14	1.0000	4	4	15	1.7705	4	5	15	0.6260	4	7	15	0.5339
4	8	15	-0.5339	5	5	15	0.1205	5	7	15	0.1888	5	8	15	-0.1888
7	7	15	0.2380	7	8	15	-0.2380	8	8	15	0.2380	11	11	15	0.6303
11	13	15	-0.5603	13	13	15	0.7140	4	4	16	0.8853	4	5	16	-0.6260
4	7	16	0.2669	4	8	16	0.5339	5	5	16	0.4426	5	7	16	-0.1888
5	8	16	-0.3775	7	7	16	0.1190	7	8	16	0.2380	8	8	16	0.4760
11	11	16	-0.0672	4	4	17	0.5828	4	6	17	1.2117	4	7	17	-0.4002
5	5	17	0.5828	5	10	17	0.5660	6	6	17	2.0637	6	7	17	-0.7818
7	7	17	0.4046	10	10	17	0.8097	11	11	17	0.5828	11	14	17	-0.5660
14	14	17	0.8097	2	2	18	0.6737	2	3	18	-0.1935	2	6	18	0.7820
2	9	18	-0.3352	3	3	18	0.0951	3	6	18	-0.2247	3	9	18	0.1647
6	6	18	0.8006	6	9	18	-0.3891	9	9	18	0.2853	1	1	19	0.6063
1	3	19	-0.1792	1	6	19	0.7512	1	9	19	0.3105	3	3	19	0.0912
3	6	19	-0.2261	3	9	19	-0.1579	6	6	19	0.8027	6	9	19	0.3916
9	9	19	0.2736	1	1	20	0.6972	1	2	20	0.7741	1	3	20	0.3521
2	2	20	0.7519	2	3	20	0.3749	3	3	20	0.2836	2	2	21	1.5053
2	5	21	-0.3904	2	4	21	0.9251	2	5	21	-0.3233	2	6	21	1.8267
2	7	21	-0.7421	2	9	21	-0.6763	2	10	21	-0.1356	3	3	21	0.3663
3	4	21	-0.2933	3	5	21	0.0066	3	6	21	-0.7137	3	7	21	0.3131
3	9	21	0.6344	3	10	21	-0.3518	4	4	21	0.4063	4	5	21	-0.2211
4	6	21	0.9946	4	7	21	-0.2924	4	9	21	-0.5080	4	10	21	-0.0670
5	5	21	0.2500	5	6	21	-0.1817	5	7	21	0.0474	5	9	21	0.0114
5	10	21	0.3661	6	6	21	2.1967	6	7	21	-0.9323	6	9	21	-1.2362
6	10	21	0.5369	7	7	21	0.5284	7	9	21	0.5422	7	10	21	-0.2606
9	9	21	1.0988	9	10	21	-0.6094	10	10	21	1.3174	11	11	21	0.5626
11	14	21	-0.4609	11	15	21	0.2902	14	14	21	0.7962	14	15	21	-0.4558
15	15	21	0.2514	1	1	22	0.4354	1	3	22	-0.2247	1	4	22	0.4204
1	5	22	-0.2973	1	6	22	0.9824	1	7	22	-0.4252	1	9	22	0.3892
1	10	22	-0.4252	3	3	22	0.2562	3	4	22	-0.2146	3	5	22	0.1517
3	6	22	-0.5862	3	7	22	0.2661	3	9	22	-0.4437	3	10	22	0.2661
4	4	22	0.1740	4	5	22	-0.1230	4	6	22	0.6236	4	7	22	-0.2026
4	9	22	0.3717	4	10	22	-0.2026	5	5	22	0.0870	5	6	22	-0.4410
5	7	22	0.1433	5	9	22	-0.2628	5	10	22	0.1433	6	6	22	1.6253
6	7	22	-0.7279	6	9	22	1.0154	6	10	22	-0.7279	7	7	22	0.3884
7	9	22	-0.4608	7	10	22	0.3884	9	9	22	0.7685	9	10	22	-0.4608
10	10	22	0.3884	11	11	22	0.2610	11	14	22	-0.4298	11	15	22	-0.2270
14	14	22	1.1653	14	15	22	0.6513	15	15	22	0.1955	7	7	23	-0.5734
8	8	23	-0.2023	8	10	23	0.3998	10	10	23	-0.2023	13	13	23	-0.2023
13	14	23	-0.3998	14	14	23	-0.2023	4	6	24	0.5773	5	6	24	0.8165
4	6	25	1.1547	5	6	25	-0.8165	2	6	26	1.0000	1	6	27	1.0000
6	7	28	0.4082	6	8	28	0.8165	6	7	29	0.8165	6	8	29	-0.8165
6	7	30	-0.8165	6	10	30	-0.8165	6	7	31	-0.4082	6	10	31	0.8165
3	6	32	0.8165	3	6	33	-0.4082	6	9	33	-0.7071	3	6	34	-0.4082
6	9	34	0.7071	4	4	35	1.3333	4	5	35	0.4714	5	5	35	-1.3333

SYMMETRIZED Z MATRIX ----------CF3-COH

4	7	36	0.2357	4	8	36	0.4714	5	7	36	0.3333	5	8	36	0.6667
4	7	37	0.4714	4	8	37	-0.4714	5	7	37	0.6667	5	8	37	-0.6667
4	7	38	-0.4714	4	10	38	-0.4714	5	7	38	-0.6667	5	10	38	-0.6667
4	7	39	-0.2357	4	10	39	0.4714	5	7	39	-0.3333	5	10	39	0.6667
4	4	40	0.6667	4	5	40	-0.4714	5	5	40	0.3333	11	11	40	-1.0000
4	7	41	0.4714	4	8	41	0.9428	5	7	41	-0.3333	5	8	41	-0.6667
4	7	42	0.4714	4	8	42	-0.4714	5	7	42	-0.3333	5	8	42	0.3333
11	13	42	1.0000	4	7	43	0.4714	4	8	43	-0.4714	5	7	43	-0.3333
5	8	43	0.3333	11	13	43	-1.0000	4	7	44	-0.4714	4	10	44	-0.4714
5	7	44	0.3333	5	10	44	0.3333	11	14	44	1.0000	4	7	45	-0.4714
4	10	45	0.9428	5	7	45	0.3333	5	10	45	-0.6667	4	7	46	-0.4714
4	10	46	-0.4714	5	7	46	0.3333	5	10	46	0.3333	11	14	46	-1.0000
1	2	47	1.0000	2	3	48	0.8165	2	3	49	-0.4082	2	9	49	-0.7071
2	3	50	-0.4082	2	9	50	0.7071	1	3	51	0.8165	1	3	52	-0.4082
1	9	52	-0.7071	1	3	53	-0.4082	1	9	53	0.7071	7	7	54	0.6667
7	8	54	0.3333	8	8	54	-1.3333	7	7	55	-0.6667	7	8	55	-0.6667
7	10	55	-0.3333	8	10	55	-0.6667	7	7	56	-0.3333	7	8	56	-0.3333
7	10	56	0.3333	8	10	56	0.6667	7	7	57	0.3333	7	8	57	-0.3333
8	8	57	0.3333	13	13	57	-1.0000	7	7	58	-0.6667	7	8	58	0.3333
7	10	58	-0.3333	8	10	58	0.3333	13	14	58	1.0000	7	7	59	-0.6667
7	8	59	0.3333	7	10	59	0.6667	8	10	59	-0.6667	7	7	60	-0.6667
7	8	60	0.3333	7	10	60	-0.3333	8	10	60	0.3333	13	14	60	-1.0000
7	7	61	0.6667	7	10	61	-0.3333	10	10	61	-1.3333	7	7	62	0.3333
7	10	62	0.3333	10	10	62	0.3333	14	14	62	-1.0000	3	7	63	-0.3333
3	10	63	0.6667	3	7	64	0.1667	3	10	64	-0.3333	7	9	64	0.2887
9	10	64	-0.5773	3	7	65	0.1667	3	10	65	-0.3333	7	9	65	-0.2887
9	10	65	0.5773	3	3	66	-0.6667	3	9	66	-0.5773	3	3	67	-0.6667
3	9	67	0.5773	3	3	68	0.3333	9	9	68	-1.0000	12	15	69	1.0000
12	14	70	-1.4142	12	13	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CF3-COH

2	2	1	1.0000	1	1	2	1.0000	6	6	3	1.0000	3	3	4	0.6667
3	4	4	-0.4714	4	4	4	0.3333	11	11	4	1.0000	3	3	5	0.3333
3	4	5	0.4714	4	4	5	0.6667	5	5	6	0.1667	5	9	6	0.2887
9	9	6	0.5000	5	5	7	0.6667	5	5	8	0.1667	5	9	8	-0.2887
9	9	8	0.5000	7	7	9	0.3333	7	8	9	-0.3333	8	8	9	0.3333
13	13	9	1.0000	7	7	10	0.1667	7	8	10	0.3333	8	8	10	0.6667
7	7	11	0.3333	7	10	11	0.3333	10	10	11	0.3333	14	14	11	1.0000
7	7	12	0.1667	7	10	12	-0.3333	10	10	12	0.6667	12	12	13	1.0000
15	15	14	1.0000	3	3	15	1.7705	3	4	15	0.6260	3	7	15	0.5339
3	8	15	-0.5339	4	4	15	0.1205	4	7	15	0.1888	4	8	15	-0.1888
7	7	15	0.2380	7	8	15	-0.2380	8	8	15	0.2380	11	11	15	0.6303
11	13	15	-0.5663	13	13	15	0.7140	3	3	16	0.8853	3	4	16	-0.6260
3	7	16	0.2669	3	8	16	0.5339	4	4	16	0.4426	4	7	16	-0.1888
4	8	16	-0.3775	7	7	16	0.1190	7	8	16	0.2380	8	8	16	0.4760
11	11	16	-0.0672	3	3	17	0.5828	3	6	17	1.2117	3	7	17	-0.4002
4	4	17	0.5828	4	10	17	0.5660	6	6	17	2.0637	6	7	17	-0.7818
7	7	17	0.4048	10	10	17	0.8097	11	11	17	0.5828	11	14	17	-0.5660
14	14	17	0.8097	2	2	18	0.6737	2	5	18	-0.1935	2	6	18	0.7820
2	9	18	-0.3352	5	5	18	0.0951	5	6	18	-0.2247	5	9	18	0.1647
6	6	18	0.8006	6	9	18	-0.3891	9	9	18	0.2853	1	1	19	0.6063
1	5	19	-0.1792	1	6	19	0.7512	1	9	19	0.3105	5	5	19	0.0912
5	6	19	-0.2261	5	9	19	-0.1579	6	6	19	0.8027	6	9	19	0.3916
9	9	19	0.2736	1	1	20	0.6972	1	2	20	0.7741	1	5	20	0.3521
2	2	20	0.7519	2	5	20	0.3749	5	5	20	0.2836	2	2	21	1.5053
2	3	21	0.9251	2	4	21	-0.3233	2	5	21	-0.3904	2	6	21	1.8267
2	7	21	-0.7421	2	9	21	-0.6763	2	10	21	-0.1356	3	3	21	0.4063
3	4	21	-0.2211	3	5	21	-0.2933	3	6	21	0.9946	3	7	21	-0.2924
3	9	21	-0.5080	3	10	21	-0.0670	4	4	21	0.2500	4	5	21	0.0066
4	6	21	-0.1817	4	7	21	0.0474	4	9	21	0.0114	4	10	21	0.3661
5	5	21	0.3663	5	6	21	-0.7137	5	7	21	0.3131	5	9	21	0.6344
5	10	21	-0.3518	6	6	21	2.1967	6	7	21	-0.9323	6	9	21	-1.2362
6	10	21	0.5369	7	7	21	0.5284	7	9	21	0.5422	7	10	21	-0.2606
9	9	21	1.0988	9	10	21	-0.6094	10	10	21	1.3174	11	11	21	0.5626
11	14	21	-0.4609	11	15	21	0.2902	14	14	21	0.7962	14	15	21	-0.4558
15	15	21	0.2514	1	1	22	0.4354	1	3	22	0.4204	1	4	22	-0.2973
1	5	22	-0.2247	1	6	22	0.9824	1	7	22	-0.4252	1	9	22	0.3892
1	10	22	-0.4252	3	3	22	0.1740	3	4	22	-0.1230	3	5	22	-0.2146
3	6	22	0.6236	3	7	22	-0.2026	3	9	22	0.3717	3	10	22	-0.2026
4	4	22	0.0870	4	5	22	0.1517	4	6	22	-0.4410	4	7	22	0.1433
4	9	22	-0.2628	4	10	22	0.1463	5	5	22	0.2562	5	6	22	-0.5862
5	7	22	0.2661	5	9	22	-0.4437	5	10	22	0.2661	6	6	22	1.6253
6	7	22	-0.7279	6	9	22	1.0154	6	10	22	-0.7279	7	7	22	0.3884
7	9	22	-0.4608	7	10	22	0.3884	9	9	22	0.7685	9	10	22	-0.4608
10	10	22	0.3884	11	11	22	0.2610	11	14	22	-0.4298	11	15	22	-0.2270
14	14	22	1.1653	14	15	22	0.6513	15	15	22	0.1955	7	7	23	-0.5734
8	8	23	-0.2023	8	10	23	0.3998	10	10	23	-0.2023	13	13	23	-0.2023
13	14	23	-0.3998	14	14	23	-0.2023	3	6	24	0.5773	4	6	24	0.8165
3	6	25	1.1547	4	6	25	-0.8165	2	6	26	1.0000	1	6	27	1.0000
6	7	28	0.4082	6	8	28	0.8165	6	7	29	0.8165	6	8	29	-0.8165
6	7	30	-0.8165	6	10	30	-0.8165	6	7	31	-0.4082	6	10	31	0.8165
5	6	32	0.8165	5	6	33	-0.4082	6	9	33	-0.7071	5	6	34	-0.4082
6	9	34	0.7071	3	3	35	1.3333	3	4	35	0.4714	4	4	35	-1.3333

SYMMETRIZED Z MATRIX ----------CF3-COD

3	7	36	0.2357	3	8	36	0.4714	4	7	36	0.3333	4	8	36	0.6667
3	7	37	0.4714	3	8	37	-0.4714	4	7	37	0.6667	4	8	37	-0.6667
3	7	38	-0.4714	3	10	38	-0.4714	4	7	38	-0.6667	4	10	38	-0.6667
3	7	39	-0.2357	3	10	39	0.4714	4	7	39	-0.3333	4	10	39	0.6667
3	3	40	0.6667	3	4	40	-0.4714	4	4	40	0.3333	11	11	40	-1.0000
3	7	41	0.4714	3	8	41	0.9428	4	7	41	-0.3333	4	8	41	-0.6667
3	7	42	0.4714	3	8	42	-0.4714	4	7	42	-0.3333	4	8	42	0.3333
11	13	42	1.0000	3	7	43	0.4714	3	8	43	-0.4714	4	7	43	-0.3333
4	8	43	0.3333	11	13	43	-1.0000	3	7	44	-0.4714	3	10	44	-0.4714
4	7	44	0.3333	4	10	44	0.3333	11	14	44	1.0000	3	7	45	-0.4714
3	10	45	0.9428	4	7	45	0.3333	4	10	45	-0.6667	3	7	46	-0.4714
3	10	46	-0.4714	4	7	46	0.3333	4	10	46	0.3333	11	14	46	-1.0000
1	2	47	1.0000	2	5	48	0.8165	2	5	49	-0.4082	2	9	49	-0.7071
2	5	50	-0.4082	2	9	50	0.7071	1	5	51	0.8165	1	5	52	-0.4082
1	9	52	-0.7071	1	5	53	-0.4082	1	9	53	0.7071	7	7	54	0.6667
7	8	54	0.3333	8	8	54	-1.3333	7	7	55	-0.6667	7	8	55	-0.6667
7	10	55	-0.3333	8	10	55	-0.6667	7	7	56	-0.3333	7	8	56	-0.3333
7	10	56	0.3333	8	10	56	0.6667	7	7	57	0.3333	7	8	57	-0.3333
8	8	57	0.3333	13	13	57	-1.0000	7	7	58	-0.6667	7	8	58	0.3333
7	10	58	-0.3333	8	10	58	0.3333	13	14	58	1.0000	7	7	59	-0.6667
7	8	59	0.3333	7	10	59	0.6667	8	10	59	-0.6667	7	7	60	-0.6667
7	8	60	0.3333	7	10	60	-0.3333	8	10	60	0.3333	13	14	60	-1.0000
7	7	61	0.6667	7	10	61	-0.3333	10	10	61	-1.3333	7	7	62	0.3333
7	10	62	0.3333	10	10	62	0.3333	14	14	62	-1.0000	5	7	63	-0.3333
5	10	63	0.6667	5	7	64	0.1667	5	10	64	-0.3333	7	9	64	0.2887
5	10	64	-0.5773	5	7	65	0.1667	5	10	65	-0.3333	7	9	65	-0.2887
9	10	65	0.5773	5	5	66	-0.6667	5	9	66	-0.5773	5	5	67	-0.6667
5	9	67	0.5773	5	5	68	0.3333	9	9	68	-1.0000	12	15	69	1.0000
12	14	70	-1.4142	12	13	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CF3-COD

1	1	1	1.0000	4	4	2	1.0000	5	5	3	1.0000	2	2	4	0.6667
2	3	4	-0.4714	3	3	4	0.3333	11	11	4	1.0000	2	2	5	0.3333
2	3	5	0.4714	3	3	5	0.6667	6	6	6	0.1667	6	9	6	0.2887
9	9	6	0.5000	6	6	7	0.6667	6	6	8	0.1667	6	9	8	-0.2887
9	9	8	0.5000	7	7	9	0.3333	7	8	9	-0.3333	8	8	9	0.3333
12	12	9	1.0000	7	7	10	0.1667	7	8	10	0.3333	8	8	10	0.6667
7	7	11	0.3333	7	10	11	0.3333	10	10	11	0.3333	14	14	11	1.0000
7	7	12	0.1667	7	10	12	-0.3333	10	10	12	0.6667	13	13	13	1.0000
15	15	14	1.0000	2	2	15	1.7341	2	3	15	0.6131	2	7	15	0.5422
2	8	15	-0.5422	3	3	15	0.1119	3	7	15	0.1917	3	8	15	-0.1917
7	7	15	0.2482	7	8	15	-0.2482	8	8	15	0.2482	11	11	15	0.6153
11	12	15	-0.5751	12	12	15	0.7447	2	2	16	0.8671	2	3	16	-0.6131
2	7	16	0.2711	2	8	16	0.5422	3	3	16	0.4335	3	7	16	-0.1917
3	8	16	-0.3834	7	7	16	0.1241	7	8	16	0.2482	8	8	16	0.4965
11	11	16	-0.0699	2	2	17	0.6059	2	5	17	1.2333	2	7	17	-0.3997
3	3	17	0.6059	3	10	17	0.5652	5	5	17	2.0811	5	7	17	-0.7651
7	7	17	0.3910	10	10	17	0.7819	11	11	17	0.6059	11	14	17	0.5652
14	14	17	0.7819	1	1	18	0.7311	1	5	18	0.8226	1	6	18	-0.1769
1	9	18	-0.3064	5	5	18	0.8407	5	6	18	-0.2026	5	9	18	-0.3509
6	6	18	0.0796	6	9	18	0.1379	9	9	18	0.2388	4	4	19	0.7685
4	5	19	0.7726	4	6	19	-0.2739	4	9	19	0.4744	5	5	19	0.6790
5	6	19	-0.2470	5	9	19	0.4278	6	6	19	0.1463	6	9	19	-0.2533
9	9	19	0.4388	1	1	20	0.5067	1	4	20	0.6970	1	6	20	0.3871
4	4	20	0.7892	4	6	20	0.5441	6	6	20	0.5025	1	1	21	1.6743
1	2	21	0.9816	1	3	21	-0.3021	1	5	21	1.9622	1	6	21	-0.3707
1	7	21	-0.7886	1	9	21	-0.6420	1	10	21	-0.1057	2	2	21	0.4275
2	3	21	-0.1994	2	5	21	1.0493	2	6	21	-0.2697	2	7	21	-0.3104
2	9	21	-0.4672	2	10	21	-0.0477	3	3	21	0.2865	3	5	21	-0.1547
3	6	21	-0.0190	3	7	21	0.0337	3	9	21	-0.0329	3	10	21	0.4052
5	5	21	2.2733	5	6	21	-0.6457	5	7	21	-0.9463	5	9	21	-1.1184
5	10	21	0.4808	6	6	21	0.3215	6	7	21	0.2793	6	9	21	0.5565
6	10	21	-0.3309	7	7	21	0.5306	7	9	21	0.4838	7	10	21	-0.2338
9	9	21	0.9646	9	10	21	-0.5732	10	10	21	1.2949	11	11	21	0.5685
11	14	21	0.4726	11	15	21	0.2591	14	14	21	0.8273	14	15	21	0.4172
15	15	21	0.1934	2	2	22	0.0909	2	3	22	-0.0643	2	4	22	0.4359
2	5	22	0.4865	2	6	22	-0.2266	2	7	22	-0.1328	2	9	22	0.3926
2	10	22	-0.1328	3	3	22	0.0454	3	4	22	-0.3082	3	5	22	-0.3440
3	6	22	0.1603	3	7	22	0.0939	3	9	22	-0.2776	3	10	22	0.0939
4	4	22	0.8639	4	5	22	1.2770	4	6	22	-0.5434	4	7	22	-0.5885
4	9	22	0.9412	4	10	22	-0.5885	5	5	22	1.5738	5	6	22	-0.7892
5	7	22	-0.7441	5	9	22	1.3670	5	10	22	-0.7441	6	6	22	0.5005
6	7	22	0.3796	6	9	22	-0.8669	6	10	22	0.3796	7	7	22	0.4106
7	9	22	-0.6575	7	10	22	0.4106	9	9	22	1.5015	9	10	22	-0.6575
10	10	22	0.4106	11	11	22	0.1363	11	14	22	0.2817	11	15	22	-0.1967
14	14	22	1.2317	14	15	22	-0.9381	15	15	22	0.3969	7	7	23	-0.4826
8	8	23	-0.2249	8	10	23	0.4211	10	10	23	-0.2249	12	12	23	-0.2249
12	14	23	0.4211	14	14	23	-0.2249	2	5	24	0.5773	3	5	24	0.8165
2	5	25	1.1547	3	5	25	-0.8165	1	5	26	1.0000	4	5	27	1.0000
5	7	28	0.4082	5	8	28	0.8165	5	7	29	0.8165	5	8	29	-0.8165
5	7	30	-0.8165	5	10	30	-0.9165	5	7	31	-0.4082	5	10	31	0.8165
5	6	32	0.8165	5	6	33	-0.4082	5	9	33	-0.7071	5	6	34	-0.4082
5	9	34	0.7071	2	2	35	1.3333	2	3	35	0.4714	3	3	35	-1.3333

SYMMETRIZED Z MATRIX ----------CF3-COF

2	7	36	0.2357	2	8	36	0.4714	3	7	36	0.3333	3	8	36	0.6667
2	7	37	0.4714	2	8	37	-0.4714	3	7	37	0.6667	3	8	37	-0.6667
2	7	38	-0.4714	2	10	38	-0.4714	3	7	38	-0.6667	3	10	38	-0.6667
2	7	39	-0.2357	2	10	39	0.4714	3	7	39	-0.3333	3	10	39	0.6667
2	2	40	0.6667	2	3	40	-0.4714	3	3	40	0.3333	11	11	40	-1.0000
2	7	41	0.4714	2	8	41	0.9428	3	7	41	-0.3333	3	8	41	-0.6667
2	7	42	0.4714	2	8	42	-0.4714	3	7	42	-0.3333	3	8	42	0.3333
11	12	42	1.0000	2	7	43	0.4714	2	8	43	-0.4714	3	7	43	-0.3333
3	8	43	0.3333	11	12	43	-1.0000	2	7	44	-0.4714	2	10	44	-0.4714
3	7	44	0.3333	3	10	44	0.3333	11	14	44	-1.0000	2	7	45	-0.4714
2	10	45	0.9428	3	7	45	0.3333	3	10	45	-0.6667	2	7	46	-0.4714
2	10	46	-0.4714	3	7	46	0.3333	3	10	46	0.3333	11	14	46	1.0000
1	4	47	1.0000	1	6	48	0.8165	1	6	49	-0.4082	1	9	49	-0.7071
1	6	50	-0.4082	1	9	50	0.7071	4	6	51	0.8165	4	6	52	-0.4082
4	9	52	-0.7071	4	6	53	-0.4082	4	9	53	0.7071	7	7	54	0.6667
7	8	54	0.3333	8	8	54	-1.3333	7	7	55	-0.6667	7	8	55	-0.6667
7	10	55	-0.3333	8	10	55	-0.6667	7	7	56	-0.3333	7	8	56	-0.3333
7	10	56	0.3333	8	10	56	0.6667	7	7	57	0.3333	7	8	57	-0.3333
8	8	57	0.3333	12	12	57	-1.0000	7	7	58	-0.6667	7	8	58	0.3333
7	10	58	-0.3333	8	10	58	0.3333	12	14	58	-1.0000	7	7	59	-0.6667
7	8	59	0.3333	7	10	59	0.6667	8	10	59	-0.6667	7	7	60	-0.6667
7	8	60	0.3333	7	10	60	-0.3333	8	10	60	0.3333	12	14	60	1.0000
7	7	61	0.6667	7	10	61	-0.3333	10	10	61	-1.3333	7	7	62	0.3333
7	10	62	0.3333	10	10	62	0.3333	14	14	62	-1.0000	6	7	63	-0.3333
6	10	63	0.6667	6	7	64	0.1667	6	10	64	-0.3333	7	9	64	0.2887
9	10	64	-0.5773	6	7	65	0.1667	6	10	65	-0.3333	7	9	65	-0.2887
9	10	65	0.5773	6	6	66	-0.6667	6	9	66	-0.5773	6	6	67	-0.6667
6	9	67	0.5773	6	6	68	0.3333	9	9	68	-1.0000	13	15	69	1.0000
13	14	70	1.4142	12	13	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CF3-COF

1	1	1	1.0000	5	5	2	1.0000	4	4	3	1.0000	2	2	4	0.6667
2	3	4	-0.4714	3	3	4	0.3333	11	11	4	1.0000	2	2	5	0.3333
2	3	5	0.4714	3	3	5	0.6667	8	8	6	0.1667	8	9	6	-0.2887
9	9	6	0.5000	8	8	7	0.6667	8	8	8	0.1667	8	9	8	0.2887
9	9	8	0.5000	6	6	9	0.3333	6	7	9	-0.3333	7	7	9	0.3333
12	12	9	1.0000	6	6	10	0.6667	6	7	10	0.3333	7	7	10	0.1667
7	7	11	0.3333	7	10	11	0.3333	10	10	11	0.3333	14	14	11	1.0000
7	7	12	0.1667	7	10	12	-0.3333	10	10	12	0.6667	13	13	13	1.0000
15	15	14	1.0000	2	2	15	1.7341	2	3	15	0.6131	2	6	15	-0.5382
2	7	15	0.5382	3	3	15	0.1119	3	6	15	-0.1903	3	7	15	0.1903
6	6	15	0.2445	6	7	15	-0.2445	7	7	15	0.2445	11	11	15	0.6153
11	12	15	-0.5708	12	12	15	0.7336	2	2	16	0.8671	2	3	16	-0.6131
2	6	16	0.5382	2	7	16	0.2691	3	3	16	0.4335	3	6	16	-0.3805
3	7	16	-0.1903	6	6	16	0.4891	6	7	16	0.2445	7	7	16	0.1223
11	11	16	-0.0699	2	2	17	0.5918	2	4	17	1.2308	2	7	17	-0.3964
3	3	17	0.5918	3	10	17	0.5607	4	4	17	2.1201	4	7	17	-0.7830
7	7	17	0.3990	10	10	17	0.7981	11	11	17	0.5918	11	14	17	-0.5607
14	14	17	0.7981	1	1	18	0.7061	1	4	18	0.8088	1	8	18	-0.1827
1	9	18	0.3164	4	4	18	0.8338	4	8	18	-0.2134	4	9	18	0.3696
8	8	18	0.0863	8	9	18	-0.1495	9	9	18	0.2590	4	4	19	0.5881
4	5	19	0.6948	4	8	19	-0.2735	4	9	19	-0.4736	5	5	19	0.6689
5	8	19	-0.2999	5	9	19	-0.5195	8	8	19	0.1839	8	9	19	0.3185
9	9	19	0.5517	1	1	20	0.6687	1	5	20	0.7969	1	8	20	0.3691
5	5	20	0.8494	5	8	20	0.4614	8	8	20	0.3865	1	1	21	1.6188
1	2	21	0.9621	1	3	21	-0.3046	1	4	21	1.9345	1	7	21	-0.7737
1	8	21	-0.3818	1	9	21	0.6614	1	10	21	-0.1122	2	2	21	0.4204
2	3	21	-0.2046	2	4	21	1.0381	2	7	21	-0.3015	2	8	21	-0.2814
2	9	21	0.4874	2	10	21	-0.0537	3	3	21	0.2757	3	4	21	-0.1645
3	7	21	0.0380	3	8	21	-0.0087	3	9	21	0.0150	3	10	21	0.3885
4	4	21	2.2743	4	7	21	-0.9439	4	8	21	-0.6772	4	9	21	1.1729
4	10	21	0.4885	7	7	21	0.5278	7	8	21	0.2913	7	9	21	-0.5045
7	10	21	-0.2364	8	8	21	0.3392	8	9	21	-0.5875	8	10	21	-0.3301
9	9	21	1.0176	9	10	21	0.5718	10	10	21	1.2921	11	11	21	0.5650
11	14	21	-0.4644	11	15	21	0.2616	14	14	21	0.8192	14	15	21	-0.4230
15	15	21	0.2063	2	2	22	0.0778	2	3	22	-0.0550	2	4	22	0.4481
2	5	22	0.3796	2	7	22	-0.1245	2	8	22	-0.2452	2	9	22	-0.4247
2	10	22	-0.1245	3	3	22	0.0389	3	4	22	-0.3168	3	5	22	-0.2684
3	7	22	0.0841	3	8	22	0.1734	3	9	22	0.3003	3	10	22	0.0881
4	4	22	1.4631	4	5	22	1.0969	4	7	22	-0.6881	4	8	22	-0.8357
4	9	22	-1.4474	4	10	22	-0.6881	5	5	22	0.6119	5	7	22	-0.4998
5	8	22	-0.5033	5	9	22	-0.8717	5	10	22	-0.4998	7	7	22	0.3750
7	8	22	0.3970	7	9	22	0.6876	7	10	22	0.3750	8	8	22	0.5715
8	9	22	0.9899	8	10	22	0.3970	9	9	22	1.7145	9	10	22	0.6876
10	10	22	0.3750	11	11	22	0.1167	11	14	22	-0.2642	11	15	22	-0.2174
14	14	22	1.1249	14	15	22	1.0229	15	15	22	0.5560	6	6	23	-0.2249
6	10	23	0.4211	7	7	23	-0.4826	10	10	23	-0.2249	12	12	23	-0.2249
12	14	23	-0.4211	14	14	23	-0.2249	2	4	24	0.5773	3	4	24	0.8165
2	4	25	1.1547	3	4	25	-0.8165	1	4	26	1.0000	4	5	27	1.0000
4	6	28	0.8165	4	7	28	0.4082	4	6	29	-0.8165	4	7	29	0.8165
4	7	30	-0.8165	4	10	30	-0.8165	4	7	31	-0.4082	4	10	31	0.8165
4	8	32	0.8165	4	8	33	-0.4082	4	9	33	0.7071	4	8	34	-0.4082
4	9	34	-0.7071	2	2	35	1.3333	2	3	35	0.4714	3	3	35	-1.3333

SYMMETRIZED Z MATRIX ----------CF3-COCL

2	6	36	0.4714	2	7	36	0.2357	3	6	36	0.6667	3	7	36	0.3333
2	6	37	-0.4714	2	7	37	0.4714	3	6	37	-0.6667	3	7	37	0.6667
2	7	38	-0.4714	2	10	38	-0.4714	3	7	38	-0.6667	3	10	38	-0.6667
2	7	39	-0.2357	2	10	39	0.4714	3	7	39	-0.3333	3	10	39	0.6667
2	2	40	0.6667	2	3	40	-0.4714	3	3	40	0.3333	11	11	40	-1.0000
2	6	41	0.9428	2	7	41	0.4714	3	6	41	-0.6667	3	7	41	-0.3333
2	6	42	-0.4714	2	7	42	0.4714	3	6	42	0.3333	3	7	42	-0.3333
11	12	42	1.0000	2	6	43	-0.4714	2	7	43	0.4714	3	6	43	0.3333
3	7	43	-0.3333	11	12	43	-1.0000	2	7	44	-0.4714	2	10	44	-0.4714
3	7	44	0.3333	3	10	44	0.3333	11	14	44	1.0000	2	7	45	-0.4714
2	10	45	0.9428	3	7	45	0.3333	3	10	45	-0.6667	2	7	46	-0.4714
2	10	46	-0.4714	3	7	46	0.3333	3	10	46	0.3333	11	14	46	-1.0000
1	5	47	1.0000	1	8	48	0.8165	1	8	49	-0.4082	1	9	49	0.7071
1	8	50	-0.4082	1	9	50	-0.7071	5	8	51	0.8165	5	8	52	-0.4082
5	9	52	0.7071	5	8	53	-0.4082	5	9	53	-0.7071	6	6	54	-1.3333
6	7	54	0.3333	7	7	54	0.6667	6	7	55	-0.6667	6	10	55	-0.6667
7	7	55	-0.6667	7	10	55	-0.3333	6	7	56	-0.3333	6	10	56	0.6667
7	7	56	-0.3333	7	10	56	0.3333	6	6	57	0.3333	6	7	57	-0.3333
7	7	57	0.3333	12	12	57	-1.0000	6	7	58	0.3333	6	10	58	0.3333
7	7	58	-0.6667	7	10	58	-0.3333	12	14	58	1.0000	6	7	59	0.3333
6	10	59	-0.6667	7	7	59	-0.6667	7	10	59	0.6667	6	7	60	0.3333
6	10	60	0.3333	7	7	60	-0.6667	7	10	60	-0.3333	12	14	60	-1.0000
7	7	61	0.6667	7	10	61	-0.3333	10	10	61	-1.3333	7	7	62	0.3333
7	10	62	0.3333	10	10	62	0.3333	14	14	62	-1.0000	7	8	63	-0.3333
8	10	63	0.6667	7	8	64	0.1667	7	9	64	-0.2887	8	10	64	-0.3333
9	10	64	0.5773	7	8	65	0.1667	7	9	65	0.2887	8	10	65	-0.3333
9	10	65	-0.5773	8	8	66	-0.6667	8	9	66	0.5773	8	8	67	-0.6667
8	9	67	-0.5773	8	8	68	0.3333	9	9	68	-1.0000	13	15	69	1.0000
13	14	70	-1.4142	12	13	71	-1.4142								

SYMMETRIZED Z MATRIX ----------CF3-COCL

D. BRADPERT and SORT

1. Frequency Fit

For each molecule the observed and calculated frequencies are listed along with their difference and percent difference. Note that in some cases the torsional frequency fit appears poor with respect to the percent difference. This fact can be misleading since the difference itself is quite small.

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE ASYM. HCH2 STRETCH ---	3010.0	3010.7	-0.7	-0.0
2 THE SYMMETRIC CH3 STRETCH	2967.0	2966.0	1.0	0.0
3 THE C-Z STRETCH ----------	2822.0	2806.1	15.9	0.6
4 THE C=O STRETCH ----------	1743.0	1749.2	-6.2	-0.4
5 THE HCH2 DEFORMATION -----	1441.0	1436.8	4.2	0.3
6 THE CH3 UMBRELLA BEND ----	1400.0	1403.2	-3.2	-0.2
7 THE SCISSORS BEND -------	1352.0	1348.4	3.6	0.3
8 THE IN-PLANE CH3 ROCK ----	1113.0	1103.9	9.0	0.8
9 THE C-C STRETCH ----------	919.0	916.4	2.6	0.3
10 THE O=C-Z ROCK ----------	509.0	509.8	-0.8	-0.2
11 THE A'' HCH2 STRETCH -----	3010.0	3001.8	8.3	0.3
12 THE A'' HCH2 DEFORMATION -	1420.0	1427.5	-7.5	-0.5
13 THE OUT-OF-PLANE CH3 WAG	867.0	817.9	49.1	5.7
14 THE OUT-OF-PLANE WAG -----	763.0	745.6	17.4	2.3
15 THE TORSION -------------	150.0	146.8	3.2	2.1

OBSERVED AND CALCULATED FREQUENCIES OF --- CH3-COH

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE C-Z STRETCH ----------	2812.0	2806.7	5.3	0.2
2 THE ASYM. DCD2 STRETCH ---	2254.0	2239.2	14.8	0.7
3 THE SYMMETRIC CD3 STRETCH	2117.0	2132.8	-15.8	-0.7
4 THE C=O STRETCH ----------	1753.0	1740.6	12.4	0.7
5 THE SCISSORS BEND -------	1390.0	1385.9	4.1	0.3
6 THE C-C STRETCH ----------	1131.0	1146.1	-15.1	-1.3
7 THE DCD2 DEFORMATION -----	1038.0	1030.7	7.3	0.7
8 THE CD3 UMBRELLA BEND ----	960.0	983.7	-23.7	-2.5
9 THE IN-PLANE CD3 ROCK ----	774.0	739.8	34.2	4.4
10 THE O=C-Z ROCK ----------	443.0	451.5	-8.5	-1.9
11 THE A'' DCD2 STRETCH -----	2223.0	2226.3	-3.3	-0.2
12 THE A'' DCD2 DEFORMATION -	1028.0	1033.0	-5.0	-0.5
13 THE OUT-OF-PLANE WAG -----	761.0	757.7	3.3	0.4
14 THE OUT-OF-PLANE CD3 WAG	626.0	614.1	11.9	1.9
15 THE TORSION ------------	122.0	117.3	4.7	3.8

OBSERVED AND CALCULATED FREQUENCIES OF --- CD3-COH

	ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1	THE ASYM. HCH2 STRETCH ---	3014.0	3010.5	3.5	0.1
2	THE SYMMETRIC CH3 STRETCH	2970.0	2965.6	4.4	0.1
3	THE C-Z STRETCH ----------	2071.0	2066.3	4.7	0.2
4	THE C=O STRETCH ----------	1743.0	1716.7	26.3	1.5
5	THE HCH2 DEFORMATION -----	1442.0	1435.3	6.7	0.5
6	THE CH3 UMBRELLA BEND ----	1353.0	1370.1	-17.1	-1.3
7	THE C-C STRETCH ----------	1109.0	1103.1	5.9	0.5
8	THE IN-PLANE CH3 ROCK ----	1043.0	1060.1	-17.1	-1.6
9	THE SCISSORS BEND -------	849.0	875.2	-26.2	-3.1
10	THE O=C-Z ROCK ----------	500.0	503.8	-3.8	-0.8
11	THE A'' HCH2 STRETCH -----	3014.0	3001.8	12.3	0.4
12	THE A'' HCH2 DEFORMATION -	1420.0	1426.1	-6.1	-0.4
13	THE OUT-OF-PLANE CH3 WAG	802.0	816.1	-14.1	-1.8
14	THE OUT-OF-PLANE WAG -----	668.0	627.9	40.1	6.0
15	THE TORSION -------------	145.0	140.4	4.6	3.1

OBSERVED AND CALCULATED FREQUENCIES OF --- CH3-COD

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE ASYM. DCD2 STRETCH ---	2265.0	2238.8	26.3	1.2
2 THE SYMMETRIC CD3 STRETCH	2130.0	2134.5	-4.5	-0.2
3 THE C-Z STRETCH ----------	2060.0	2063.9	-3.9	-0.2
4 THE C=O STRETCH ----------	1737.0	1710.5	26.5	1.5
5 THE C-C STRETCH ----------	1151.0	1165.8	-14.8	-1.3
6 THE DCD2 DEFORMATION -----	1045.0	1033.3	11.7	1.1
7 THE CD3 UMBRELLA BEND ----	1028.0	1029.1	-1.1	-0.1
8 THE SCISSORS BEND -------	938.0	961.9	-23.9	-2.5
9 THE IN-PLANE CD3 ROCK ----	747.0	727.9	19.1	2.6
10 THE O=C-Z ROCK ----------	436.0	446.4	-10.4	-2.4
11 THE A'' DCD2 STRETCH -----	2225.0	2226.3	-1.3	-0.1
12 THE A'' DCD2 DEFORMATION -	1028.0	1029.1	-1.1	-0.1
13 THE OUT-OF-PLANE WAG -----	676.0	681.9	-5.9	-0.9
14 THE OUT-OF-PLANE CD3 WAG	573.0	570.5	2.5	0.4
15 THE TORSION -------------	116.0	110.2	5.8	5.0

OBSERVED AND CALCULATED FREQUENCIES OF --- CD3-COD

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE ASYM. HCH2 STRETCH ---	3043.0	3070.3	-27.3	-0.9
2 THE SYMMETRIC CH3 STRETCH	2953.0	2962.7	-9.7	-0.3
3 THE C=O STRETCH ----------	1870.0	1875.3	-5.3	-0.3
4 THE HCH2 DEFORMATION -----	1437.0	1468.3	-31.3	-2.2
5 THE CH3 UMBRELLA BEND ----	1378.0	1372.4	5.6	0.4
6 THE C-Z STRETCH ----------	1187.0	1210.2	-23.2	-2.0
7 THE IN-PLANE CH3 ROCK ----	1000.0	1001.4	-1.4	-0.1
8 THE C-C STRETCH ----------	826.0	824.7	1.3	0.2
9 THE SCISSORS BEND -------	598.0	602.4	-4.4	-0.7
10 THE O=C-Z ROCK ----------	420.0	420.3	-0.3	-0.1
11 THE A'' HCH2 STRETCH -----	3004.0	3008.1	-4.1	-0.1
12 THE A'' HCH2 DEFORMATION -	1440.0	1448.7	-8.7	-0.6
13 THE OUT-OF-PLANE CH3 WAG	1053.0	1070.1	-17.1	-1.6
14 THE OUT-OF-PLANE WAG -----	567.0	572.9	-5.9	-1.0
15 THE TORSION -------------	122.0	119.1	2.9	2.4

OBSERVED AND CALCULATED FREQUENCIES OF --- CH3-COF

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE ASYM. DCD2 STRETCH ---	2274.0	2272.0	2.0	0.1
2 THE SYMMETRIC CD3 STRETCH	2144.0	2138.9	5.1	0.2
3 THE C=O STRETCH ----------	1869.0	1872.1	-3.1	-0.2
4 THE C-Z STRETCH ----------	1204.0	1192.3	11.8	1.0
5 THE CD3 UMBRELLA BEND ----	1149.0	1127.5	21.5	1.9
6 THE DCD2 DEFORMATION -----	1030.0	1015.8	14.2	1.4
7 THE IN-PLANE CD3 ROCK ----	839.0	819.0	20.0	2.4
8 THE C-C STRETCH ----------	778.0	772.3	5.7	0.7
9 THE SCISSORS BEND -------	577.0	572.5	4.5	0.8
10 THE O=C-Z ROCK ----------	378.0	379.8	-1.8	-0.5
11 THE A'' DCD2 STRETCH -----	2243.0	2239.0	4.0	0.2
12 THE A'' DCD2 DEFORMATION -	1057.0	1068.6	-11.6	-1.1
13 THE OUT-OF-PLANE CD3 WAG	915.0	909.8	5.2	0.6
14 THE OUT-OF-PLANE WAG -----	491.0	478.6	12.4	2.5
15 THE TORSION -------------	93.0	89.3	3.7	4.0

OBSERVED AND CALCULATED FREQUENCIES OF --- CD3-COF

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE ASYM. HCH2 STRETCH ---	3029.0	3025.3	3.7	0.1
2 THE SYMMETRIC CH3 STRETCH	2934.0	2923.6	10.3	0.4
3 THE C=O STRETCH ----------	1822.0	1833.2	-11.2	-0.6
4 THE HCH2 DEFORMATION -----	1432.0	1472.1	-40.1	-2.8
5 THE CH3 UMBRELLA BEND ----	1370.0	1349.5	20.5	1.5
6 THE IN-PLANE CH3 RCCK ----	1109.0	1098.7	10.3	0.9
7 THE C-C STRETCH ----------	958.0	975.4	-17.4	-1.8
8 THE C-Z STRETCH ----------	608.0	609.5	-1.5	-0.3
9 THE SCISSORS BEND -------	436.0	440.9	-4.9	-1.1
10 THE O=C-Z ROCK ----------	348.0	344.6	3.4	1.0
11 THE A'' HCH2 STRETCH -----	3029.0	3030.4	-1.4	-0.0
12 THE A'' HCH2 DEFORMATICN -	1432.0	1430.9	1.1	0.1
13 THE OUT-OF-PLANE CH3 WAG	1029.0	1030.2	-1.2	-0.1
14 THE OUT-OF-PLANE WAG -----	514.0	525.1	-11.1	-2.2
15 THE TORSION ------------	137.0	146.9	-9.9	-7.2

OBSERVED ANC CALCULATEC FREQUENCIES OF --- CH3-CCCL

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE ASYM. DCD2 STRETCH ---	2280.0	2258.1	21.9	1.0
2 THE SYMMETRIC CD3 STRETCH	2104.0	2096.2	7.8	0.4
3 THE C=O STRETCH ----------	1820.0	1826.8	-6.8	-0.4
4 THE DCD2 DEFORMATION -----	1132.0	1093.1	38.9	3.4
5 THE CD3 UMBRELLA BEND ----	1040.0	1061.0	-21.0	-2.0
6 THE C-C STRETCH ----------	962.0	978.4	-16.4	-1.7
7 THE IN-PLANE CD3 ROCK ----	818.0	834.7	-16.7	-2.0
8 THE C-Z STRETCH ----------	563.0	570.8	-7.8	-1.4
9 THE SCISSORS BEND -------	437.0	426.6	10.4	2.4
10 THE O=C-Z ROCK ----------	317.0	308.8	8.2	2.6
11 THE A'' DCD2 STRETCH -----	2280.0	2263.5	16.5	0.7
12 THE A'' DCD2 DEFORMATION -	1040.0	1015.6	24.4	2.3
13 THE OUT-OF-PLANE CD3 WAG	877.0	842.8	34.2	3.9
14 THE OUT-OF-PLANE WAG -----	498.0	482.0	16.0	3.2
15 THE TORSION -------------	102.0	106.0	-4.0	-4.0

OBSERVED AND CALCULATED FREQUENCIES OF --- CD3-COCL

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE ASYM. HCH2 STRETCH ---	3026.0	3030.3	-4.3	-0.1
2 THE SYMMETRIC CH3 STRETCH	2945.0	2936.8	8.2	0.3
3 THE C=O STRETCH ----------	1821.0	1824.5	-3.5	-0.2
4 THE HCH2 DEFORMATION -----	1425.0	1439.5	-14.5	-1.0
5 THE CH3 UMBRELLA BEND ----	1362.0	1348.1	13.9	1.0
6 THE IN-PLANE CH3 ROCK ----	1092.0	1087.5	4.5	0.4
7 THE C-C STRETCH ----------	942.0	945.5	-3.5	-0.4
8 THE C-Z STRETCH ----------	570.0	571.0	-1.0	-0.2
9 THE SCISSORS BEND -------	347.0	345.7	1.3	0.4
10 THE O=C-Z ROCK ----------	304.0	311.4	-7.4	-2.4
11 THE A'' HCH2 STRETCH -----	3025.0	3026.8	-1.8	-0.1
12 THE A'' HCH2 DEFORMATION -	1438.0	1443.1	-5.1	-0.4
13 THE OUT-OF-PLANE CH3 WAG	1021.0	1039.8	-18.8	-1.8
14 THE OUT-OF-PLANE WAG -----	492.0	490.4	1.6	0.3
15 THE TORSION -------------	137.0	142.4	-5.4	-4.0

OBSERVED AND CALCULATED FREQUENCIES OF --- CH3-COBR

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE ASYM. DCD2 STRETCH ---	2275.0	2258.3	16.6	0.7
2 THE SYMMETRIC CD3 STRETCH	2105.0	2107.8	-2.8	-0.1
3 THE C=O STRETCH ----------	1825.0	1817.8	7.2	0.4
4 THE DCD2 DEFORMATION -----	1122.0	1119.6	2.4	0.2
5 THE CD3 UMBRELLA BEND ----	1010.0	1023.9	-13.9	-1.4
6 THE IN-PLANE CD3 ROCK ----	951.0	951.0	-0.0	-0.0
7 THE C-C STRETCH ----------	808.0	804.7	3.3	0.4
8 THE C-Z STRETCH ----------	525.0	522.5	2.4	0.5
9 THE SCISSORS BEND -------	345.0	342.1	2.9	0.8
10 THE O=C-Z ROCK ----------	275.0	278.5	-3.5	-1.3
11 THE A'' DCD2 STRETCH -----	2275.0	2258.6	16.4	0.7
12 THE A'' DCD2 DEFORMATION -	1043.0	1026.5	16.5	1.6
13 THE OUT-OF-PLANE CD3 WAG	855.0	850.5	4.5	0.5
14 THE OUT-OF-PLANE WAG -----	440.0	448.2	-8.2	-1.9
15 THE TORSION -------------	101.0	102.5	-1.5	-1.5

OBSERVED AND CALCULATED FREQUENCIES OF --- CD3-COBR

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE C-Z STRETCH ----------	2864.0	2876.9	-12.9	-0.5
2 THE C=O STRETCH ----------	1788.0	1799.8	-11.8	-0.7
3 THE SCISSORS BEND -------	1384.0	1414.9	-30.9	-2.2
4 THE SYMMETRIC CF3 STRETCH	1310.0	1271.9	38.1	2.9
5 THE ASYM. FCF2 STRETCH ---	1202.0	1163.5	38.5	3.2
6 THE C-C STRETCH ----------	840.0	848.7	-8.7	-1.0
7 THE CF3 UMBRELLA BEND ----	706.0	690.6	15.3	2.2
8 THE FCF2 DEFORMATION -----	580.0	579.5	0.5	0.1
9 THE O=C-Z ROCK ----------	431.0	434.8	-3.8	-0.9
10 THE IN-PLANE CF3 ROCK ----	256.0	255.5	0.5	0.2
11 THE A'' FCF2 STRETCH -----	1183.0	1221.4	-38.4	-3.2
12 THE OUT-OF-PLANE WAG -----	958.0	859.3	98.7	10.3
13 THE A'' FCF2 DEFORMATION -	531.0	525.5	5.5	1.0
14 THE OUT-OF-PLANE CF3 WAG	322.0	362.7	-40.7	-12.7
15 THE TORSION -------------	55.0	59.9	-4.9	-8.9

OBSERVED AND CALCULATED FREQUENCIES CF --- CF3-COH

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE C-Z STRETCH ----------	2150.0	2155.1	-5.1	-0.2
2 THE C=O STRETCH ----------	1770.0	1761.6	8.4	0.5
3 THE SYMMETRIC, CF3 STRETCH	1302.0	1304.6	-2.6	-0.2
4 THE ASYM. FCF2 STRETCH ---	1244.0	1264.8	-20.8	-1.7
5 THE SCISSORS BEND -------	1033.0	999.3	33.6	3.3
6 THE C-C STRETCH ----------	811.0	794.3	16.7	2.1
7 THE CF3 UMBRELLA BEND ----	693.0	687.9	5.1	0.7
8 THE FCF2 DEFORMATION -----	580.0	576.2	3.8	0.7
9 THE O=C-Z ROCK -----------	428.0	416.4	11.6	2.7
10 THE IN-PLANE CF3 ROCK ----	253.0	255.0	-2.0	-0.8
11 THE A'' FCF2 STRETCH -----	1177.0	1219.0	-42.0	-3.6
12 THE OUT-OF-PLANE WAG -----	842.0	844.8	-2.8	-0.3
13 THE A'' FCF2 DEFORMATION -	521.0	525.5	-4.5	-0.9
14 THE OUT-OF-PLANE CF3 WAG	318.0	306.8	11.2	3.5
15 THE TORSION -------------	52.0	52.3	-0.3	-0.7

OBSERVED AND CALCULATED FREQUENCIES OF --- CF3-COD

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE C=O STRETCH ----------	1899.0	1869.9	29.1	1.5
2 THE SYMMETRIC CF3 STRETCH	1340.0	1359.7	-19.7	-1.5
3 THE ASYM. FCF2 STRETCH ---	1254.0	1274.3	-20.3	-1.6
4 THE C-Z STRETCH ----------	1099.0	1116.7	-17.7	-1.6
5 THE C-C STRETCH ----------	806.0	800.7	5.3	0.7
6 THE SCISSORS BEND -------	761.0	723.7	37.3	4.9
7 THE CF3 UMBRELLA BEND ----	692.0	660.7	31.3	4.5
8 THE FCF2 DEFORMATION -----	595.0	576.4	18.5	3.1
9 THE O=C-Z ROCK ----------	390.0	391.8	-1.8	-0.5
10 THE IN-PLANE CF3 ROCK ----	228.0	227.2	0.8	0.4
11 THE A'' FCF2 STRETCH -----	1214.0	1199.1	14.9	1.2
12 THE A'' FCF2 DEFORMATION -	519.0	537.2	-18.2	-3.5
13 THE OUT-OF-PLANE WAG -----	427.0	428.6	-1.6	-0.4
14 THE OUT-OF-PLANE CF3 WAG	242.0	241.7	0.3	0.1
15 THE TORSION -------------	50.0	58.3	-8.3	-16.6

OBSERVED AND CALCULATED FREQUENCIES OF --- CF3-COF

ASSIGNMENT	OBSERVED	CALCULATED	DIFF.	PERCENT
1 THE C=O STRETCH ----------	1811.0	1812.2	-1.2	-0.1
2 THE SYMMETRIC CF3 STRETCH	1284.0	1315.0	-31.0	-2.4
3 THE ASYM. FCF2 STRETCH ---	1240.0	1253.8	-13.8	-1.1
4 THE C-C STRETCH ----------	937.0	947.0	-10.0	-1.1
5 THE C-Z STRETCH ----------	750.0	735.3	14.7	2.0
6 THE FCF2 DEFORMATION -----	703.0	669.4	33.6	4.8
7 THE CF3 UMBRELLA BEND ----	583.0	606.8	-23.8	-4.1
8 THE SCISSORS BEND -------	511.0	496.7	14.3	2.8
9 THE O=C-Z ROCK ----------	334.0	350.3	-16.3	-4.9
10 THE IN-PLANE CF3 ROCK ----	198.0	198.0	-0.0	-0.0
11 THE A'' FCF2 STRETCH -----	1202.0	1168.0	34.0	2.8
12 THE A'' FCF2 DEFORMATION -	517.0	527.8	-10.8	-2.1
13 THE OUT-OF-PLANE WAG -----	390.0	399.3	-9.3	-2.4
14 THE OUT-OF-PLANE CF3 WAG	234.0	234.3	-0.3	-0.1
15 THE TORSION -------------	50.0	44.0	5.9	11.9

OBSERVED AND CALCULATED FREQUENCIES CF --- CF3-COCL

2. Urey-Bradley Force Field

The following table lists all of the simple valence force constants, the Urey-Bradley non-bonded repulsion force constants, and the interaction force constants for each of the seven types of molecules. Each row of the table is labeled with an abbreviation of an internal coordinate or combination of internal coordinates, in the case of the interaction force constants. The force constant numbering system corresponds with that displayed in Figure 2-3, page II-12.

		CH_3COZ				CF_3COZ		
	LABEL	H	F	CL	BR	H	F	CL
1	K (C=O)	10.500	12.100	11.950	11.950	12.300	12.600	12.100
2	K (C-Z)	3.590	3.500	2.400	2.400	4.250	3.500	3.000
3	K (C-C)	3.293	3.100	3.000	3.000	1.500	2.000	2.000
4	K (C-X)	4.650	4.720	4.550	4.570	5.100	5.230	5.100
5	K(C-X)'	4.650	4.620	4.600	4.650	5.200	5.200	5.100
6	H(CCO)	1.040	0.420	0.420	0.420	0.900	0.900	0.800
7	H (OCZ)	0.471	0.870	0.442	0.442	0.500	0.500	0.400
8	H (CCZ)	0.230	0.500	0.630	0.530	0.550	0.630	0.630
9	H (XCX)	0.471	0.550	0.474	0.474	0.450	0.650	0.600
10	H(XCX)'	0.471	0.590	0.434	0.434	0.350	0.800	0.650
11	H (XCC)	0.340	0.340	0.470	0.470	0.600	0.480	0.450
12	H(XCC)'	0.528	0.408	0.510	0.428	0.500	0.450	0.450
13	H (WAG)	1.050	0.570	0.480	0.430	0.750	0.160	0.155
14	H (TORS)	0.040	0.100	0.015	0.015	0.050	0.130	0.150
15	F (X--X)	0.110	0.020	0.090	0.090	2.200	2.000	2.000
16	F(X--X)'	0.110	0.100	0.070	0.070	2.200	2.300	2.200
17	F (X--C)	0.301	0.451	0.371	0.371	2.100	1.250	1.200
18	F (O--C)	0.349	0.349	0.200	0.200	0.050	0.300	0.300
19	F(C-Z)	0.600	0.700	0.270	0.300	0.250	0.270	0.270
20	F(O--Z)	0.630	1.150	0.860	0.360	0.100	1.100	0.900
21	C (X--O)	-0.060	0.0	0.010	0.010	-0.070	0.350	0.230
22	C(X--X')	0.0	0.030	0.080	0.080	0.100	-0.080	0.0
23	MOL.TEN.	0.051	0.049	0.070	0.070	0.600	0.600	0.600

THE UREY-BRADLEY FORCE CONSTANTS

		CH_3COZ				CF_3COZ		
	LABEL	H	F	CL	BR	H	F	CL
24	CC..CX'	0.0	0.0	0.0	0.0	-0.050	-0.100	-0.100
25	CC..CX	0.0	0.0	0.0	0.0	-0.250	-0.250	-0.250
26	CC..CO	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27	CC..CZ	0.0	-0.100	-0.070	-0.050	-0.100	-0.050	-0.050
28	CC..XCX'	0.0	0.200	0.070	-0.130	-0.400	-0.200	-0.250
29	CC..XCX	0.0	0.0	0.020	0.080	-0.250	-0.150	-0.250
30	CC..CCX	0.050	0.0	0.130	0.130	-0.100	-0.150	-0.050
31	CC..CCX'	0.0	0.0	-0.050	0.0	0.0	-0.150	-0.050
32	CC..OCZ	0.0	0.0	-0.050	-0.050	-0.160	-0.050	-0.100
33	CC..OCC	0.0	0.200	0.050	0.050	0.200	0.200	0.200
34	CC..ZCC	0.0	0.0	0.0	0.0	0.200	0.200	0.200
35	CX'..CH	0.0	0.010	-0.030	-0.020	0.100	0.300	0.250
36	CX'.XCX'	0.0	0.0	0.0	0.0	-0.200	-0.200	-0.200
37	CX'..XCX	0.0	0.0	0.0	0.0	-0.100	-0.250	-0.200
38	CX'..CCX	0.0	0.0	0.0	0.0	0.300	0.250	0.250
39	CX'.CCX'	0.0	0.0	-0.250	-0.200	0.0	0.0	0.100
40	CX..CX5	0.0	0.150	0.010	0.010	0.400	0.370	0.400
41	CX..XCX'	0.0	0.0	0.0	0.0	-0.100	-0.030	-0.100
42	CX..XCX	0.0	0.050	0.180	0.130	-0.400	-0.200	-0.300
43	CX4.XCX4	0.0	-0.050	-0.130	-0.130	-0.300	-0.300	-0.300
44	CX4.CCX5	0.0	0.0	0.0	0.0	0.050	0.100	0.100
45	CX4.CCX'	0.0	0.0	0.0	0.0	0.200	0.030	0.100
46	CX4.CCX4	0.0	0.0	0.0	0.0	0.150	0.200	0.100
47	CO..CZ	0.0	0.0	0.0	0.0	0.0	0.0	0.0
48	CO..OCZ	0.0	0.0	0.0	0.0	0.200	0.0	0.200
49	CO..OCC	0.0	0.0	0.0	0.0	0.200	0.0	0.200
50	CO..ZCC	0.0	0.0	0.0	0.0	-0.200	0.0	-0.200
51	CZ..OCZ	0.0	0.0	0.100	0.0	0.0	0.250	0.350
52	CZ..OCC	0.0	0.0	0.0	0.0	0.0	-0.200	-0.350
53	CZ..ZCC	0.0	0.0	0.0	0.0	0.0	0.100	0.100
54	XCX'.XCX	0.0	0.080	-0.020	0.0	0.050	-0.400	-0.150
55	XCX'.CCX	0.0	0.110	0.025	0.030	0.100	-0.200	0.0
56	XCX'CCX'	0.0	0.020	0.080	0.0	0.200	0.100	0.250
57	XCX..XCX	0.0	0.050	0.020	0.020	0.370	0.400	0.400
58	XCX..CCX	0.0	-0.010	-0.020	-0.020	0.160	0.050	0.0
59	XCX.CCX'	0.0	-0.005	0.050	0.030	0.015	0.015	0.015
60	XCX5CCX4	0.0	0.010	0.030	0.030	0.200	0.050	0.100
61	CCX.CCX'	0.0	-0.010	0.060	0.060	0.500	0.150	0.200
62	CCX5CCX4	0.050	0.050	0.030	0.030	-0.300	-0.100	-0.050
63	CCX'.OCZ	0.0	0.200	0.100	0.0	-0.130	0.050	-0.100
64	CCX'.OCC	0.0	-0.050	-0.140	-0.130	-0.080	-0.080	-0.080
65	CCX'.ZCC	0.138	0.138	0.140	0.130	-0.100	-0.100	-0.100
66	OCZ..OCC	0.0	0.100	0.0	0.0	0.230	0.050	0.050
67	OCZ..ZCC	0.0	-0.140	0.0	0.0	0.160	0.160	0.100
68	OCC..ZCC	0.0	-0.100	0.0	0.0	-0.400	-0.200	-0.400
69	WAG.TORS	0.030	0.200	0.030	0.050	0.170	0.100	0.090
70	M.RK.WAG	0.050	-0.135	-0.020	0.010	-0.250	0.240	0.250
71	M.OF.WAG	0.080	0.065	0.040	0.030	0.0	0.050	0.020

THE INTERACTION FORCE CONSTANTS

3. Symmetrized F Matrix

The symmetrized F matrix is formed by the operation of the symmetrized Z matrix on the Urey-Bradley force field. The F matrix is given in terms of its two symmetry blocks. The symmetry coordinate labels of the rows and columns are listed above the appropriate symmetry blocks.

```
 1 THE ASYM. HCH2 STRETCH ---
 2 THE SYMMETRIC CH3 STRETCH
 3 THE C-Z STRETCH ----------
 4 THE C=C STRETCH ----------
 5 THE HCH2 DEFORMATION -----
 6 THE CH3 UMBRELLA BEND ----
 7 THE SCISSORS BEND -------
 8 THE IN-PLANE CH3 ROCK ----
 9 THE C-C STRETCH ----------
10 THE O=C-Z ROCK -----------
-----------------------------
```

1	4.8570	0.0135	0.0	0.0186	-0.0510	-0.0039	-0.0023	0.1227	0.0143	-0.0040
2	0.0135	5.0763	0.0	-0.0547	0.C	-0.0119	0.0156	0.0056	0.3045	0.0271
3	0.0	0.0	4.3911	0.4818	0.0	0.0	0.1185	0.0	0.4493	0.1918
4	0.0186	-0.0547	0.4818	11.1093	0.0	0.0416	0.2029	0.0024	0.1576	-0.0689
5	-0.0510	0.0	0.0	0.0	0.5130	0.0	0.0	0.0208	0.0	0.0
6	-0.0039	-0.0119	0.0	0.0416	C.0	0.5222	0.0076	-0.0357	-0.2093	-0.0665
7	-0.0023	0.0156	0.1185	0.2029	0.0	0.0076	0.7821	-0.0298	-0.1689	0.1559
8	0.1227	0.0056	0.0	0.0024	0.0208	-0.0357	-0.0298	0.6010	-0.0666	0.1077
9	0.0143	0.3045	0.4493	C.1576	C.0	-0.2093	-0.1689	-0.0666	4.5858	0.1774
10	-0.0040	0.0271	0.1918	-0.0689	0.C	-0.0665	0.1559	0.1077	0.1774	0.8347

```
11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

11	4.8378	-0.C510	-C.1148	0.0	-0.0130
12	-0.0510	C.5130	-0.0208	-0.1131	0.0
13	-0.1148	-C.0208	0.4295	-0.0707	0.0203
14	0.0	-C.1131	-0.0707	1.0500	0.0300
15	-0.0130	0.0	0.0203	0.0300	0.0291

F MATRIX FOR THE MOLECULE CH3-COH

```
 1 THE C-Z STRETCH ----------
 2 THE ASYM. DCD2 STRETCH ---
 3 THE SYMMETRIC CD3 STRETCH
 4 THE C=O STRETCH ----------
 5 THE SCISSORS BEND -------
 6 THE C-C STRETCH ----------
 7 THE DCD2 DEFORMATION -----
 8 THE CD3 UMBRELLA BEND ----
 9 THE IN-PLANE CD3 ROCK ----
10 THE O=C-Z ROCK -----------
-----------------------------
```

1	4.3911	0.0	0.0	0.4818	0.1185	0.4493	0.0	0.0	0.0	0.1918
2	0.0	4.8570	0.0135	0.0186	-0.0023	0.0143	-0.0510	-0.0039	0.1227	-0.0040
3	0.0	0.0135	5.0763	-0.0547	0.0156	0.3045	0.0	-0.0119	0.0056	0.0271
4	0.4818	0.0186	-0.0547	11.1093	0.2029	0.1576	0.0	0.0416	0.0024	-0.0689
5	0.1185	-0.0023	0.0156	0.2029	0.7821	-0.1689	0.0	0.0076	-0.0298	0.1559
6	0.4493	0.0143	0.3045	0.1576	-0.1689	4.5858	0.0	-0.2093	-0.0666	0.1774
7	0.0	-0.0510	0.0	0.0	0.0	0.0	0.5130	0.0	0.0208	0.0
8	0.0	-0.0039	-0.0119	0.0416	0.0076	-0.2093	0.0	0.5222	-0.0357	-0.0665
9	0.0	0.1227	0.0056	0.0024	-0.0298	-0.0666	0.0208	-0.0357	0.6010	0.1077
10	0.1918	-0.0040	0.0271	-0.0689	0.1559	0.1774	0.0	-0.0665	0.1077	0.8347

```
11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CD3 WAG
15 THE TORSION --------------
-----------------------------
```

11	4.8378	-0.0510	0.0	-0.1148	-0.0130
12	-0.0510	0.5130	-0.1131	-0.0208	0.0
13	0.0	-0.1131	1.0500	-0.0707	0.0300
14	-0.1148	-0.0208	-0.0707	0.4295	0.0203
15	-0.0130	0.0	0.0300	0.0203	0.0291

F MATRIX FOR THE MOLECULE CD3-COH

```
 1 THE ASYM. HCH2 STRETCH ---
 2 THE SYMMETRIC CH3 STRETCH
 3 THE C-Z STRETCH ----------
 4 THE C=C STRETCH ----------
 5 THE HCH2 DEFORMATION -----
 6 THE CH3 UMBRELLA BEND ----
 7 THE C-C STRETCH ----------
 8 THE IN-PLANE CH3 ROCK ----
 9 THE SCISSORS BEND -------
10 THE C=C-Z ROCK ----------
-----------------------------
```

```
 1  4.8570 0.0135 0.0    0.0186-0.0510-0.0039 0.0143 0.1227-0.0023-0.0040
 2  0.0135 5.0763 0.0   -0.0547 0.0   -0.0119 0.3045 0.0056 0.0156 0.0271
 3  0.0    0.0    4.3911 0.4818 0.0    0.0    0.4493 0.0    0.1185 0.1918
 4  0.0186-0.0547 0.481811.1093 0.C    0.0416 0.1576 0.0024 0.2029-0.0689
 5 -0.0510 0.0    0.0    0.0    0.5130 0.0    0.0    0.0208 0.0    0.0
 6 -0.0039-0.0119 0.0    0.0416 0.0    0.5222-0.2093-0.0357 0.0076-0.0665
 7  0.0143 0.3045 0.4493 0.1576 C.0   -0.2093 4.5858-0.0666-0.1689 0.1774
 8  0.1227 0.0056 0.0    0.0024 0.0208-0.0357-0.0666 0.6010-0.0298 0.1077
 9 -0.0023 0.0156 0.1185 0.2029 0.0    0.0076-0.1689-0.0298 0.7821 0.1559
10 -0.0040 0.0271 0.1918-0.0689 0.0   -0.0665 0.1774 0.1077 0.1559 0.8347
-------------------------------------------------------------------------
```

```
11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

```
11  4.8378-0.0510-C.1148 0.0   -0.0130
12 -0.0510 C.5130-0.0208-0.1131 0.0
13 -0.1148-0.0208 0.4295-0.0707 0.0203
14  0.0   -0.1131-C.0707 1.0500 0.0300
15 -0.0130 0.0    0.0203 0.0300 0.0291
---------------------------------------
```

F MATRIX FOR THE MOLECULE CH3-COD

```
 1 THE ASYM. DCD2 STRETCH ---
 2 THE SYMMETRIC CD3 STRETCH
 3 THE C-Z STRETCH ----------
 4 THE C=O STRETCH ----------
 5 THE C-C STRETCH ----------
 6 THE DCD2 DEFORMATION -----
 7 THE CD3 UMBRELLA BEND ----
 8 THE SCISSORS BEND -------
 9 THE IN-PLANE CD3 ROCK ----
10 THE O=C-Z ROCK -----------
-----------------------------
```

1	4.8570	0.0135	0.0	0.0186	0.0143	-0.0510	-0.0039	-0.0023	0.1227	-0.0040
2	0.0135	5.0763	0.0	-0.0547	0.3045	0.0	-0.0119	0.0156	0.0056	0.0271
3	0.0	0.0	4.3911	0.4818	0.4493	0.0	0.0	0.1185	0.0	0.1918
4	0.0186	-0.0547	0.4818	11.1093	0.1576	0.0	0.0416	0.2029	0.0024	-0.0689
5	0.0143	0.3045	0.4493	0.1576	4.5858	0.0	-0.2093	-0.1689	-0.0666	0.1774
6	-0.0510	0.0	0.0	0.0	0.0	0.5130	0.0	0.0	0.0208	0.0
7	-0.0039	-0.0119	0.0	0.0416	-0.2093	0.0	0.5222	0.0076	-0.0357	-0.0665
8	-0.0023	0.0156	0.1185	0.2029	-0.1689	0.0	0.0076	0.7821	-0.0298	0.1559
9	0.1227	0.0056	0.0	0.0024	-0.0666	0.0208	-0.0357	-0.0298	0.6010	0.1077
10	-0.0040	0.0271	0.1918	-0.0689	0.1774	0.0	-0.0665	0.1559	0.1077	0.8347

```
11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CD3 WAG
15 THE TORSION --------------
-----------------------------
```

11	4.8378	-0.0510	0.0	-0.1148	-0.0130
12	-0.0510	0.5130	-0.1131	-0.0208	0.0
13	0.0	-0.1131	1.0500	-0.0707	0.0300
14	-0.1148	-0.0208	-0.0707	0.4295	0.0203
15	-0.0130	0.0	0.0300	0.0203	0.0291

F MATRIX FOR THE MOLECULE CD3-COD

```
 1 THE ASYM. HCH2 STRETCH ---
 2 THE SYMMETRIC CH3 STRETCH
 3 THE C=C STRETCH ----------
 4 THE HCH2 DEFORMATION -----
 5 THE CH3 UMBRELLA BEND ----
 6 THE C-Z STRETCH ----------
 7 THE IN-PLANE CH3 ROCK ----
 8 THE C-C STRETCH ----------
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK -----------
-----------------------------
```

```
 1  4.9715-0.1627 0.0   -0.0339-0.0091-0.0077 0.2059-0.0055 0.0041-0.0072
 2 -0.1627 5.1584 0.0    0.0349-0.1174 0.0108-0.0047 0.5491-0.0058 0.0101
 3  0.0    0.0   13.1648 0.0    0.0    0.9003 0.0    0.2871 0.3734-0.1082
 4 -0.0339 0.0349 0.0    0.5122-0.0459 0.0   -0.0375 0.1633 0.0    0.0
 5 -0.0091-0.1174 0.0   -0.0459 0.5996-0.0124-0.0232-0.2663-0.0437-0.0686
 6 -0.0077 0.0108 0.9003 0.0   -0.0124 4.8232-0.0124 0.4276 0.2972 0.3001
 7  0.2059-0.0047 0.0   -0.0375-0.0232-0.0124 0.6967-0.0225 0.1123 0.0942
 8 -0.0055 0.5491 0.2871 0.1633-0.2663 0.4276-0.0225 4.9218-0.3509 0.0802
 9  0.0041-0.0058 0.3734 0.0   -0.0437 0.2972 0.1123-0.3509 1.2408-0.2909
10 -0.0072 0.0101-0.1082 0.0   -0.0686 0.3001 0.0942 0.0802-0.2909 0.9515
-----------------------------------------------------------------------
```

```
11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

```
11  4.8085 0.0907-0.2126 0.0   -0.0045
12  0.0907 0.4996-0.0393-0.0919 0.0
13 -0.2126-0.0393 0.5960 0.1909 0.0193
14  0.0   -0.0919 0.1909 0.5700 0.2000
15 -0.0045 0.0    0.0193 0.2000 0.1085
-------------------------------------
```

F MATRIX FOR THE MOLECULE CH3-COF

```
 1 THE ASYM. DCD2 STRETCH ---
 2 THE SYMMETRIC CD3 STRETCH
 3 THE C=O STRETCH ----------
 4 THE C-Z STRETCH ----------
 5 THE CD3 UMBRELLA BEND ----
 6 THE CCD2 DEFORMATION -----
 7 THE IN-PLANE CD3 ROCK ----
 8 THE C-C STRETCH ----------
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------
-----------------------------
```

1	4.9715	-0.1627	0.0	-0.0077	-0.0091	-0.0339	0.2059	-0.0055	0.0041	-0.0072
2	-0.1627	5.1584	0.0	0.0108	-0.1174	0.0349	-0.0047	0.5491	-0.0058	0.0101
3	0.0	0.0	13.1648	0.9003	0.0	0.0	0.0	0.2871	0.3734	-0.1082
4	-0.0077	0.0108	0.9003	4.8232	-0.0124	0.0	-0.0124	0.4276	0.2972	0.3001
5	-0.0091	-0.1174	0.0	-0.0124	0.5996	-0.0459	-0.0232	-0.2663	-0.0437	-0.0686
6	-0.0339	0.0349	0.0	0.0	-0.0459	0.5122	-0.0375	0.1633	0.0	0.0
7	0.2059	-0.0047	0.0	-0.0124	-0.0232	-0.0375	0.6967	-0.0225	0.1123	0.0942
8	-0.0055	0.5491	0.2871	0.4276	-0.2663	0.1633	-0.0225	4.9218	-0.3509	0.0802
9	0.0041	-0.0058	0.3734	0.2972	-0.0437	0.0	0.1123	-0.3509	1.2408	-0.2909
10	-0.0072	0.0101	-0.1082	0.3001	-0.0686	0.0	0.0942	0.0802	-0.2909	0.9515

```
11 THE A'' DCD2 STRETCH -----
12 THE A'' CCD2 DEFORMATION -
13 THE OUT-OF-PLANE CD3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

11	4.8085	0.0907	-0.2126	0.0	-0.0045
12	0.0907	0.4996	-0.0393	-0.0919	0.0
13	-0.2126	-0.0393	0.5960	0.1909	0.0193
14	0.0	-0.0919	0.1909	0.5700	0.2000
15	-0.0045	0.0	0.0193	0.2000	0.1085

F MATRIX FOR THE MOLECULE CD3-COF

```
 1 THE ASYM. HCH2 STRETCH ---
 2 THE SYMMETRIC CH3 STRETCH
 3 THE C=O STRETCH ----------
 4 THE HCH2 DEFORMATION -----
 5 THE CH3 UMBRELLA BEND ----
 6 THE IN-PLANE CH3 ROCK ----
 7 THE C-C STRETCH ----------
 8 THE C-Z STRETCH ----------
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------
-----------------------------
```

```
 1  4.8650 0.0133-0.0030-0.0187 0.0733 0.0055-0.0227-0.0201 0.0104-0.0170
 2  0.0133 4.9528 0.0093-0.0323 0.0127-0.1229 0.4838 0.0284-0.0167 0.0205
 3 -0.0030 0.009312.6401 0.0   -0.0072-0.0004 0.1843 0.6557 0.2908-0.0704
 4 -0.0187-0.0323 0.0    0.5025-0.0532 0.0352 0.0408 0.0    0.0    0.0
 5  0.0733 0.0127-0.0072-0.0532 0.5540 0.0451-0.3639-0.0392-0.0055-0.1207
 6  0.0055-0.1229-0.0004 0.0352 0.0451 0.6718-0.1902-0.0392 0.0895 0.1131
 7 -0.0227 0.4838 0.1843 0.0408-0.3639-0.1902 4.3047 0.2246-0.2406 0.1104
 8 -0.0201 0.0284 0.6557 0.0   -0.0392-0.0392 0.2246 3.3751 0.3864 0.2167
 9  0.0104-0.0167 0.2908 0.0   -0.0055 0.0895-0.2406 0.3864 0.9533-0.1765
10 -0.0170 0.0205-0.0704 0.0   -0.1207 0.1131 0.1104 0.2167-0.1765 0.8430
```

```
11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

```
11  4.7940 0.2684-0.1793 0.0    0.0051
12  0.2684 0.4822-0.0785-0.0566 0.0
13 -0.1793-0.0785 0.7254 0.0283-0.0557
14  0.0   -0.0566 0.0283 0.4800 0.0300
15  0.0051 0.0   -0.0557 0.0300 0.0460
---------------------------------------
```

F MATRIX FOR THE MOLECULE CH3-COCL

```
 1 THE ASYM. DCD2 STRETCH ---
 2 THE SYMMETRIC CD3 STRETCH
 3 THE C=C STRETCH ----------
 4 THE DCD2 DEFORMATION -----
 5 THE CD3 UMBRELLA BEND ----
 6 THE C-C STRETCH ----------
 7 THE IN-PLANE CD3 ROCK ----
 8 THE C-Z STRETCH ----------
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK -----------
-----------------------------
```

1	4.8650	0.0133	-0.0030	-0.0187	0.0733	-0.0227	0.0055	-0.0201	0.0104	-0.0170
2	0.0133	4.9528	0.0093	-0.0323	0.0127	0.4838	-0.1229	0.0284	-0.0167	0.0205
3	-0.0030	0.0093	12.6401	0.0	-0.0072	0.1843	-0.0004	0.6557	0.2908	-0.0704
4	-0.0187	-0.0323	0.0	0.5025	-0.0532	0.0408	0.0352	0.0	0.0	0.0
5	0.0733	0.0127	-0.0072	-0.0532	0.5540	-0.3639	0.0451	-0.0392	-0.0055	-0.1207
6	-0.0227	0.4838	0.1843	0.0408	-0.3639	4.3047	-0.1902	0.2246	-0.2406	0.1104
7	0.0055	-0.1229	-0.0004	0.0352	0.0451	-0.1902	0.6718	-0.0392	0.0895	0.1131
8	-0.0201	0.0284	0.6557	0.0	-0.0392	0.2246	-0.0392	3.3751	0.3864	0.2167
9	0.0104	-0.0167	0.2908	0.0	-0.0055	-0.2406	0.0895	0.3864	0.9533	-0.1765
10	-0.0170	0.0205	-0.0704	0.0	-0.1207	0.1104	0.1131	0.2167	-0.1765	0.8430

```
11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE CD3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

11	4.7940	0.2684	-0.1793	0.0	0.0051
12	0.2684	0.4822	-0.0785	-0.0566	0.0
13	-0.1793	-0.0785	0.7254	0.0283	-0.0557
14	0.0	-0.0566	0.0283	0.4800	0.0300
15	0.0051	0.0	-0.0557	0.0300	0.0460

F MATRIX FOR THE MOLECULE CD3-COCL

```
     1 THE ASYM. HCH2 STRETCH ---
     2 THE SYMMETRIC CH3 STRETCH
     3 THE C=O STRETCH ----------
     4 THE HCH2 DEFORMATION -----
     5 THE CH3 UMBRELLA BEND ----
     6 THE IN-PLANE CH3 ROCK ----
     7 THE C-C STRETCH ----------
     8 THE C-Z STRETCH ----------
     9 THE SCISSORS BEND -------
    10 THE O=C-Z ROCK -----------
   ------------------------------
```

```
 1  4.8910 0.0331-0.0030-0.0354 0.0723 0.0378-0.0205-0.0192 0.0097-0.0158
 2  0.0331 4.9948 0.0093-0.0087-0.0212-0.0978 0.4806 0.0272-0.0158 0.0188
 3 -0.0030 0.009312.3247 0.0   -0.0072-0.0004 0.1843 0.2721 0.0963-0.0704
 4 -0.0354-0.0087 0.0    0.4758-0.0298-0.0081-0.1715 0.0    0.0    0.0
 5  0.0723-0.0212-0.0072-0.0298 0.5901 0.0305-0.4161-0.0409 0.0289-0.1168
 6  0.0378-0.0978-0.0004-0.0081 0.0305 0.6170-0.1485-0.0409 0.0239 0.0997
 7 -0.0205 0.4806 0.1843-0.1715-0.4161-0.1485 4.3095 0.2675-0.2496 0.1259
 8 -0.0192 0.0272 0.2721 0.0   -0.0409-0.0409 0.2675 3.0051 0.0436 0.2519
 9  0.0097-0.0158 0.0963 0.0    0.0289 0.0239-0.2496 0.0436 0.7419-0.1711
10 -0.0158 0.0188-0.0704 0.0   -0.1168 0.0997 0.1259 0.2519-0.1711 0.8337
-----------------------------------------------------------------------
```

```
    11 THE A'' HCH2 STRETCH -----
    12 THE A'' HCH2 DEFORMATION -
    13 THE OUT-OF-PLANE CH3 WAG
    14 THE OUT-OF-PLANE WAG -----
    15 THE TORSION --------------
   ------------------------------
```

```
11  4.8120 0.2184-0.1761 0.0    0.0029
12  0.2184 0.4822-0.0785-0.0424 0.0
13 -0.1761-0.0785 0.7247-0.0141-0.0589
14  0.0   -0.0424-0.0141 0.4300 0.0500
15  0.0029 0.0   -0.0589 0.0500 0.0493
---------------------------------------
```

F MATRIX FOR THE MOLECULE CH3-COBR

```
 1 THE ASYM. DCD2 STRETCH ---
 2 THE SYMMETRIC CD3 STRETCH
 3 THE C=C STRETCH ----------
 4 THE DCD2 DEFORMATION -----
 5 THE CD3 UMBRELLA BEND ----
 6 THE IN-PLANE CD3 ROCK ----
 7 THE C-C STRETCH ----------
 8 THE C-Z STRETCH ----------
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK -----------
-----------------------------
```

```
 1  4.8910 0.0331-0.0030-0.0354 0.0723 0.0378-0.0205-0.0192 0.0097-0.0158
 2  0.0331 4.9948 0.0093-0.0087-0.0212-0.0978 0.4806 0.0272-0.0158 0.0188
 3 -0.0030 0.009312.3247 0.0   -0.0072-0.0004 0.1843 0.2721 0.0963-0.0704
 4 -0.0354-0.0087 0.0    0.4758-0.0298-0.0081-0.1715 0.0    0.0    0.0
 5  0.0723-0.0212-0.0072-0.0298 0.5901 0.0305-0.4161-0.0409 0.0289-0.1168
 6  0.0378-0.0978-0.0004-0.0081 0.0305 0.6170-0.1485-0.0409 0.0239 0.0997
 7 -0.0205 0.4806 0.1843-0.1715-0.4161-0.1485 4.3095 0.2675-0.2496 0.1259
 8 -0.0192 0.0272 0.2721 0.0   -0.0409-0.0409 0.2675 3.0051 0.0436 0.2519
 9  0.0097-0.0158 0.0963 0.0    0.0289 0.0239-0.2496 0.0436 0.7419-0.1711
10 -0.0158 0.0188-0.0704 0.0   -0.1168 0.0997 0.1259 0.2519-0.1711 0.8337
-----------------------------------------------------------------------
```

```
11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE CD3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

```
11  4.8120 0.2184-0.1761 0.0    0.0029
12  0.2184 0.4822-0.0785-0.0424 0.0
13 -0.1761-0.0785 0.7247-0.0141-0.0589
14  0.0   -0.0424-0.0141 0.4300 0.0500
15  0.0029 0.0   -0.0589 0.0500 0.0493
---------------------------------------
```

F MATRIX FOR THE MOLECULE CD3-COBR

1 THE C-Z STRETCH ----------
2 THE C=O STRETCH ----------
3 THE SCISSORS BEND -------
4 THE SYMMETRIC CF3 STRETCH
5 THE ASYM. FCF2 STRETCH ---
6 THE C-C STRETCH ----------
7 THE CF3 UMBRELLA BEND ----
8 THE FCF2 DEFORMATION -----
9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----

1	4.5148	0.0774	-0.0321	0.0420	-0.0297	0.1860	-0.0425	0.0	0.1165 -0.0425
2	0.0774	12.3035	0.2184	-0.0648	0.0226	-0.0888	0.0519	0.0	-0.2523 0.0095
3	-0.0321	0.2184	0.2376	-0.0009	0.0147	-0.3704	0.0180	0.0	-0.0594 0.0246
4	0.0420	-0.0648	-0.0009	12.5889	-0.0911	2.2198	0.1201	0.1886	0.0727 -0.0627
5	-0.0297	0.0226	0.0147	-0.0911	7.6206	0.1319	0.0777	-1.4791	-0.0271 0.9107
6	0.1860	-0.0888	-0.3704	2.2198	0.1319	6.0832	-1.9351	-0.1225	0.2665 -0.0287
7	-0.0425	0.0519	0.0180	0.1201	0.0777	-1.9351	1.7918	-0.1483	-0.0783 -0.2529
8	0.0	0.0	0.0	0.1886	-1.4791	-0.1225	-0.1483	1.8895	0.0 0.4166
9	0.1165	-0.2523	-0.0594	0.0727	-0.0271	0.2665	-0.0783	0.0	1.2076 -0.0150
10	-0.0425	0.0095	0.0246	-0.0627	0.9107	-0.0287	-0.2529	0.4166	-0.0150 1.2922

11 THE A'' FCF2 STRETCH -----
12 THE OUT-OF-PLANE WAG -----
13 THE A'' FCF2 DEFORMATION -
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION --------------

11	7.1495	0.0	-1.3458	-1.2994	-0.0430
12	0.0	0.7500	0.0	0.3536	0.1700
13	-1.3458	0.0	1.5295	-0.2799	0.0
14	-1.2994	0.3536	-0.2799	2.5397	0.0970
15	-0.0430	0.1700	0.0	0.0970	0.0519

F MATRIX FOR THE MOLECULE CF3-COH

1 THE C-Z STRETCH ----------
2 THE C=O STRETCH ----------
3 THE SYMMETRIC CF3 STRETCH
4 THE ASYM. FCF2 STRETCH ---
5 THE SCISSORS BEND -------
6 THE C-C STRETCH ----------
7 THE CF3 UMBRELLA BEND ----
8 THE FCF2 DEFORMATION -----
9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----

1	4.5148	0.0774	0.0420	-0.0297	-0.0321	0.1860	-0.0425	0.0	0.1165	-0.0425
2	0.0774	12.3035	-0.0648	0.0226	0.2184	-0.0888	0.0519	0.0	-0.2523	0.0095
3	0.0420	-0.0648	12.5889	-0.0911	-0.0009	2.2198	0.1201	0.1886	0.0727	-0.0627
4	-0.0297	0.0226	-0.0911	7.6206	0.0147	0.1319	0.0777	-1.4791	-0.0271	0.9107
5	-0.0321	0.2184	-0.0009	0.0147	0.2376	-0.3704	0.0180	0.0	-0.0594	0.0246
6	0.1860	-0.0888	2.2198	0.1319	-0.3704	6.0832	-1.9351	-0.1225	0.2665	-0.0287
7	-0.0425	0.0519	0.1201	0.0777	0.0180	-1.9351	1.7918	-0.1483	-0.0783	-0.2529
8	0.0	0.0	0.1886	-1.4791	0.0	-0.1225	-0.1483	1.8895	0.0	0.4166
9	0.1165	-0.2523	0.0727	-0.0271	-0.0594	0.2665	-0.0783	0.0	1.2076	-0.0150
10	-0.0425	0.0095	-0.0627	0.9107	0.0246	-0.0287	-0.2529	0.4166	-0.0150	1.2922

11 THE A'' FCF2 STRETCH -----
12 THE OUT-OF-PLANE WAG -----
13 THE A'' FCF2 DEFORMATION -
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION --------------

11	7.1495	0.0	-1.3458	-1.2994	-0.0430
12	0.0	0.7500	0.0	0.3536	0.1700
13	-1.3458	0.0	1.5295	-0.2799	0.0
14	-1.2994	0.3536	-0.2799	2.5397	0.0970
15	-0.0430	0.1700	0.0	0.0970	0.0519

F MATRIX FOR THE MOLECULE CF3-COO

```
 1 THE C=C STRETCH ----------
 2 THE SYMMETRIC CF3 STRETCH
 3 THE ASYM. FCF2 STRETCH ---
 4 THE C-Z STRETCH ----------
 5 THE C-C STRETCH ----------
 6 THE SCISSORS BEND -------
 7 THE CF3 UMBRELLA BEND ----
 8 THE FCF2 DEFORMATION -----
 9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----
-----------------------------
```

1	13.9627	0.3436	-0.1057	0.7668	0.9336	0.2430	-0.2760	0.0	-0.3166	-0.0370
2	0.3436	12.2289	-0.2957	-0.0349	1.5236	-0.0763	0.4221	0.3937	-0.1949	-0.2370
3	-0.1057	-0.2957	7.0082	0.0247	0.0959	-0.0195	-0.1666	-1.3786	0.0107	0.7542
4	0.7668	-0.0349	0.0247	4.5062	0.0564	0.8130	0.0471	0.0	0.2649	0.0471
5	0.9336	1.5236	0.0959	0.0564	5.7067	-0.4945	-1.2484	-0.0408	-0.4906	0.2278
6	0.2430	-0.0763	-0.0195	0.8130	-0.4945	1.0703	0.0207	0.0	0.3787	-0.0529
7	-0.2760	0.4221	-0.1666	0.0471	-1.2484	0.0207	1.6756	-0.0039	0.2277	-0.1113
8	0.0	0.3937	-1.3786	0.0	-0.0408	0.0	-0.0039	2.9201	0.0	0.4760
9	-0.3166	-0.1949	0.0107	0.2649	-0.4906	0.3787	0.2277	0.0	1.3726	-0.1596
10	-0.0370	-0.2370	0.7542	0.0471	0.2278	-0.0529	-0.1113	0.4760	-0.1596	1.4895

```
11 THE A'' FCF2 STRETCH -----
12 THE A'' FCF2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION --------------
-----------------------------
```

11	6.8752	-1.0502	0.0	0.9494	0.1064
12	-1.0502	1.6045	-0.0707	0.2527	0.0
13	0.0	-0.0707	0.1600	0.3394	0.1000
14	0.9494	0.2527	0.3394	1.6135	0.2210
15	0.1064	0.0	0.1000	0.2210	0.1677

F MATRIX FOR THE MOLECULE CF3-COF

```
 1 THE C=O STRETCH ----------
 2 THE SYMMETRIC CF3 STRETCH
 3 THE ASYM. FCF2 STRETCH ---
 4 THE C-C STRETCH ----------
 5 THE C-Z STRETCH ----------
 6 THE FCF2 DEFORMATION -----
 7 THE CF3 UMBRELLA BEND ----
 8 THE SCISSORS BEND -------
 9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----
-----------------------------
```

1	13.2860	0.2213	-0.0701	0.6876	0.7172	0.0	-0.1780	0.3529	0.5299	-0.0258
2	0.2213	11.8827	-0.2404	1.3693	0.0	0.2962	0.3690	-0.0647	0.1121	-0.0831
3	-0.0701	-0.2404	8.8511	0.0847	0.0	-1.3511	-0.0960	-0.0020	0.0035	0.6621
4	0.6876	1.3693	0.0847	5.4762	0.1376	0.0	-1.4017	-0.5386	0.2528	0.1123
5	0.7172	0.0	0.0	0.1376	3.9451	0.0	0.0	0.7221	-0.4585	0.0
6	0.0	0.2962	-1.3511	0.0	0.0	2.3968	-0.1628	0.0	0.0	0.4427
7	-0.1780	0.3690	-0.0960	-1.4017	0.0	-0.1628	1.5921	0.0703	-0.1218	-0.0777
8	0.3529	-0.0647	-0.0020	-0.5386	0.7221	0.0	0.0703	0.7731	-0.1719	-0.0826
9	0.5299	0.1121	0.0035	0.2528	-0.4585	0.0	-0.1218	-0.1719	1.5757	0.1431
10	-0.0258	-0.0831	0.6621	0.1123	0.0	0.4427	-0.0777	-0.0826	0.1431	1.2866

```
11 THE A'' FCF2 STRETCH -----
12 THE A'' FCF2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION --------------
-----------------------------
```

11	6.6169	-1.1416	0.0	-0.7796	0.0602
12	-1.1416	1.5323	-0.0283	-0.3527	0.0
13	0.0	-0.0283	0.1550	-0.3536	0.0900
14	-0.7796	-0.3527	-0.3536	1.5112	-0.0973
15	0.0602	0.0	0.0900	-0.0973	0.1975

F MATRIX FOR THE MOLECULE CF3-COCL

4. L Matrix

The L matrix is the transformation matrix from normal coordinate space to symmetry coordinate space. Above each symmetry block are the symmetry coordinate labels for the rows. Each column corresponds to a given normal coordinate.

1 THE ASYM. HCH2 STRETCH ---
2 THE SYMMETRIC CH3 STRETCH
3 THE C-Z STRETCH ----------
4 THE C=O STRETCH ----------
5 THE HCH2 DEFORMATION -----
6 THE CH3 UMBRELLA BEND ----
7 THE SCISSORS BEND -------
8 THE IN-PLANE CH3 ROCK ----
9 THE C-C STRETCH ----------
10 THE O=C-Z ROCK ----------

1	1.0469	-0.0739	0.0171	-0.0024	-0.0089	-0.0099	0.0024	0.0003	0.0082	-0.0088
2	0.0702	1.0070	0.0534	-0.0100	-0.0054	0.0075	0.0151	-0.0119	-0.0033	0.0000
3	-0.0205	-0.0536	1.0347	-0.0128	0.0105	-0.0147	-0.0116	-0.0259	-0.0184	0.0058
4	-0.0001	-0.0018	-0.0402	-0.3526	-0.0682	0.1051	-0.0337	0.0050	0.0523	0.0163
5	0.1476	-0.0097	-0.0053	-0.0990	1.3761	0.4863	0.0709	-0.1845	0.2278	-0.0631
6	-0.0065	-0.1322	0.0170	0.1274	-0.2875	0.7370	1.1895	-0.0426	-0.2020	-0.0541
7	0.0111	0.0124	-0.0528	0.5552	-0.1717	0.8362	-0.6367	0.2476	-0.1426	-0.0968
8	-0.0988	0.0130	-0.0662	-0.2979	0.3740	0.0384	0.0141	0.5293	-0.6735	0.2001
9	-0.0026	-0.0450	-0.0251	0.1847	-0.0104	0.0899	0.1086	0.2810	0.1627	0.0672
10	-0.0925	0.0100	-0.1065	-0.4542	0.0273	-0.3827	0.3015	0.3179	0.0699	-0.3578

11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------

11	1.0497	-0.0106	0.0140	0.0058	0.0008
12	0.1457	1.4678	0.2754	-0.0727	-0.0052
13	0.0932	-0.3633	0.9085	0.2258	-0.0391
14	0.0312	-0.0456	0.2416	-0.5331	-0.0118
15	0.0030	0.0306	-0.0369	0.3494	0.6813

L MATRIX FOR THE MOLECULE CH3-COH

```
 1 THE C-Z STRETCH ----------
 2 THE ASYM. DCD2 STRETCH ---
 3 THE SYMMETRIC CD3 STRETCH
 4 THE C=C STRETCH ----------
 5 THE SCISSORS BEND -------
 6 THE C-C STRETCH ----------
 7 THE DCD2 DEFORMATION -----
 8 THE CD3 UMBRELLA BEND ----
 9 THE IN-PLANE CD3 ROCK ----
10 THE O=C-Z ROCK -----------
-----------------------------
```

```
 1  1.0362-0.0070 0.0186 0.C11C-0.0098-0.0322 0.0026 0.0117-0.0090 0.0056
 2 -0.0050-0.7775-0.0083 0.0247-0.0181 0.0086-0.0211-0.0144-0.0043-0.0086
 3 -0.0124-0.0076 0.7248 0.CC37-0.0009 0.0290 0.0025 0.C184-0.0009 0.0008
 4 -0.0399 0.0090-0.0038 0.3582 0.1141 0.0335-0.0039 0.0098 0.0390 0.0107
 5 -0.0541-0.0367 0.0090-0.5507 1.0783-0.0156-0.0149-0.2161-0.1199-0.0687
 6 -0.0218-0.0017-0.0779-0.1840 0.0403 0.3100 0.0154-0.1229 0.1009 0.0548
 7 -0.0049-0.2109-0.0024 0.CC78 0.0174-0.0822 1.0708-0.0074 0.1228-0.0778
 8  0.0211-0.0045-0.1978-0.0776 0.0631 0.8336 0.0978 0.6289-0.3146-0.0676
 9 -0.0588 0.1589 0.0036 0.2030-0.0048 0.0959 0.1786-0.3686-0.5395 0.2452
10 -0.1038 0.1554-0.0055 0.4436-0.4672 0.2570-0.0705-0.2883-0.0617-0.3006
```

```
11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CD3 WAG
15 THE TORSION --------------
-----------------------------
```

```
11  0.7785-0.0180-0.0039 0.0057 0.0006
12  0.2057 1.0488 0.2607 0.0964-0.0045
13  0.0443-0.1003 0.5692-0.0984-0.0092
14  0.1398-0.2234 0.2746 0.6725-0.0334
15  0.0044 0.0667-0.3071 0.1854 0.5442
-----------------------------------
```

L MATRIX FOR THE MOLECULE CD3-COH

```
 1 THE ASYM. HCH2 STRETCH ---
 2 THE SYMMETRIC CH3 STRETCH
 3 THE C-Z STRETCH ----------
 4 THE C=O STRETCH ----------
 5 THE HCH2 DEFORMATION -----
 6 THE CH3 UMBRELLA BEND ----
 7 THE C-C STRETCH ----------
 8 THE IN-PLANE CH3 ROCK ----
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK -----------
-----------------------------
```

1	-1.0474	-0.0693	-0.0020	-0.0004	-0.0108	-0.0035	-0.0010	0.0001	0.0081	-0.0089
2	-0.0668	1.0086	-0.0083	-0.0110	-0.0046	0.0164	-0.0121	-0.0023	-0.0026	0.0001
3	0.0018	-0.0070	-0.7514	-0.1205	0.0108	-0.0181	0.0046	0.0038	-0.0138	0.0023
4	0.0005	-0.0033	0.1074	-0.3522	-0.0437	0.0413	0.0468	-0.0548	0.0343	0.0159
5	-0.1476	-0.0094	0.0251	-0.0995	1.4361	0.2607	-0.0749	-0.2352	0.1710	-0.0631
6	0.0057	-0.1315	-0.0506	0.1093	-0.2110	1.3997	-0.1729	0.1744	-0.1479	-0.0524
7	0.0029	-0.0460	0.0159	0.1952	-0.0031	0.1494	0.2595	0.0829	0.1601	0.0631
8	0.0997	0.0101	0.1436	-0.2643	0.3766	-0.0068	0.2823	0.6117	-0.5309	0.2005
9	-0.0041	0.0090	0.0459	0.3679	0.0122	0.0716	0.6606	-0.4583	-0.3769	-0.0780
10	0.0906	0.0063	0.1969	-0.3109	-0.0582	-0.0191	0.0449	0.4273	0.1841	-0.3643

```
11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

11	1.0497	-0.0107	0.0147	-0.0033	0.0008
12	0.1457	1.4703	0.2613	0.0755	-0.0055
13	0.0932	-0.3636	0.9301	-0.1059	-0.0369
14	0.0308	-0.0275	0.1667	0.4665	-0.0153
15	0.0034	0.0126	0.0181	-0.1833	0.6539

L MATRIX FOR THE MOLECULE CH3-COD

```
  1 THE ASYM. DCD2 STRETCH ---
  2 THE SYMMETRIC CD3 STRETCH
  3 THE C-Z STRETCH ----------
  4 THE C=O STRETCH ----------
  5 THE C-C STRETCH ----------
  6 THE DCD2 DEFORMATION -----
  7 THE CD3 UMBRELLA BEND ----
  8 THE SCISSORS BEND -------
  9 THE IN-PLANE CD3 ROCK ----
 10 THE O=C-Z ROCK -----------
-----------------------------
```

```
 1 -0.7779-0.0065 0.0085 0.0164 0.0005-0.0187-0.0127-0.0171-0.0031 0.0087
 2 -0.0072 0.7176-0.1026 0.0046 0.0255-0.0138 0.0139 0.0120-0.0004-0.0007
 3 -0.0049-0.1066-0.7451 0.1138-0.0098 0.0099-0.0041-0.0068-0.0093-0.0033
 4  0.0078 0.0110 0.1054 0.3570 0.0676 0.0208-0.0208 0.0194 0.0350-0.0105
 5 -0.0009-0.0739 0.0283-0.1942 0.2976-0.0217 0.0309-0.1369 0.1064-0.0516
 6 -0.2108-0.0012 0.0067 0.0079-0.0507 0.7148 0.8013 0.0099 0.1149 0.0777
 7 -0.0043-0.2002-0.0011-0.0755 0.7428-0.4157 0.4492 0.4301-0.3032 0.0636
 8 -0.0130 0.0119 0.0471-0.3680 0.4568 0.5766-0.4631 0.0463-0.1969 0.0535
 9  0.1576 0.0207 0.1156 0.1805 0.0445 0.0868 0.1513-0.4263-0.5030-0.2445
10  0.1414 0.0258 0.1909 0.3066 0.0095-0.2800 0.1171-0.4016-0.0209 0.3058
-------------------------------------------------------------------------
```

```
 11 THE A'' DCD2 STRETCH -----
 12 THE A'' DCD2 DEFORMATION -
 13 THE OUT-OF-PLANE WAG -----
 14 THE OUT-OF-PLANE CD3 WAG
 15 THE TORSION --------------
-----------------------------
```

```
11  0.7785-0.0184-0.0005-0.0055 0.0006
12  0.2057 1.0611-0.2256-0.0164-0.0045
13  0.0435-0.0506-0.4083 0.2756-0.0116
14  0.1398-0.2187-0.5614-0.4633-0.0303
15  0.0052 0.0242 0.0931-0.1733 0.5129
-----------------------------------------
```

L MATRIX FOR THE MOLECULE CD3-COD

```
 1 THE ASYM. HCH2 STRETCH ---
 2 THE SYMMETRIC CH3 STRETCH
 3 THE C=C STRETCH ----------
 4 THE HCH2 DEFORMATION -----
 5 THE CH3 UMBRELLA BEND ----
 6 THE C-Z STRETCH ----------
 7 THE IN-PLANE CH3 ROCK ----
 8 THE C-C STRETCH ----------
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------
-----------------------------

 1  0.9153 0.5137 0.0006-0.0234-0.0146 0.0092 0.0157-0.0046 0.0014 0.0094
 2 -0.4935 0.8788 0.0177-0.0494 0.0175 0.0143-0.0191-0.0106-0.0059 0.0007
 3  0.0025-0.0059 0.3750-0.0080 0.0301 0.0134 0.0531 0.0334-0.0054-0.0099
 4  0.1364 0.1016-0.0600 0.9629 1.0278 0.4747-0.0644-0.0918-0.0066 0.0366
 5  0.0751-0.1503-0.0731-1.0168 0.9619-0.0844-0.1307-0.0741-0.0677 0.0518
 6  0.0005-0.0029-0.1235-0.0537-0.0475 0.2225-0.1225 0.2255-0.0055 0.0135
 7 -0.0748-0.0359 0.2301 0.3161 0.2168-0.5578-0.6729 0.1586 0.0285-0.1370
 8  0.0189-0.0350-0.1794-0.0327 0.1486-0.2282 0.1935 0.1261 0.0657-0.0033
 9 -0.0048 0.0136-0.1987 0.0974 0.0611-0.3353 0.2127 0.0322-0.3545 0.1157
10 -0.0750-0.0428 0.2959 0.0280 0.0008-0.2828-0.0177-0.0940 0.0585 0.3294
-------------------------------------------------------------------------

11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------

11  1.0480-0.0745 0.0011-0.0171 0.0035
12  0.2364 1.3754 0.5882 0.0071-0.0357
13  0.0636-0.5269 0.7495-0.3876 0.0532
14  0.0538-0.1407 0.4185 0.4616-0.2139
15  0.0146-0.0204 0.1291 0.2638 0.5095
-----------------------------------

   L MATRIX FOR THE MOLECULE CH3-COF
```

```
  1 THE ASYM. DCD2 STRETCH ---
  2 THE SYMMETRIC CD3 STRETCH
  3 THE C=O STRETCH ----------
  4 THE C-Z STRETCH ----------
  5 THE CD3 UMBRELLA BEND ----
  6 THE DCD2 DEFORMATION -----
  7 THE IN-PLANE CD3 ROCK ----
  8 THE C-C STRETCH ----------
  9 THE SCISSORS BEND -------
 10 THE O=C-Z ROCK ----------
 -----------------------------

 1 -0.7537 0.1931 0.0258-0.0042 0.0100-0.0293 0.0042-0.0014 0.0030-0.0106
 2  0.1797 0.6984 0.0221 0.0058 0.0541-0.0033-0.0173-0.0042-0.0064-0.0006
 3  0.0083-0.0150 0.3759 0.0267 0.0262 0.0267 0.0452 0.0081-0.0013 0.0079
 4 -0.0045-0.0008-0.1223-0.2378 0.1341 0.0800 0.0396 0.1961 0.0026-0.0062
 5 -0.0497-0.2124-0.0677 0.4605 0.9007 0.0538-0.3082-0.0612-0.1480-0.0490
 6 -0.2169 0.0726-0.0269 0.1562-0.2372 1.0109-0.2504-0.0329-0.0125-0.0468
 7  0.1437-0.0346 0.1867 0.2562-0.2415-0.0969-0.4603 0.4086 0.0075 0.1634
 8 -0.0193-0.0611-0.1808 0.3191 0.0623-0.0073 0.1249 0.0572 0.0726 0.0027
 9 -0.0026 0.0195-0.2011 0.3548-0.1818-0.0677 0.1782 0.0469-0.3199-0.0999
10  0.1281-0.0368 0.2869 0.2137-0.1290-0.1832-0.1191 0.0272 0.0403-0.2906
-------------------------------------------------------------------------

 11 THE A'' DCD2 STRETCH -----
 12 THE A'' DCD2 DEFORMATION -
 13 THE OUT-OF-PLANE CD3 WAG
 14 THE OUT-OF-PLANE WAG -----
 15 THE TORSION --------------
 -----------------------------

11  0.7777-0.0480-0.0340-0.0142 0.0026
12  0.2686 0.8081 0.7191-0.0055-0.0266
13  0.1266-0.4912 0.4154-0.3905 0.0391
14  0.0818-0.3221 0.4345 0.3637-0.1582
15  0.0212-0.0629 0.1154 0.1620 0.3829
-----------------------------------------

    L MATRIX FOR THE MOLECULE CD3-COF
```

1 THE ASYM. HCH2 STRETCH ---
2 THE SYMMETRIC CH3 STRETCH
3 THE C=O STRETCH ----------
4 THE HCH2 DEFORMATION -----
5 THE CH3 UMBRELLA BEND ----
6 THE IN-PLANE CH3 ROCK ----
7 THE C-C STRETCH ----------
8 THE C-Z STRETCH ----------
9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------

1	1.0481	-0.0456	0.0132	0.0052	-0.0256	-0.0199	-0.0124	0.0029	0.0016	0.0028
2	0.0435	1.0092	0.0268	0.0187	0.0145	0.0013	-0.0296	-0.0008	-0.0002	-0.0036
3	-0.0041	-0.0074	0.3752	-0.0302	-0.0107	0.0187	0.0577	0.0172	-0.0002	-0.0066
4	0.1519	-0.0355	0.0721	1.2698	0.6305	0.4247	0.2061	-0.0638	-0.0156	0.0469
5	0.0321	-0.1095	-0.0357	-0.6715	1.2809	0.0102	0.1298	-0.0580	-0.0422	0.0731
6	-0.1283	-0.0265	0.2770	0.3909	0.2847	-0.6410	-0.4778	0.1992	0.0831	-0.1017
7	0.0020	-0.0382	-0.1678	-0.0132	0.1035	-0.2104	0.2741	0.0753	0.0326	0.0016
8	0.0030	0.0002	-0.1154	-0.0261	0.0010	0.1797	-0.1127	0.2264	-0.0096	0.0348
9	-0.0004	0.0088	-0.1407	0.0628	-0.0028	-0.2814	0.2060	-0.0778	-0.3372	-0.0119
10	-0.0956	-0.0006	0.2647	-0.0070	-0.0192	-0.3030	0.0228	-0.1664	-0.0730	0.2695

11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION -------------

11	1.0408	-0.1351	-0.0262	-0.0037	-0.0010
12	0.3247	1.3368	0.5959	0.1454	-0.0008
13	0.0541	-0.5991	0.8046	0.1111	-0.0459
14	-0.0592	0.0271	-0.2924	0.5536	0.0508
15	-0.0108	0.0132	-0.0858	0.1561	-0.5649

L MATRIX FOR THE MOLECULE CH3-COCL

```
  1 THE ASYM. DCD2 STRETCH ---
  2 THE SYMMETRIC CD3 STRETCH
  3 THE C=O STRETCH ----------
  4 THE DCD2 DEFORMATION -----
  5 THE CD3 UMBRELLA BEND ----
  6 THE C-C STRETCH ----------
  7 THE IN-PLANE CD3 ROCK ----
  8 THE C-Z STRETCH ----------
  9 THE SCISSORS BEND -------
 10 THE O=C-Z ROCK -----------
-----------------------------

 1  0.7762-0.0159 0.0401-0.0062-0.0020-0.0357-0.0244 0.0083 0.0033 0.0031
 2  0.0132 0.7243 0.0350 0.0031-0.0068 0.0174-0.0199 0.0023 0.0010-0.0035
 3 -0.0181-0.0168 0.3769 0.0248-0.0045 0.0019 0.0490 0.0106 0.0006-0.0053
 4  0.2155-0.0211 0.0128-0.4882-0.5835 0.7528 0.1585-0.0669-0.0197 0.0589
 5  0.0271-0.1686-0.0506 0.9482-0.1188 0.5272-0.1452-0.0823-0.0740 0.0675
 6  0.0086-0.0590-0.1712 0.2105-0.2457-0.0775 0.1355 0.0579 0.0375-0.0001
 7 -0.1830-0.0245 0.1951-0.0544-0.3943-0.0540-0.5390 0.2291 0.0975-0.1225
 8  0.0102 0.0037-0.1133-0.0387 0.1881 0.1347 0.0088 0.2071 0.0071 0.0228
 9  0.0013 0.0114-0.1443 0.0586-0.2933-0.2107 0.0674-0.0135-0.3252-0.0016
10 -0.1448-0.0091 0.2548 0.0647-0.2040-0.2288-0.1542-0.0813-0.0664 0.2421
-------------------------------------------------------------------------

 11 THE A'' DCD2 STRETCH -----
 12 THE A'' DCD2 DEFORMATION -
 13 THE OUT-OF-PLANE CD3 WAG
 14 THE OUT-OF-PLANE WAG -----
 15 THE TORSION --------------
-----------------------------

11  0.7717-0.0978-0.0369-0.0058 0.0007
12  0.3252 0.9433 0.4472 0.1742 0.0007
13  0.1251-0.4354 0.6034 0.1749 0.0330
14 -0.0865 0.0524-0.4036 0.4737-0.0356
15 -0.0163 0.0156-0.0989 0.1187 0.4080
---------------------------------------

    L MATRIX FOR THE MOLECULE CD3-COCL
```

```
 1 THE ASYM. HCH2 STRETCH ---
 2 THE SYMMETRIC CH3 STRETCH
 3 THE C=C STRETCH ----------
 4 THE HCH2 DEFORMATION -----
 5 THE CH3 UMBRELLA BEND ----
 6 THE IN-PLANE CH3 ROCK ----
 7 THE C-C STRETCH ----------
 8 THE C-Z STRETCH ----------
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------
-----------------------------
```

```
 1  1.0430-0.1153 0.0077-0.0180-0.0227-0.0102-0.0073 0.0004-0.0006 0.0034
 2  0.1112 1.0042 0.0230 0.0088 0.0183-0.0004-0.0264-0.0018 0.0006-0.0025
 3 -0.0031-0.0065 0.3747 0.0302-0.0326 0.0193 0.0511 0.0194 0.0054-0.0037
 4  0.1458-0.0241 0.1233-0.8319 1.1903 0.0194 0.3483 0.0022-0.0079 0.0323
 5  0.0236-0.1313-0.0379 1.2002 0.8012-0.1078 0.1243-0.0385-0.0019 0.0539
 6 -0.1217-0.0091 0.2740-0.1724 0.2640-0.7420-0.4871 0.1998 0.0002-0.0793
 7 -0.0019-0.0399-0.1693 0.0900 0.0068-0.2303 0.2615 0.0823-0.0086 0.0053
 8  0.0024-0.0007-0.1134 0.0007 0.0387 0.1707-0.1052 0.1879 0.0616 0.0465
 9 -0.0006 0.0087-0.1297-0.0195-0.0506-0.2748 0.1970-0.1883 0.2749-0.0126
10 -0.0926 0.0064 0.2521 0.0297-0.0964-0.2889 0.0141-0.2299 0.0101 0.2303
-------------------------------------------------------------------------
```

```
11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
-----------------------------
```

```
11  1.0431-0.1162-0.0217-0.0001-0.0013
12  0.2971 1.3368 0.6159 0.1192 0.0009
13  0.0598-0.6067 0.7947 0.1358-0.0431
14 -0.0584 0.0426-0.2920 0.5330 0.0802
15 -0.0109 0.0182-0.0940 0.1964-0.5506
---------------------------------------
```

L MATRIX FOR THE MOLECULE CH3-COBR

```
 1 THE ASYM. OCO2 STRETCH ---
 2 THE SYMMETRIC CO3 STRETCH
 3 THE C=O STRETCH ----------
 4 THE OCO2 DEFORMATION -----
 5 THE CO3 UMBRELLA BEND ----
 6 THE IN-PLANE CO3 ROCK ----
 7 THE C-C STRETCH ----------
 8 THE C-Z STRETCH ----------
 9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------
----------------------------
```

1	-0.7761	-0.0415	0.0272	-0.0012	-0.0324	-0.0112	-0.0194	0.0045	-0.0002	-0.0041
2	-0.0381	0.7236	0.0274	0.0158	0.0183	0.0044	-0.0183	0.0014	-0.0000	0.0024
3	0.0130	-0.0130	0.3774	0.0280	-0.0018	-0.0058	0.0454	0.0134	0.0043	0.0033
4	-0.2110	-0.0103	0.0327	-0.4744	0.3304	0.8947	0.2088	0.0031	-0.0042	-0.0417
5	-0.0198	-0.1868	-0.0496	0.8800	0.6032	0.2595	-0.0962	-0.0766	0.0149	-0.0458
6	0.1752	-0.0104	0.1973	0.0216	-0.2058	0.3325	-0.5553	0.2454	-0.0078	0.0953
7	-0.0021	-0.0627	-0.1703	0.2533	-0.1454	0.1619	0.1310	0.0703	-0.0097	-0.0049
8	-0.0087	0.0018	-0.1130	-0.0812	0.1749	-0.1087	0.0063	0.1702	0.0638	-0.0301
9	0.0017	0.0099	-0.1312	0.1290	-0.2853	0.1701	0.0516	-0.1567	0.2703	0.0279
10	0.1389	-0.0018	0.2473	0.1292	-0.2659	0.0903	-0.1641	-0.1583	0.0400	-0.2060

```
11 THE A'' OCO2 STRETCH -----
12 THE A'' OCO2 DEFORMATION -
13 THE OUT-OF-PLANE CO3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------
----------------------------
```

11	-0.7734	-0.0834	-0.0364	-0.0015	0.0009
12	-0.3065	0.9309	0.4959	0.1395	-0.0005
13	-0.1284	-0.4561	0.5852	0.1815	0.0310
14	0.0856	0.0823	-0.3866	0.4629	-0.0559
15	0.0164	0.0248	-0.1049	0.1459	0.3970

L MATRIX FOR THE MOLECULE CO3-COBR

```
 1 THE C-Z STRETCH ----------
 2 THE C=O STRETCH ----------
 3 THE SCISSORS BEND -------
 4 THE SYMMETRIC CF3 STRETCH
 5 THE ASYM. FCF2 STRETCH ---
 6 THE C-C STRETCH ----------
 7 THE CF3 UMBRELLA BEND ----
 8 THE FCF2 DEFORMATION -----
 9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----
-----------------------------
```

```
 1  1.0356 0.0520 0.0132-0.0092 0.0003 0.0119-0.0062-0.0012-0.0053 0.0009
 2 -0.0598 0.3716 0.0459-0.0157-0.0014 0.0341 0.0139 0.0027 0.0212 0.0040
 3 -0.0738-0.3594 0.6802-0.1701-0.4777 0.7175-0.1449-0.1317-0.3593-0.2597
 4 -0.0015-0.0121 0.0275-0.2703 0.0658-0.0448 0.0301-0.0091 0.0042 0.0034
 5 -0.0009-0.0227 0.2531 0.0998 0.2926-0.0339-0.0258 0.0265 0.0138-0.0208
 6 -0.0318-0.1366-0.0886 0.1510 0.0583 0.3120 0.1109 0.0422-0.0393-0.0023
 7  0.0035 0.0047-0.0566 0.3234-0.0109 0.1260 0.3896 0.0732-0.1774-0.0085
 8 -0.0006-0.0189 0.1951 0.0484 0.1676-0.0332-0.0576 0.3475 0.0110-0.0537
 9 -0.1170 0.3802-0.6601-0.0115 0.2884-0.0740-0.0875-0.0463-0.0799-0.0845
10 -0.0658 0.1704-0.2051-0.0791-0.1175 0.0808-0.0845-0.0658-0.2301 0.1343
-----------------------------------------------------------------------
```

```
11 THE A'' FCF2 STRETCH -----
12 THE OUT-OF-PLANE WAG -----
13 THE A'' FCF2 DEFORMATION -
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION --------------
-----------------------------
```

```
11  0.3954-0.0726 0.0350 0.0217 0.0021
12  0.1709 0.3939-0.0074-0.3680-0.0821
13  0.2638 0.0109 0.3547 0.0392 0.0012
14  0.3081 0.2653 0.0214 0.1366-0.0040
15 -0.0369-0.1218-0.0008 0.3475 0.3975
-------------------------------------
```

L MATRIX FOR THE MOLECULE CF3-COH

```
 1 THE C-Z STRETCH ----------
 2 THE C=O STRETCH ----------
 3 THE SYMMETRIC CF3 STRETCH
 4 THE ASYM. FCF2 STRETCH ---
 5 THE SCISSORS BEND -------
 6 THE C-C STRETCH ----------
 7 THE CF3 UMBRELLA BEND ----
 8 THE FCF2 DEFORMATION -----
 9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----
-----------------------------
```

```
 1  0.7333-0.2012-0.0069-0.0195 0.0252 0.0199-0.0120-0.0012-0.0075 0.0005
 2 -0.1530-0.3460 0.0167-0.0221 0.0033 0.0382 0.0109 0.0002 0.0187 0.0041
 3 -0.0025 0.0140-0.0407-0.2774 0.0032-0.0372 0.0315-0.0079 0.0051 0.0035
 4  0.0037 0.0156 0.3781-0.0504 0.1147-0.0480-0.0241 0.0281 0.0171-0.0206
 5 -0.0340 0.3110 0.1425-0.1290-0.2606 0.7105-0.1714-0.1454-0.3881-0.2637
 6 -0.0190 0.1558-0.0052 0.1619 0.1919 0.2572 0.0976 0.0395-0.0414-0.0028
 7  0.0063-0.0053 0.0519 0.3243 0.0990 0.1043 0.3865 0.0848-0.1650-0.0095
 8  0.0038 0.0122 0.2604-0.0528 0.0202-0.0106-0.0599 0.3447 0.0231-0.0533
 9 -0.2350-0.2673-0.3681 0.0660 0.4115-0.2131-0.0743-0.0226-0.0551-0.0843
10 -0.1239-0.1325-0.2665 0.0208 0.0455 0.0224-0.0809-0.0517-0.2253 0.1324
-------------------------------------------------------------------------
```

```
11 THE A'' FCF2 STRETCH -----
12 THE OUT-OF-PLANE WAG -----
13 THE A'' FCF2 DEFORMATION -
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION --------------
-----------------------------
```

```
11  0.3970-0.0644-0.0351 0.0179 0.0020
12  0.1466 0.3399 0.0090-0.2958-0.0746
13  0.2642 0.0177-0.3548 0.0312 0.0013
14  0.3061 0.2793-0.0222 0.1107-0.0026
15 -0.0120-0.0507-0.0013 0.1891 0.3496
--------------------------------------
```

L MATRIX FOR THE MOLECULE CF3-COD

```
 1 THE C=O STRETCH ----------
 2 THE SYMMETRIC CF3 STRETCH
 3 THE ASYM. FCF2 STRETCH ---
 4 THE C-Z STRETCH ----------
 5 THE C-C STRETCH ----------
 6 THE SCISSORS BEND -------
 7 THE CF3 UMBRELLA BEND ----
 8 THE FCF2 DEFORMATION -----
 9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----
-----------------------------
```

```
 1 -0.3803-0.0043-0.0157 0.0046-0.0240-0.0034 0.0045-0.0179-0.0017 0.0001
 2 -0.0022-0.2401 0.1549-0.0381-0.0423-0.0177-0.0206 0.0141 0.0077 0.0000
 3  0.0132-0.1974-0.3322-0.0931 0.0099-0.0402 0.0047 0.0309-0.0085 0.0088
 4  0.0944-0.0591-0.0405 0.3090-0.1014-0.0530 0.0970 0.0337 0.0476 0.0240
 5  0.1471 0.2310-0.0777-0.2177-0.1874-0.0119 0.0352-0.0403 0.0070 0.0080
 6  0.1351 0.0816 0.0709-0.3467-0.0131-0.0818 0.2617 0.0273-0.1666-0.1193
 7  0.0140 0.3418-0.1939-0.0204-0.3198 0.0158-0.1701 0.1724-0.0585-0.0337
 8  0.0097-0.1669-0.2418-0.0636-0.0346 0.2791 0.0987 0.0520-0.0311 0.0219
 9 -0.2709 0.1902 0.2417-0.2378 0.1172-0.0807 0.0354 0.1815 0.0344 0.1099
10 -0.1633 0.1773 0.2473-0.0894 0.0718-0.0182 0.0001 0.1177 0.1990-0.0732
```

```
11 THE A'' FCF2 STRETCH -----
12 THE A'' FCF2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CF3 WAG .
15 THE TORSION --------------
-----------------------------
```

```
11  0.3991-0.0048-0.0279 0.0294-0.0068
12  0.2601-0.3177-0.0943 0.0762-0.0139
13  0.1042 0.0994-0.2797 0.5790-0.1504
14 -0.2374-0.0314 0.3384-0.1391 0.0175
15  0.0064 0.0194-0.0142 0.1515 0.1370
-----------------------------------
```

L MATRIX FOR THE MOLECULE CF3-COF

```
 1 THE C=O STRETCH ----------
 2 THE SYMMETRIC CF3 STRETCH
 3 THE ASYM. FCF2 STRETCH ---
 4 THE C-C STRETCH ----------
 5 THE C-Z STRETCH ----------
 6 THE FCF2 DEFORMATION -----
 7 THE CF3 UMBRELLA BEND ----
 8 THE SCISSORS BEND -------
 9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----
-----------------------------
```

```
 1  0.3806-0.0001-0.0103-0.0012 0.0240 0.0060-0.0159-0.0070 0.0010 0.0031
 2  0.0019-0.2643 0.1168 0.0226 0.0349-0.0202 0.0137 0.0008 0.0045 0.0006
 3 -0.0080-0.1563-0.3647 0.0416-0.0083-0.0240 0.0114 0.0286-0.0079 0.0116
 4 -0.1409 0.2088-0.0631 0.2702 0.1533 0.0472-0.0226-0.0022-0.0010-0.0009
 5 -0.1374-0.0169-0.0177-0.2417 0.1247 0.0080-0.0887 0.0782 0.0585 0.0250
 6 -0.0048-0.1335-0.2538 0.0144-0.0299 0.2953 0.0833 0.0812-0.0381 0.0263
 7 -0.0105 0.3568-0.1338 0.0799 0.3175-0.0250 0.2479 0.0930-0.0444-0.0209
 8 -0.1237 0.0300 0.0405 0.3947-0.0511 0.0215-0.1854 0.1525-0.1735-0.1295
 9 -0.2545-0.1163-0.2326-0.2440 0.1581 0.1216-0.0364-0.1327 0.0010-0.0693
10  0.1570 0.1219 0.2566 0.1227-0.1043-0.0585 0.0574 0.0741 0.1879-0.0747
-------------------------------------------------------------------------
```

```
11 THE A'' FCF2 STRETCH -----
12 THE A'' FCF2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION --------------
-----------------------------
```

```
11 -0.3989-0.0175-0.0275 0.0272-0.0102
12 -0.2505-0.3189-0.1284 0.0698-0.0217
13 -0.0811 0.1076-0.2104 0.5271-0.1844
14 -0.2356 0.0572-0.3234 0.1374-0.0462
15 -0.0186 0.0198-0.0269 0.1753 0.1002
---------------------------------------
```

L MATRIX FOR THE MOLECULE CF3-COCL

5. Potential Energy Distribution Matrix

As was done with the G, F, and L matrices, the potential energy distribution matrix is separated into its two symmetry blocks with symmetry coordinate labels listed above each block. See page I-39 for definition of the P.E.D. matrix.

1 THE ASYM. HCH2 STRETCH ---
2 THE SYMMETRIC CH3 STRETCH
3 THE C-Z STRETCH ----------
4 THE C=O STRETCH ----------
5 THE HCH2 DEFORMATION -----
6 THE CH3 UMBRELLA BEND ----
7 THE SCISSORS BEND -------
8 THE IN-PLANE CH3 ROCK ----
9 THE C-C STRETCH ----------
10 THE O=C-Z ROCK ----------

1	0.9974	0.0051	0.0003	0.0000	0.0003	0.0004	0.0000	0.0000	0.0007	0.0025
2	0.0047	0.9938	0.0031	0.0003	0.0001	0.0002	0.0011	0.0010	0.0001	0.0
3	0.0003	0.0024	1.0139	0.0004	0.0004	0.0008	0.0006	0.0041	0.0030	0.0010
4	0.0	0.0000	0.0039	0.7668	0.0425	0.1059	0.0118	0.0004	0.0616	0.0193
5	0.0021	0.0000	0.0000	0.0028	0.7992	0.1047	0.0024	0.0243	0.0538	0.0134
6	0.0000	0.0018	0.0000	0.0047	0.0355	0.2447	0.6901	0.0013	0.0431	0.0100
7	0.0000	0.0000	0.0005	0.1338	0.0190	0.4717	0.2961	0.0668	0.0321	0.0479
8	0.0011	0.0000	0.0006	0.0296	0.0691	0.0008	0.0001	0.2346	0.5513	0.1572
9	0.0000	0.0018	0.0006	0.0868	0.0004	0.0320	0.0505	0.5045	0.2454	0.1352
10	0.0013	0.0000	0.0020	0.0956	0.0005	0.1054	0.0709	0.1175	0.0082	0.6980

11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------

11	1.0046	0.0005	0.0024	0.0005	0.0003
12	0.0021	0.9212	0.0987	0.0083	0.0011
13	0.0007	0.0472	0.8998	0.0669	0.0518
14	0.0002	0.0018	0.1556	0.9115	0.0115
15	0.0	0.0000	0.0001	0.0109	1.0661

P.E.D. - FOR THE MOLECULE CH3-COH

1 THE C-Z STRETCH ----------
2 THE ASYM. DCD2 STRETCH ---
3 THE SYMMETRIC CD3 STRETCH
4 THE C=O STRETCH ----------
5 THE SCISSORS BEND -------
6 THE C-C STRETCH ----------
7 THE DCD2 DEFORMATION -----
8 THE CD3 UMBRELLA BEND ----
9 THE IN-PLANE CD3 ROCK ----
10 THE O=C-Z ROCK ----------

1	1.0163	0.0001	0.0006	0.0003	0.0004	0.0059	0.0000	0.0010	0.0011	0.0012
2	0.0000	0.9945	0.0001	0.0017	0.0014	0.0005	0.0035	0.0018	0.0003	0.0030
3	0.0002	0.0001	0.9955	0.0000	0.0000	0.0055	0.0001	0.0030	0.0000	0.0000
4	0.0038	0.0003	0.0001	0.7988	0.1278	0.0162	0.0003	0.0019	0.0523	0.0107
5	0.0005	0.0004	0.0000	0.1329	0.8039	0.0002	0.0003	0.0641	0.0349	0.0307
6	0.0005	0.0000	0.0104	0.0870	0.0066	0.5699	0.0017	0.1216	0.1448	0.1147
7	0.0000	0.0077	0.0000	0.0000	0.0001	0.0045	0.9404	0.0000	0.0240	0.0259
8	0.0000	0.0000	0.0076	0.0018	0.0018	0.4692	0.0080	0.3624	0.1604	0.0199
9	0.0004	0.0051	0.0000	0.0139	0.0000	0.0071	0.0306	0.1433	0.5428	0.3011
10	0.0019	0.0068	0.0000	0.0921	0.1611	0.0712	0.0066	0.1218	0.0098	0.6281

11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CD3 WAG
15 THE TORSION -------------

11	1.0046	0.0025	0.0002	0.0007	0.0002
12	0.0074	0.8981	0.1031	0.0215	0.0013
13	0.0007	0.0168	1.0065	0.0457	0.0109
14	0.0029	0.0341	0.0958	0.8744	0.0591
15	0.0	0.0002	0.0081	0.0045	1.0642

P.E.D. - FOR THE MOLECULE CD3-COH

1 THE ASYM. HCH2 STRETCH ---
2 THE SYMMETRIC CH3 STRETCH
3 THE C-Z STRETCH ----------
4 THE C=O STRETCH ----------
5 THE HCH2 DEFORMATION -----
6 THE CH3 UMBRELLA BEND ----
7 THE C-C STRETCH ----------
8 THE IN-PLANE CH3 ROCK ----
9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------

1	0.9984	0.0045	0.0000	0.0000	0.0005	0.0001	0.0000	0.0	0.0007	0.0026
2	0.0042	0.9972	0.0001	0.0004	0.0001	0.0012	0.0010	0.0000	0.0001	0.0
3	0.0000	0.0000	0.9862	0.0367	0.0004	0.0013	0.0001	0.0001	0.0019	0.0002
4	0.0000	0.0000	0.0510	0.7942	0.0175	0.0172	0.0339	0.0505	0.0290	0.0188
5	0.0021	0.0000	0.0001	0.0029	0.8722	0.0315	0.0040	0.0429	0.0333	0.0137
6	0.0000	0.0017	0.0005	0.0036	0.0192	0.9254	0.0218	0.0240	0.0253	0.0096
7	0.0000	0.0019	0.0005	0.1007	0.0000	0.0926	0.4310	0.0476	0.2605	0.1223
8	0.0011	0.0000	0.0049	0.0242	0.0703	0.0000	0.0668	0.3398	0.3756	0.1617
9	0.0000	0.0000	0.0007	0.0610	0.0001	0.0036	0.4763	0.2482	0.2463	0.0318
10	0.0013	0.0000	0.0129	0.0465	0.0023	0.0003	0.0023	0.2302	0.0627	0.7410

11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION -------------

11	1.0046	0.0005	0.0026	0.0002	0.0003
12	0.0021	0.9261	0.0893	0.0126	0.0014
13	0.0007	0.0474	0.9472	0.0207	0.0503
14	0.0002	0.0007	0.0744	0.9840	0.0213
15	0.0	0.0000	0.0000	0.0042	1.0728

P.E.D. - FOR THE MOLECULE CH3-COO

1 THE ASYM. DCD2 STRETCH ---
2 THE SYMMETRIC CD3 STRETCH
3 THE C-Z STRETCH ----------
4 THE C=O STRETCH ----------
5 THE C-C STRETCH ----------
6 THE DCD2 DEFORMATION -----
7 THE CD3 UMBRELLA BEND ----
8 THE SCISSORS BEND -------
9 THE IN-PLANE CD3 ROCK ----
10 THE O=C-Z ROCK ----------

1	0.9959	0.0001	0.0001	0.0008	0.0000	0.0027	0.0013	0.0026	0.0001	0.0031
2	0.0001	0.9743	0.0213	0.0001	0.0041	0.0015	0.0016	0.0013	0.0000	0.0000
3	0.0000	0.0186	0.9719	0.0330	0.0005	0.0007	0.0001	0.0004	0.0012	0.0004
4	0.0002	0.0005	0.0492	0.8216	0.0635	0.0076	0.0077	0.0076	0.0436	0.0105
5	0.0000	0.0093	0.0015	0.1003	0.5074	0.0034	0.0070	0.1577	0.1664	0.1040
6	0.0077	0.0	0.0000	0.0000	0.0016	0.4169	0.5281	0.0001	0.0217	0.0264
7	0.0000	0.0078	0.0	0.0017	0.3600	0.1435	0.1689	0.1773	0.1539	0.0180
8	0.0000	0.0000	0.0007	0.0615	0.2039	0.4135	0.2690	0.0031	0.0972	0.0190
9	0.0051	0.0001	0.0032	0.0114	0.0015	0.0072	0.0221	0.2004	0.4873	0.3062
10	0.0057	0.0002	0.0121	0.0455	0.0001	0.1041	0.0183	0.2471	0.0012	0.6652

11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CD3 WAG
15 THE TORSION ----------

11	1.0046	0.0026	0.0000	0.0008	0.0003
12	0.0074	0.9264	0.0954	0.0007	0.0015
13	0.0007	0.0043	0.6394	0.4163	0.0199
14	0.0029	0.0330	0.4944	0.4809	0.0551
15	0.0	0.0000	0.0009	0.0046	1.0715

P.E.D. - FOR THE MOLECULE CD3-COD

1	THE ASYM. HCH2 STRETCH ---
2	THE SYMMETRIC CH3 STRETCH
3	THE C=O STRETCH ----------
4	THE HCH2 DEFORMATION -----
5	THE CH3 UMBRELLA BEND ----
6	THE C-Z STRETCH ----------
7	THE IN-PLANE CH3 ROCK ----
8	THE C-C STRETCH ----------
9	THE SCISSORS BEND -------
10	THE O=C-Z ROCK ----------

1	0.7503	0.2538	0.0000	0.0021	0.0010	0.0005	0.0021	0.0003	0.0000	0.0042
2	0.2263	0.7708	0.0008	0.0099	0.0014	0.0012	0.0032	0.0014	0.0008	0.0000
3	0.0000	0.0001	0.8939	0.0007	0.0107	0.0027	0.0628	0.0367	0.0018	0.0124
4	0.0017	0.0010	0.0009	0.3740	0.4879	0.1338	0.0036	0.0108	0.0001	0.0066
5	0.0006	0.0026	0.0015	0.4883	0.5002	0.0049	0.0173	0.0082	0.0129	0.0155
6	0.0	0.0000	0.0355	0.0109	0.0098	0.2769	0.1226	0.6122	0.0007	0.0084
7	0.0007	0.0002	0.0178	0.0548	0.0295	0.2514	0.5342	0.0437	0.0026	0.1256
8	0.0003	0.0012	0.0765	0.0041	0.0980	0.2972	0.3121	0.1954	0.0993	0.0005
9	0.0000	0.0000	0.0237	0.0093	0.0042	0.1617	0.0951	0.0032	0.7298	0.1596
10	0.0010	0.0003	0.0402	0.0006	0.0000	0.0883	0.0005	0.0210	0.0153	0.9923

11	THE A'' HCH2 STRETCH -----
12	THE A'' HCH2 DEFORMATION -
13	THE OUT-OF-PLANE CH3 WAG
14	THE OUT-OF-PLANE WAG -----
15	THE TORSION -------------

11	0.9913	0.0216	0.0000	0.0072	0.0071
12	0.0052	0.7648	0.2564	0.0001	0.0763
13	0.0005	0.1339	0.4966	0.4634	0.2015
14	0.0003	0.0091	0.1480	0.6285	3.1206
15	0.0000	0.0000	0.0027	0.0391	3.3692

P.E.D. - FOR THE MOLECULE CH3-COF

1 THE ASYM. DCD2 STRETCH ---
2 THE SYMMETRIC CD3 STRETCH
3 THE C=C STRETCH ----------
4 THE C-Z STRETCH ----------
5 THE CD3 UMBRELLA BEND ----
6 THE DCD2 DEFORMATION -----
7 THE IN-PLANE CD3 ROCK ----
8 THE C-C STRETCH ----------
9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------

1	0.9290	0.0688	0.0016	0.0001	0.0007	0.0070	0.0002	0.0000	0.0002	0.0065
2	0.0548	0.9341	0.0012	0.0002	0.0202	0.0001	0.0039	0.0003	0.0011	0.0000
3	0.0003	0.0011	0.9011	0.0112	0.0120	0.0154	0.0682	0.0025	0.0001	0.0097
4	0.0000	0.0000	0.0350	0.3257	0.1159	0.0508	0.0191	0.5283	0.0002	0.0022
5	0.0005	0.0100	0.0013	0.1519	0.6499	0.0029	0.1442	0.0064	0.0681	0.0170
6	0.0079	0.0010	0.0002	0.0149	0.0385	0.8613	0.0813	0.0016	0.0004	0.0132
7	0.0047	0.0003	0.0118	0.0546	0.0543	0.0108	0.3736	0.3312	0.0002	0.2191
8	0.0006	0.0068	0.0780	0.5936	0.0256	0.0004	0.1943	0.0458	0.1343	0.0004
9	0.0000	0.0002	0.0243	0.1867	0.0548	0.0094	0.0998	0.0078	0.6579	0.1457
10	0.0051	0.0005	0.0379	0.0519	0.0212	0.0525	0.0341	0.0020	0.0080	0.9461

11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE CD3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION ------------

11	0.9853	0.0165	0.0114	0.0072	0.0068
12	0.0122	0.4852	0.5302	0.0001	0.0752
13	0.0032	0.2138	0.2110	0.6738	0.1940
14	0.0013	0.0880	0.2208	0.5591	3.0374
15	0.0000	0.0006	0.0030	0.0211	3.3863

P.E.D. - FOR THE MOLECULE CD3-COF

1 THE ASYM. HCH2 STRETCH ---
2 THE SYMMETRIC CH3 STRETCH
3 THE C=O STRETCH ----------
4 THE HCH2 DEFORMATION -----
5 THE CH3 UMBRELLA BEND ----
6 THE IN-PLANE CH3 ROCK ----
7 THE C-C STRETCH ----------
8 THE C-Z STRETCH ----------
9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------

1	0.9917	0.0020	0.0004	0.0001	0.0030	0.0027	0.0013	0.0002	0.0001	0.0006
2	0.0017	1.0021	0.0018	0.0014	0.0010	0.0000	0.0077	0.0000	0.0000	0.0009
3	0.0000	0.0001	0.8990	0.0090	0.0014	0.0062	0.0750	0.0170	0.0000	0.0078
4	0.0022	0.0001	0.0013	0.6349	0.1863	0.1275	0.0381	0.0093	0.0011	0.0158
5	0.0001	0.0013	0.0004	0.1957	0.8474	0.0001	0.0167	0.0085	0.0086	0.0423
6	0.0021	0.0001	0.0260	0.0804	0.0508	0.3883	0.2737	0.1219	0.0405	0.0994
7	0.0000	0.0012	0.0613	0.0006	0.0430	0.2681	0.5774	0.1115	0.0359	0.0002
8	0.0000	0.0	0.0227	0.0018	0.0000	0.1532	0.0765	0.7908	0.0027	0.0585
9	0.0	0.0000	0.0095	0.0029	0.0000	0.1062	0.0722	0.0264	0.9469	0.0019
10	0.0014	0.0	0.0299	0.0000	0.0003	0.1089	0.0008	0.1067	0.0392	0.8752

11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------

11	0.9602	0.0726	0.0053	0.0004	0.0004
12	0.0094	0.7148	0.2740	0.0628	0.0000
13	0.0004	0.2160	0.7514	0.0552	0.1201
14	0.0003	0.0003	0.0657	0.9059	0.0975
15	0.0000	0.0000	0.0005	0.0069	1.1559

P.E.D. - FOR THE MOLECULE CH3-COCL

1 THE ASYM. CCD2 STRETCH ---
2 THE SYMMETRIC CD3 STRETCH
3 THE C=O STRETCH ----------
4 THE CCD2 DEFORMATION -----
5 THE CD3 UMBRELLA BEND ----
6 THE C-C STRETCH ----------
7 THE IN-PLANE CD3 ROCK ----
8 THE C-Z STRETCH ----------
9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------

1	0.9763	0.0005	0.0040	0.0003	0.0000	0.0110	0.0071	0.0017	0.0005	0.0008
2	0.0003	1.0042	0.0031	0.0001	0.0003	0.0027	0.0048	0.0001	0.0000	0.0011
3	0.0014	0.0014	0.9138	0.0111	0.0004	0.0001	0.0739	0.0074	0.0000	0.0063
4	0.0078	0.0001	0.0000	0.1702	0.2581	0.5051	0.0308	0.0117	0.0018	0.0310
5	0.0001	0.0061	0.0007	0.7078	0.0118	0.2732	0.0285	0.0196	0.0283	0.0450
6	0.0001	0.0058	0.0642	0.2711	0.3920	0.0459	0.1925	0.0752	0.0563	0.0000
7	0.0075	0.0002	0.0130	0.0028	0.1576	0.0035	0.4757	0.1838	0.0596	0.1795
8	0.0001	0.0000	0.0221	0.0072	0.1801	0.1086	0.0006	0.7546	0.0016	0.0313
9	0.0000	0.0000	0.0101	0.0046	0.1237	0.0751	0.0106	0.0009	0.9410	0.0000
10	0.0059	0.0000	0.0279	0.0050	0.0529	0.0783	0.0489	0.0290	0.0347	0.8797

11 THE A'' CCD2 STRETCH -----
12 THE A'' OCD2 DEFORMATION -
13 THE OUT-OF-PLANE CD3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------

11	0.9462	0.0755	0.0156	0.0012	0.0004
12	0.0169	0.7064	0.2306	0.1070	0.0000
13	0.0038	0.2264	0.6316	0.1622	0.1191
14	0.0012	0.0022	0.1869	0.7875	0.0919
15	0.0000	0.0000	0.0011	0.0047	1.1576

P.E.D. - FOR THE MOLECULE CD3-COCL

1 THE ASYM. HCH2 STRETCH ---
2 THE SYMMETRIC CH3 STRETCH
3 THE C=O STRETCH ----------
4 THE HCH2 DEFORMATION -----
5 THE CH3 UMBRELLA BEND ----
6 THE IN-PLANE CH3 ROCK ----
7 THE C-C STRETCH ----------
8 THE C-Z STRETCH ----------
9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------

1	0.9839	0.0128	0.0001	0.0013	0.0024	0.0007	0.0005	0.0000	0.0000	0.0010
2	0.0114	0.9918	0.0013	0.0003	0.0016	0.0000	0.0066	0.0001	0.0000	0.0006
3	0.0000	0.0001	0.8830	0.0092	0.0123	0.0066	0.0610	0.0242	0.0050	0.0029
4	0.0019	0.0001	0.0037	0.2699	0.6300	0.0003	0.1096	0.0000	0.0004	0.0087
5	0.0001	0.0020	0.0004	0.6966	0.3540	0.0099	0.0173	0.0046	0.0000	0.0301
6	0.0017	0.0000	0.0236	0.0150	0.0402	0.4878	0.2781	0.1283	0.0	0.0679
7	0.0000	0.0013	0.0630	0.0286	0.0002	0.3281	0.5596	0.1520	0.0046	0.0021
8	0.0000	0.0	0.0197	0.0000	0.0042	0.1258	0.0632	0.5527	0.1620	0.1139
9	0.0	0.0000	0.0064	0.0002	0.0018	0.0804	0.0547	0.1370	0.7969	0.0021
10	0.0013	0.0000	0.0270	0.0006	0.0072	0.0999	0.0003	0.2296	0.0012	0.7744

11 THE A'' HCH2 STRETCH -----
12 THE A'' HCH2 DEFORMATION -
13 THE OUT-OF-PLANE CH3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------

11	0.9705	0.0530	0.0036	0.0	0.0006
12	0.0079	0.7027	0.2873	0.0484	0.0000
13	0.0005	0.2176	0.7188	0.0943	0.1127
14	0.0003	0.0006	0.0576	0.8626	0.2313
15	0.0000	0.0000	0.0007	0.0134	1.2519

P.E.D. - FOR THE MOLECULE CH3-COBR

1 THE ASYM. DCD2 STRETCH ---
2 THE SYMMETRIC CD3 STRETCH
3 THE C=O STRETCH ----------
4 THE DCD2 DEFORMATION -----
5 THE CD3 UMBRELLA BEND ----
6 THE IN-PLANE CD3 ROCK ----
7 THE C-C STRETCH ----------
8 THE C-Z STRETCH ----------
9 THE SCISSORS BEND -------
10 THE O=C-Z ROCK ----------

1	0.9810	0.0032	0.0019	0.0000	0.0083	0.0011	0.0048	0.0006	0.0000	0.0018
2	0.0024	0.9997	0.0019	0.0017	0.0027	0.0002	0.0044	0.0001	0.0	0.0007
3	0.0007	0.0008	0.9022	0.0131	0.0001	0.0008	0.0666	0.0138	0.0034	0.0030
4	0.0071	0.0000	0.0003	0.1451	0.0841	0.7153	0.0544	0.0000	0.0001	0.0181
5	0.0001	0.0079	0.0007	0.6190	0.3477	0.0746	0.0143	0.0215	0.0019	0.0270
6	0.0063	0.0000	0.0123	0.0004	0.0423	0.1281	0.4991	0.2311	0.0005	0.1226
7	0.0000	0.0065	0.0642	0.3746	0.1475	0.2121	0.1939	0.1325	0.0059	0.0023
8	0.0001	0.0000	0.0197	0.0268	0.1489	0.0666	0.0003	0.5417	0.1778	0.0596
9	0.0000	0.0000	0.0066	0.0167	0.0978	0.0403	0.0052	0.1133	0.7870	0.0126
10	0.0054	0.0000	0.0262	0.0189	0.0955	0.0128	0.0589	0.1300	0.0193	0.7748

11 THE A'' DCD2 STRETCH -----
12 THE A'' DCD2 DEFORMATION -
13 THE OUT-OF-PLANE CD3 WAG
14 THE OUT-OF-PLANE WAG -----
15 THE TORSION --------------

11	0.9582	0.0539	0.0150	0.0001	0.0006
12	0.0151	0.6735	0.2784	0.0793	0.0000
13	0.0040	0.2429	0.5826	0.2019	0.1124
14	0.0010	0.0047	0.1509	0.7791	0.2167
15	0.0000	0.0000	0.0013	0.0089	1.2558

P.E.D. - FOR THE MOLECULE CD3-COBR

1 THE C-Z STRETCH ----------
2 THE C=O STRETCH ----------
3 THE SCISSORS BEND -------
4 THE SYMMETRIC CF3 STRETCH
5 THE ASYM. FCF2 STRETCH ---
6 THE C-C STRETCH ----------
7 THE CF3 UMBRELLA BEND ----
8 THE FCF2 DEFORMATION -----
9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----

1	0.9934	0.0064	0.0007	0.0004	0.0	0.0015	0.0006	0.0000	0.0011	0.0001
2	0.0090	0.8907	0.0220	0.0032	0.0000	0.0338	0.0085	0.0005	0.0495	0.0052
3	0.0003	0.0161	0.0932	0.0072	0.0680	0.2884	0.0177	0.0208	0.2755	0.4170
4	0.0000	0.0010	0.0081	0.9657	0.0683	0.0595	0.0406	0.0052	0.0020	0.0039
5	0.0000	0.0021	0.4142	0.0796	0.8184	0.0207	0.0180	0.0272	0.0130	0.0861
6	0.0013	0.0595	0.0405	0.1455	0.0259	1.3958	0.2664	0.0548	0.0844	0.0009
7	0.0000	0.0000	0.0049	0.1968	0.0003	0.0671	0.9684	0.0485	0.5068	0.0034
8	0.0	0.0004	0.0610	0.0046	0.0666	0.0049	0.0223	1.1541	0.0021	0.1419
9	0.0034	0.0915	0.4463	0.0002	0.1260	0.0156	0.0329	0.0131	0.0692	0.2244
10	0.0011	0.0197	0.0461	0.0085	0.0224	0.0199	0.0328	0.0283	0.6145	0.6067

11 THE A'' FCF2 STRETCH -----
12 THE OUT-OF-PLANE WAG -----
13 THE A'' FCF2 DEFORMATION -
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION ------------

11	1.2722	0.0867	0.0539	0.0436	0.0146
12	0.0249	0.2676	0.0003	1.3108	2.3904
13	0.1212	0.0004	1.1830	0.0303	0.0011
14	0.2745	0.4110	0.0072	0.6116	0.0193
15	0.0001	0.0018	0.0	0.0810	3.8859

P.E.D. - FOR THE MOLECULE CF3-COH

1	THE C-Z STRETCH ----------
2	THE C=O STRETCH ----------
3	THE SYMMETRIC CF3 STRETCH
4	THE ASYM. FCF2 STRETCH ---
5	THE SCISSORS BEND -------
6	THE C-C STRETCH ----------
7	THE CF3 UMBRELLA BEND ----
8	THE FCF2 DEFORMATION -----
9	THE O=C-Z ROCK ----------
10	THE IN-PLANE CF3 ROCK ----

1	0.8877	0.1000	0.0002	0.0018	0.0049	0.0048	0.0023	0.0000	0.0025	0.0000
2	0.1053	0.8061	0.0034	0.0064	0.0002	0.0484	0.0052	0.0000	0.0421	0.0054
3	0.0000	0.0014	0.0208	1.0287	0.0002	0.0470	0.0449	0.0040	0.0032	0.0041
4	0.0000	0.0010	1.0871	0.0206	0.1704	0.0472	0.0158	0.0308	0.0217	0.0846
5	0.0001	0.0126	0.0048	0.0042	0.0274	0.3228	0.0251	0.0257	0.3503	0.4313
6	0.0008	0.0808	0.0002	0.1692	0.3809	1.0832	0.2080	0.0485	0.1021	0.0013
7	0.0000	0.0000	0.0048	0.2000	0.0298	0.0525	0.9608	0.0659	0.4780	0.0042
8	0.0000	0.0002	0.1278	0.0056	0.0013	0.0006	0.0243	1.1480	0.0099	0.1401
9	0.0244	0.0472	0.1633	0.0056	0.3477	0.1476	0.0239	0.0032	0.0359	0.2238
10	0.0073	0.0124	0.0916	0.0006	0.0046	0.0018	0.0303	0.0176	0.6425	0.5913

11	THE A'' FCF2 STRETCH -----
12	THE OUT-OF-PLANE WAG -----
13	THE A'' FCF2 DEFORMATION -
14	THE OUT-OF-PLANE CF3 WAG
15	THE TORSION -------------

11	1.2877	0.0706	0.0541	0.0413	0.0173
12	0.0184	0.2062	0.0004	1.1844	2.5843
13	0.1221	0.0011	1.1843	0.0269	0.0017
14	0.2720	0.4713	0.0077	0.5618	0.0108
15	0.0000	0.0003	0.0000	0.0335	3.9344

P.E.D. - FOR THE MOLECULE CF3-COD

1 THE C=C STRETCH ----------
2 THE SYMMETRIC CF3 STRETCH
3 THE ASYM. FCF2 STRETCH ---
4 THE C-Z STRETCH ----------
5 THE C-C STRETCH ----------
6 THE SCISSORS BEND -------
7 THE CF3 UMBRELLA BEND ----
8 THE FCF2 DEFORMATION -----
9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----

1	0.9808	0.0002	0.0036	0.0004	0.0213	0.0005	0.0011	0.0229	0.0005	0.0000
2	0.0000	0.6473	0.3070	0.0242	0.0580	0.0124	0.0201	0.0123	0.0081	0.0
3	0.0006	0.2508	0.8089	0.0828	0.0018	0.0367	0.0006	0.0342	0.0056	0.0179
4	0.0195	0.0144	0.0077	0.5858	0.1228	0.0410	0.1648	0.0262	0.1129	0.0853
5	0.0599	0.2797	0.0360	0.3684	0.5308	0.0026	0.0276	0.0473	0.0031	0.0121
6	0.0095	0.0065	0.0056	0.1752	0.0005	0.0232	0.2851	0.0041	0.3286	0.5015
7	0.0002	0.1798	0.0659	0.0010	0.4540	0.0013	0.1886	0.2546	0.0634	0.0627
8	0.0001	0.0747	0.1785	0.0161	0.0093	0.7378	0.1106	0.0403	0.0312	0.0462
9	0.0489	0.0456	0.0838	0.1057	0.0499	0.0290	0.0067	0.2310	0.0180	0.5452
10	0.0193	0.0430	0.0953	0.0162	0.0204	0.0016	0.0	0.1054	0.6522	0.2624

11 THE A'' FCF2 STRETCH -----
12 THE A'' FCF2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION --------------

11	1.2936	0.0009	0.0494	0.1726	0.1566
12	0.1282	0.9532	0.1319	0.2710	0.1547
13	0.0021	0.0093	0.1157	1.5590	1.8086
14	0.1074	0.0094	1.7086	0.9075	0.2462
15	0.0000	0.0004	0.0003	0.1119	1.5743

P.E.D. - FOR THE MOLECULE CF3-COF

1 THE C=O STRETCH ----------
2 THE SYMMETRIC CF3 STRETCH
3 THE ASYM. FCF2 STRETCH ---
4 THE C-C STRETCH ----------
5 THE C-Z STRETCH ----------
6 THE FCF2 DEFORMATION -----
7 THE CF3 UMBRELLA BEND ----
8 THE SCISSORS BEND -------
9 THE O=C-Z ROCK -----------
10 THE IN-PLANE CF3 ROCK ----

1	0.9950	0.0	0.0015	0.0000	0.0239	0.0018	0.0154	0.0045	0.0002	0.0055
2	0.0000	0.8154	0.1751	0.0115	0.0455	0.0184	0.0103	0.0001	0.0033	0.0002
3	0.0002	0.1644	0.9844	0.0224	0.0015	0.0149	0.0041	0.0387	0.0060	0.0398
4	0.0562	0.2344	0.0235	0.7572	0.4041	0.0462	0.0129	0.0002	0.0001	0.0002
5	0.0385	0.0011	0.0013	0.4365	0.1926	0.0010	0.1431	0.1660	0.1867	0.1071
6	0.0000	0.0420	0.1668	0.0009	0.0067	0.7921	0.0767	0.1087	0.0481	0.0720
7	0.0001	0.1991	0.0308	0.0193	0.5040	0.0038	0.4513	0.0947	0.0435	0.0303
8	0.0061	0.0007	0.0014	0.2281	0.0063	0.0014	0.1226	0.1237	0.3220	0.5611
9	0.0528	0.0209	0.0921	0.1777	0.1237	0.0883	0.0096	0.1910	0.0000	0.3274
10	0.0164	0.0188	0.0915	0.0367	0.0439	0.0167	0.0195	0.0486	0.6288	0.3111

11 THE A'' FCF2 STRETCH -----
12 THE A'' FCF2 DEFORMATION -
13 THE OUT-OF-PLANE WAG -----
14 THE OUT-OF-PLANE CF3 WAG
15 THE TORSION ------------

11	1.3106	0.0123	0.0533	0.1517	0.5986
12	0.1197	0.9497	0.2690	0.2309	0.6343
13	0.0013	0.0109	0.0730	1.3321	4.6149
14	0.1044	0.0301	1.6834	0.8820	2.8237
15	0.0001	0.0005	0.0015	0.1877	1.7338

P.E.D. - FOR THE MOLECULE CF3-COCL

6. Cartesian Displacements

In the following matrices the columns correspond to the normal coordinates Q(n). The rows are divided into groups of three, each group corresponding to the x, y, and z Cartesian coordinates of a given atom in the molecule. See diagrams on page IV-116 for Cartesian coordinate descriptions.

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	Q(14)	Q(15)
	X	0.0	0.0	0.0	-0.001	0.006	0.0	-0.002	0.0	0.0	0.0	0.0	0.026	-0.104	0.145	-0.086
C	Y	0.0	-0.005	0.075	0.092	0.220	-0.061	0.022	-0.163	-0.045	0.117	0.0	0.001	0.005	0.001	0.0
	Z	0.0	-0.004	0.0	-0.202	-0.022	0.0	0.006	-0.113	-0.049	-0.002	0.0	0.0	-0.001	0.0	0.0
	X	0.0	0.0	0.0	0.0	-0.007	-0.002	0.0	0.0	-0.001	0.0	0.090	0.056	0.121	0.0	0.009
C	Y	-0.084	-0.013	0.002	-0.004	-0.044	-0.014	0.049	0.124	-0.038	-0.015	0.0	0.004	0.0	0.0	0.0
	Z	0.033	-0.050	0.004	0.037	0.001	0.079	0.118	0.067	0.131	0.123	0.002	0.005	0.009	0.001	0.0
	X	0.001	0.0	-0.002	-0.010	0.045	0.013	0.002	0.009	-0.011	0.004	0.006	-0.669	-0.239	-0.053	-0.432
H	Y	0.808	0.512	0.045	-0.024	-0.032	-0.042	0.023	0.142	-0.063	-0.003	0.0	-0.002	-0.006	-0.001	0.0
	Z	-0.039	-0.006	-0.012	-0.134	0.375	-0.295	-0.439	0.417	-0.321	0.449	-0.004	0.016	-0.040	-0.010	0.002
	X	0.280	-0.474	-0.020	0.012	-0.295	-0.237	-0.204	0.051	-0.013	0.018	-0.542	-0.073	-0.130	-0.093	0.285
H	Y	0.097	-0.162	-0.011	-0.024	0.402	-0.041	-0.267	-0.075	0.353	-0.167	-0.195	0.421	-0.177	-0.115	-0.349
	Z	-0.101	0.314	0.012	0.038	-0.247	-0.319	-0.392	0.024	0.324	0.074	0.334	0.018	-0.535	-0.219	0.242
	X	-0.280	0.475	0.016	-0.027	0.308	0.237	0.204	-0.022	-0.024	-0.007	-0.543	-0.099	-0.121	-0.089	0.284
H	Y	0.105	-0.173	-0.006	-0.001	0.396	0.026	-0.175	-0.110	0.378	-0.183	0.189	-0.486	0.165	0.118	0.349
	Z	-0.195	0.301	0.013	0.051	-0.372	-0.280	-0.276	0.047	0.269	0.078	-0.344	-0.066	0.483	0.212	-0.240
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.004	0.013	-0.047	0.070
O	Y	0.0	0.0	0.001	-0.067	-0.028	0.064	-0.035	0.037	0.027	-0.062	0.0	0.0	0.0	0.0	0.0
	Z	0.0	0.002	0.0	0.113	0.032	-0.049	0.0	0.012	-0.066	-0.136	0.0	0.0	0.0	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.002	-0.066	0.145	-0.750	-0.341
H	Y	0.020	0.048	-0.956	0.071	0.019	-0.099	0.075	-0.140	-0.011	0.102	0.0	0.0	0.0	0.0	0.0
	Z	0.006	0.005	-0.074	0.215	-0.159	0.626	-0.476	-0.098	-0.213	0.099	0.0	0.0	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CH3-COH

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	Q(14)	Q(15)
	X	0.0	0.0	0.0	0.0	0.0	0.0	-0.002	0.0	0.0	0.0	0.0	0.043	-0.177	-0.017	-0.105
C	Y	0.087	-0.009	0.0	-0.043	-0.194	-0.113	0.003	0.188	0.020	0.123	0.0	0.0	0.0	-0.002	0.0
	Z	0.017	-0.018	0.001	0.143	0.053	-0.114	0.009	0.136	-0.037	0.041	0.0	0.0	0.0	0.0	0.0
	X	0.0	0.001	0.0	0.0	0.0	0.003	-0.002	0.0	-0.004	0.001	0.123	0.067	0.071	0.111	0.0
C	Y	0.003	0.114	-0.026	-0.042	0.063	0.095	-0.068	-0.070	-0.093	0.025	0.0	0.0	0.0	0.0	0.0
	Z	0.008	-0.043	-0.073	-0.015	-0.022	0.182	0.028	0.051	0.097	0.087	0.0	-0.004	0.0	0.003	0.0
	X	0.0	0.005	-0.005	-0.002	0.001	0.023	-0.025	0.016	-0.011	0.0	-0.010	-0.499	-0.109	-0.117	-0.259
D	Y	-0.007	-0.519	0.387	0.027	-0.032	0.114	-0.074	-0.079	-0.098	0.027	0.0	0.0	0.0	0.0	0.0
	Z	-0.007	0.004	0.006	0.050	-0.045	-0.178	0.264	-0.440	-0.149	0.410	0.003	0.056	0.0	-0.025	0.001
	X	0.003	-0.209	-0.319	0.011	-0.014	-0.092	-0.251	-0.085	0.011	0.021	-0.368	-0.020	0.015	-0.071	0.187
D	Y	0.003	-0.088	-0.123	-0.005	-0.006	-0.096	0.259	-0.075	0.219	-0.148	-0.124	0.337	0.046	-0.133	-0.209
	Z	-0.003	0.136	0.207	-0.017	-0.002	-0.100	-0.215	-0.120	0.285	0.045	0.237	0.105	-0.061	-0.381	0.178
	X	-0.004	0.213	0.314	-0.010	0.019	0.114	0.257	0.091	-0.032	-0.017	-0.369	-0.049	0.016	-0.057	0.187
D	Y	0.003	-0.094	-0.123	-0.006	-0.002	-0.100	0.286	-0.077	0.223	-0.150	0.123	-0.343	-0.047	0.132	0.209
	Z	-0.008	0.139	0.218	-0.002	-0.005	-0.139	-0.184	-0.172	0.276	0.059	-0.228	-0.059	0.073	0.386	-0.178
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.009	0.045	-0.017	0.089
O	Y	-0.007	0.008	0.0	0.066	0.109	0.038	-0.011	-0.057	0.010	-0.085	0.0	0.0	0.0	0.0	0.0
	Z	-0.005	0.004	0.0	-0.119	-0.024	-0.006	-0.002	-0.045	-0.093	-0.143	0.0	0.0	0.0	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.003	-0.141	0.685	-0.347	-0.400
H	Y	-0.948	-0.012	-0.017	-0.118	-0.075	-0.083	0.006	0.154	0.022	0.109	0.0	0.0	0.0	0.0	0.0
	Z	-0.305	0.258	0.002	0.455	0.257	0.269	-0.150	-0.532	-0.298	-0.475	0.0	0.0	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CD3-COH

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	C(14)	Q(15)
	X	0.0	0.0	0.0	C.0	0.0	C.C06	0.0	0.004	-0.003	0.0	0.002	0.032	-0.085	-C.189	-0.056
C	Y	0.0	-0.002	-0.121	0.074	-0.001	-0.028	-0.157	-0.031	-0.031	0.112	0.0	-0.003	-0.003	0.0	0.0
	Z	0.0	-0.004	0.022	-0.207	-0.019	-0.002	-0.124	-0.008	-0.028	-0.002	0.0	0.002	0.0	C.0	0.0
	X	-0.001	0.0	0.0	0.0	0.003	-0.006	-0.001	-0.006	0.005	-0.001	0.089	0.053	0.118	0.017	0.C06
C	Y	0.083	-0.014	-0.002	0.002	-0.043	0.042	0.072	0.118	-0.011	-0.021	0.001	0.001	0.008	0.0	0.0
	Z	-0.034	-0.047	-0.007	0.030	0.037	0.125	0.068	0.016	0.135	0.121	-0.007	-0.067	-0.017	-C.003	0.C
	X	0.003	0.C07	0.002	-0.002	-0.026	-0.078	0.013	-0.004	0.002	0.004	0.003	-0.654	-C.279	0.C49	-C.462
H	Y	-0.807	0.513	-0.004	-0.013	-0.C46	0.029	0.075	0.141	-0.026	-0.015	0.0	0.004	0.0	0.0	0.0
	Z	0.028	-0.012	0.058	-0.142	0.508	-0.425	0.300	0.428	-0.277	0.453	-0.004	0.016	-0.041	0.005	0.002
	X	-0.271	-0.473	C.004	0.018	-0.409	-0.303	0.054	0.048	-0.025	0.024	-0.53C	0.064	-C.130	0.101	0.283
H	Y	-0.096	-0.178	0.011	-0.015	0.388	-0.113	0.024	-0.183	0.266	-0.175	-0.194	0.406	-0.147	C.082	-0.377
	Z	0.189	0.305	-0.004	0.043	-0.320	-0.412	0.111	-0.113	0.260	0.069	0.348	0.229	-0.558	C.188	0.227
	X	0.274	0.470	-0.001	-0.023	0.413	0.339	-0.053	-0.026	0.009	-0.020	-0.547	-0.050	-C.195	C.099	0.285
H	Y	-0.096	-0.165	0.004	0.0	0.307	-0.268	0.024	-0.236	0.313	-0.182	0.186	-0.552	0.165	-0.093	0.376
	Z	0.181	0.301	-0.005	0.038	-0.252	-0.364	0.098	-0.118	0.267	0.064	-0.343	-0.067	0.498	-0.172	-0.224
	X	0.0	0.0	0.0	0.0	0.C	0.C	0.0	0.0	0.0	0.0	0.0	-0.004	0.007	0.058	0.063
O	Y	0.0	0.0	0.012	-0.074	-0.014	0.017	0.081	-0.050	-0.006	-0.058	0.0	0.0	0.0	0.0	0.0
	Z	0.0	0.0	-0.017	0.116	0.018	-0.014	-0.021	0.052	-0.054	-0.138	0.0	0.0	0.0	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.001	0.0	0.0	0.0	0.0	0.0	-0.030	0.030	0.453	-0.257
D	Y	-0.002	0.005	0.629	0.171	-0.CC6	-0.007	-0.195	-0.001	0.013	0.100	0.0	0.0	0.0	0.0	0.0
	Z	-0.003	0.0	0.052	0.101	-0.021	0.054	0.273	-0.455	-0.389	0.109	0.0	-0.004	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CH3-COD

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	C(14)	C(15)
	X	0.0	0.0	0.0	0.0	0.0	0.002	0.001	0.0	0.0	0.0	0.0	0.037	0.187	-0.092	-0.073
C	Y	-0.013	-0.018	-0.130	-0.100	-0.106	-0.017	0.019	0.147	-0.002	-0.114	0.0	-0.003	0.0	0.0	0.0
	Z	0.026	0.004	0.042	0.293	-0.132	-0.148	0.103	0.013	-0.022	0.047	0.0	0.0	-0.001	0.0	0.0
	X	0.001	0.0	0.0	0.0	0.0	-0.002	-0.004	-0.002	0.0	0.0	0.125	0.066	-0.117	-0.074	0.0
C	Y	0.130	-0.024	0.017	0.047	0.044	-0.133	0.025	-0.133	-0.061	0.010	0.0	-0.002	0.002	0.001	0.0
	Z	-0.042	-0.067	-0.001	-0.041	0.145	-0.038	0.035	0.007	0.106	-0.090	0.0	0.007	0.002	0.003	0.0
	X	-0.005	0.005	0.0	0.002	-0.020	0.029	0.009	-0.011	0.011	0.0	-0.009	-0.503	0.120	0.082	-0.287
D	Y	-0.519	0.382	-0.049	0.016	0.088	-0.107	-0.016	-0.105	-0.084	-0.015	0.0	0.0	0.0	0.0	0.0
	Z	0.033	0.009	0.021	0.045	-0.157	0.184	0.011	-0.428	-0.161	-0.419	0.009	0.047	-0.010	0.0	0.0
	X	-0.192	-0.309	0.053	0.018	-0.103	-0.130	-0.286	-0.089	-0.004	-0.035	-0.364	0.006	0.009	0.080	0.187
D	Y	-0.087	-0.110	0.020	0.005	-0.126	0.273	0.132	-0.083	0.220	0.146	-0.114	0.367	0.0	0.105	-0.235
	Z	0.147	0.209	-0.026	-0.010	-0.091	-0.043	-0.274	-0.098	0.272	-0.046	0.233	0.050	0.204	0.300	0.160
	X	0.197	0.320	-0.050	-0.008	0.066	0.150	0.267	0.056	0.008	0.026	-0.356	0.028	-0.008	0.071	0.187
D	Y	-0.092	-0.121	0.017	-0.005	-0.087	0.251	0.150	-0.049	0.217	0.156	0.151	-0.303	-0.095	-0.167	0.231
	Z	0.143	0.198	-0.029	-0.017	-0.056	-0.068	-0.254	-0.065	0.270	-0.037	-0.227	-0.060	-0.229	-0.320	-0.162
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.007	-0.038	0.044	0.083
D	Y	0.002	0.002	0.011	0.078	0.061	0.053	-0.050	-0.007	0.009	0.060	0.0	0.0	0.0	0.0	0.0
	Z	0.0	-0.001	-0.018	-0.120	-0.036	-0.008	0.007	-0.032	-0.082	0.129	0.0	0.0	0.0	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	-0.054	-0.272	0.376	-0.311
D	Y	0.008	0.088	0.632	-0.134	-0.140	-0.134	0.102	0.093	0.031	-0.066	0.0	0.0	0.0	0.0	0.0
	Z	-0.085	0.004	-0.014	-0.368	0.331	0.742	-0.532	0.485	-0.262	-0.257	0.0	0.002	-0.002	-0.001	0.0

CARTESIAN DISPLACEMENTS FOR --- C03-C0D

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	C(13)	C(14)	Q(15)
	X	0.0	0.0	0.0	0.0	C.005	-0.001	-0.003	0.0	0.0	0.0	0.002	0.064	-C.144	-0.183	0.089
C	Y	0.0	0.002	-0.202	-0.019	-0.C26	0.102	-0.034	0.086	-0.023	-0.079	0.0	0.005	C.0	0.001	0.0
	Z	0.0	-0.010	0.137	-C.048	-0.C36	0.164	-0.115	-C.007	0.076	-0.012	0.0	0.0	0.0	C.0	C.0
	X	0.0	0.0	0.0	0.006	0.0	0.001	0.0	0.0	0.0	0.0	0.093	0.019	0.127	-C.013	-0.003
C	Y	-0.083	-0.041	0.028	-0.030	-0.066	-0.091	-0.112	0.017	0.028	0.112	0.0	0.003	-0.004	0.002	0.0
	Z	0.010	-0.052	-0.027	-0.102	0.113	-0.089	0.071	0.114	0.143	0.0	0.0	0.0	0.0	0.0	0.0
	X	-0.003	-0.004	-0.008	-0.07C	-C.0e5	0.004	0.037	-0.003	0.0	0.005	-0.045	-0.654	-0.430	-0.046	-0.531
H	Y	0.340	0.740	-0.004	-0.422	0.016	0.052	0.132	-0.089	0.017	0.255	0.008	0.084	-0.007	0.017	-0.004
	Z	0.190	0.453	0.063	0.544	-0.113	-0.351	-0.379	0.300	0.156	-0.251	0.0	0.0	0.0	0.0	0.0
	X	0.484	-0.253	0.032	-0.101	-0.455	-C.157	0.024	0.048	0.017	-0.020	-0.546	-0.014	-0.078	C.238	0.225
H	Y	0.328	-0.124	-0.026	0.523	0.355	C.274	0.039	-0.076	0.032	0.204	-0.319	0.343	0.169	-0.213	-0.445
	Z	-0.172	0.119	-0.033	0.409	-0.393	0.216	0.456	0.042	0.183	0.120	0.210	0.420	-0.343	C.350	-C.158
	X	-0.493	0.245	-0.017	0.070	C.439	0.109	-0.057	-0.039	-0.015	0.015	-0.549	-0.056	-0.067	0.226	0.227
H	Y	0.328	-0.134	-0.023	0.465	0.389	0.250	0.017	-0.074	0.031	0.202	0.330	-0.306	-0.123	0.202	0.445
	Z	-0.179	0.124	-0.027	0.437	-0.468	0.210	0.464	0.048	0.188	0.116	-0.200	-0.359	0.369	-0.350	C.156
	X	0.0	0.0	0.0	0.0	C.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.014	0.033	0.085	C.012
O	Y	0.0	0.0	0.122	0.002	0.020	0.002	0.068	0.105	-0.106	-0.002	0.0	0.0	0.0	0.0	0.0
	Z	0.0	0.0	-0.070	0.013	-0.014	-0.027	-0.037	-0.037	-0.070	0.132	0.0	0.0	0.0	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.008	0.014	0.029	-0.060
F	Y	0.0	0.0	0.011	0.005	0.004	-0.040	0.022	-0.140	0.083	-0.055	0.0	0.0	0.0	0.0	0.0
	Z	0.0	0.0	-0.004	0.008	0.004	-0.031	0.032	-0.059	-0.103	-0.097	0.0	0.0	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CH3-COF

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	Q(14)	Q(15)
	X	0.0	0.0	-0.001	0.0	0.006	-0.002	0.001	-0.002	0.0	0.0	-0.001	0.131	-0.150	-0.149	0.070
C	Y	-0.006	0.005	-0.193	-0.113	0.061	0.043	0.034	0.055	-0.010	0.082	0.0	0.005	0.0	0.002	0.0
	Z	0.0	-0.010	0.129	-0.185	0.079	0.040	-0.079	-0.003	0.052	0.018	0.0	0.0	0.0	0.0	0.0
	X	0.013	-0.004	0.011	0.010	-0.008	-0.031	-0.018	0.023	0.0	0.010	0.141	0.030	0.168	-0.055	0.005
C	Y	0.127	-0.027	0.025	0.025	-0.041	-0.093	-0.115	0.114	0.015	-0.060	0.0	0.010	0.0	0.004	0.0
	Z	-0.007	-0.082	-0.030	0.171	0.160	0.028	0.015	0.060	0.122	0.002	-0.016	-0.013	-0.047	0.016	0.0
	X	0.0	-0.005	0.007	0.029	0.004	0.023	-0.038	0.018	-0.004	0.006	-0.035	-0.374	-0.375	-0.019	-0.363
D	Y	-0.351	0.431	0.014	0.024	0.284	-0.186	0.033	-0.089	-0.004	-0.204	-0.012	-0.036	-0.032	0.0	0.001
	Z	-0.172	0.256	0.048	0.082	-0.348	-0.027	-0.161	0.398	0.168	0.253	-0.018	-0.093	-0.045	-0.017	0.004
	X	-0.275	-0.257	0.014	-0.103	-0.076	-0.274	0.113	0.018	0.026	0.015	-0.356	0.020	0.045	0.132	0.166
D	Y	-0.191	-0.136	-0.006	-0.015	-0.177	0.325	-0.050	-0.023	0.033	-0.161	-0.218	0.125	0.159	-0.146	-0.311
	Z	0.101	0.105	-0.021	-0.112	-0.154	-0.002	0.347	-0.103	0.199	-0.113	0.147	0.288	-0.100	0.316	-0.102
	X	0.273	0.264	-0.017	0.085	0.060	0.274	-0.093	-0.027	-0.023	-0.018	-0.386	-0.030	-0.036	0.150	0.166
D	Y	-0.182	-0.151	-0.008	0.001	-0.116	0.274	-0.054	-0.024	0.026	-0.161	0.211	-0.218	-0.174	0.115	0.316
	Z	0.099	0.106	-0.017	-0.101	-0.167	0.021	0.329	-0.094	0.199	-0.110	-0.129	-0.274	0.150	-0.333	0.102
	X	0.0	0.0	0.0	0.0	-0.001	0.002	0.0	0.0	0.0	0.0	0.001	-0.033	0.038	0.085	0.034
D	Y	0.003	-0.004	0.120	0.033	0.019	0.029	0.111	0.068	-0.094	-0.002	0.0	0.0	0.0	0.0	0.0
	Z	0.0	0.003	-0.074	0.003	-0.038	-0.034	-0.046	0.004	-0.078	-0.134	0.0	0.0	0.0	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.001	0.0	0.0	0.0	0.0	0.0	-0.015	0.015	0.028	-0.073
F	Y	0.0	0.0	0.010	0.041	-0.035	-0.025	-0.054	-0.137	0.068	0.048	0.0	0.0	0.0	0.0	0.0
	Z	-0.002	0.002	-0.002	0.034	-0.032	-0.004	0.013	-0.055	-0.109	0.096	0.0	0.0	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CO3-COF

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	Q(14)	Q(15)
	X	0.0	0.0	0.0	0.001	-0.006	-0.001	0.0	0.0	0.0	0.0	0.001	0.020	-0.099	0.236	0.031
C	Y	0.001	-0.009	0.203	-0.035	0.013	0.087	-0.082	-0.032	0.081	0.053	-0.001	-0.002	-0.004	0.0	0.0
	Z	-0.002	0.0	-0.086	-0.034	0.002	0.147	-0.110	0.124	0.029	-0.020	0.0	-0.002	0.002	0.0	0.0
	X	0.0	0.0	0.0	-0.003	0.004	0.001	0.001	0.0	0.0	0.0	0.098	0.018	0.130	-0.015	-0.009
C	Y	0.041	-0.039	-0.020	-0.022	0.078	-0.035	0.180	0.063	0.075	-0.018	-0.001	0.003	-0.011	-0.002	0.0
	Z	-0.084	-0.019	0.013	-0.042	0.034	-0.126	-0.002	0.073	0.079	0.158	-0.001	0.0	-0.006	-0.001	0.0
	X	0.0	-0.006	0.016	0.037	0.084	-0.015	0.011	-0.010	-0.012	0.014	-0.098	-0.644	-0.450	-0.166	-0.567
H	Y	-0.128	-0.105	0.075	0.679	-0.130	-0.355	-0.253	0.340	0.168	-0.295	-0.002	0.026	-0.036	-0.005	0.002
	Z	0.780	0.524	0.043	0.067	-0.027	-0.201	-0.094	0.120	0.085	0.109	0.003	0.011	0.005	0.001	0.0
	X	0.283	-0.466	-0.013	-0.247	-0.336	-0.107	-0.073	0.030	0.028	-0.019	-0.546	0.031	-0.108	-0.149	0.276
H	Y	-0.201	0.329	-0.061	-0.189	-0.523	0.0	0.169	0.054	0.098	-0.021	0.365	0.110	-0.431	-0.230	0.243
	Z	0.083	-0.133	-0.025	0.362	-0.234	0.241	0.288	-0.083	0.030	0.291	-0.078	0.594	-0.056	-0.042	-0.421
	X	-0.284	0.466	0.023	0.261	0.331	0.118	0.059	-0.025	-0.010	0.018	-0.537	0.097	-0.117	-0.148	0.277
H	Y	-0.197	0.324	-0.060	-0.184	-0.463	0.010	0.179	0.050	0.096	-0.017	-0.372	-0.191	0.460	0.232	-0.246
	Z	0.089	-0.145	-0.011	0.420	-0.091	0.240	0.267	-0.067	0.044	0.279	0.055	-0.527	0.092	0.050	0.421
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.003	0.016	-0.089	0.031
O	Y	0.0	0.002	-0.131	0.023	-0.003	-0.028	-0.078	-0.093	-0.019	0.093	0.0	-0.002	0.002	0.0	0.0
	Z	-0.002	-0.001	0.069	-0.002	0.0	-0.016	0.034	0.045	-0.173	0.035	0.001	0.002	0.004	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	0.003	-0.021	-0.021
CL	Y	0.001	0.0	-0.003	-0.002	0.010	0.005	0.002	0.018	-0.057	-0.043	0.0	-0.005	0.0	0.0	0.0
	Z	0.0	0.0	0.002	0.0	0.003	-0.016	0.009	-0.091	0.037	-0.073	0.0	0.0	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CH3-COCL

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	Q(14)	Q(15)
	X	0.001	0.0	0.0	0.0	0.0	0.003	0.001	0.0	0.0	0.0	0.0	0.030	-0.144	0.211	-0.029
C	Y	-0.012	-0.011	0.223	-0.024	0.058	0.038	-0.063	-0.054	0.062	0.066	0.002	0.004	0.004	0.001	0.0
	Z	0.006	0.0	-0.062	-0.029	0.193	0.132	-0.015	0.095	0.052	-0.026	-0.001	-0.001	-0.003	0.0	0.0
	X	0.002	0.0	0.0	-0.009	-0.003	0.005	0.004	-0.002	0.0	0.001	0.134	0.024	0.138	0.032	0.006
C	Y	0.087	-0.063	-0.037	0.175	-0.037	0.092	0.151	0.004	0.077	-0.020	0.013	0.039	0.019	0.007	0.0
	Z	-0.106	-0.037	-0.013	0.123	-0.043	-0.064	-0.048	0.093	0.089	0.104	0.002	0.005	0.002	0.0	0.0
	X	-0.016	0.0	0.004	0.023	0.020	-0.040	-0.022	0.009	0.004	-0.006	-0.083	-0.455	-0.287	-0.168	0.395
D	Y	-0.143	-0.108	0.019	-0.406	-0.318	-0.017	-0.171	0.292	0.187	-0.291	-0.014	-0.042	-0.020	-0.008	0.0
	Z	0.495	0.375	0.059	-0.050	-0.112	-0.131	-0.161	0.177	0.124	0.034	0.0	0.001	-0.002	0.0	0.0
	X	0.186	-0.306	0.011	-0.081	0.127	-0.322	-0.022	0.036	0.003	-0.018	-0.356	0.011	0.034	-0.083	-0.188
D	Y	-0.143	0.247	-0.031	-0.040	0.210	-0.317	0.228	0.015	0.096	-0.030	0.264	0.053	-0.226	-0.203	-0.195
	Z	0.050	-0.058	-0.011	-0.321	-0.078	-0.003	0.256	-0.031	0.071	0.227	-0.025	0.411	-0.043	-0.079	0.275
	X	-0.181	0.311	-0.024	0.061	-0.129	0.300	0.044	-0.040	-0.020	0.018	-0.362	0.030	0.008	-0.090	-0.190
D	Y	-0.151	0.250	-0.007	-0.071	0.180	-0.331	0.222	0.008	0.091	-0.009	-0.239	-0.049	0.299	0.226	0.198
	Z	0.065	-0.056	-0.028	-0.327	-0.088	0.009	0.291	-0.045	0.049	0.235	0.011	-0.453	0.024	0.071	-0.275
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	0.002	0.030	-0.089	-0.047
D	Y	0.003	0.006	-0.138	-0.033	-0.002	-0.018	-0.103	-0.077	-0.012	0.095	0.0	0.0	0.0	0.0	0.0
	Z	-0.003	0.002	0.047	-0.016	-0.019	-0.032	0.024	0.063	-0.170	0.040	0.0	-0.004	0.0	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	0.006	-0.022	0.029
CL	Y	0.0	0.0	-0.001	-0.001	0.0	0.005	0.007	0.030	-0.061	-0.038	0.0	0.0	0.0	0.0	0.0
	Z	0.0	-0.004	0.0	0.026	-0.022	0.0	-0.010	-0.099	0.014	-0.073	0.0	0.0	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CD3-CDCL

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	Q(14)	Q(15)
	X	0.0	0.0	0.002	-0.004	0.003	-0.001	0.0	0.0	0.0	0.0	0.0	0.028	-0.104	0.232	0.047
C	Y	0.008	-0.008	0.189	0.010	0.022	0.121	-0.095	0.020	-0.103	0.035	0.0	0.002	0.004	0.0	0.0
	Z	0.013	-0.003	-0.114	0.005	0.048	0.235	-0.131	0.201	-0.011	-0.019	0.0	-0.004	-0.002	0.0	0.0
	X	-0.002	0.0	0.003	-0.007	-0.007	-0.008	-0.006	0.001	0.0	0.0	0.095	0.008	0.129	-0.015	-0.012
C	Y	0.043	-0.046	-0.029	0.071	0.059	-0.018	0.169	0.121	-0.070	-0.022	0.003	0.018	0.002	0.0	0.0
	Z	-0.081	-0.016	-0.006	0.083	-0.004	-0.122	-0.010	0.075	-0.044	0.177	0.0	-0.002	-0.004	0.0	0.0
	X	0.014	0.0	-0.029	0.017	-0.011	0.076	0.032	0.0	-0.007	-0.004	-0.079	-0.582	-0.482	-0.129	-0.575
H	Y	-0.147	-0.058	0.098	-0.487	-0.137	-0.564	-0.354	0.393	-0.001	-0.246	0.003	-0.027	0.035	0.006	-0.002
	Z	0.817	0.475	0.032	-0.016	-0.059	-0.187	-0.099	0.109	-0.041	0.153	0.0	-0.007	0.003	0.0	0.0
	X	0.258	-0.486	-0.051	0.046	-0.417	0.003	-0.079	0.0	0.018	-0.020	-0.552	0.031	-0.154	-0.175	0.269
H	Y	-0.174	0.340	-0.084	-0.141	-0.576	0.148	0.146	0.070	-0.067	-0.013	0.336	0.078	-0.520	-0.268	0.219
	Z	0.057	-0.138	0.024	-0.478	-0.033	0.129	0.229	-0.039	-0.086	0.284	-0.107	0.562	-0.044	-0.026	-0.435
	X	-0.250	0.484	0.029	-0.023	0.427	0.022	0.098	0.0	-0.012	0.012	-0.529	0.106	-0.082	-0.162	0.268
H	Y	-0.184	0.344	-0.047	-0.158	-0.609	0.152	0.142	0.050	-0.087	0.019	-0.392	-0.288	0.376	0.241	-0.217
	Z	0.067	-0.141	0.0	-0.444	-0.013	0.158	0.277	-0.062	-0.072	0.290	0.127	-0.499	0.105	0.038	0.434
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.017	-0.092	0.024
O	Y	-0.002	0.002	-0.126	-0.024	0.012	-0.042	-0.066	-0.121	-0.002	0.084	0.0	0.0	0.0	0.0	0.0
	Z	-0.006	0.0	0.076	0.011	-0.018	-0.036	0.043	-0.022	0.207	0.054	0.0	-0.004	-0.002	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	-0.008	-0.009
BR	Y	0.0	0.0	0.0	0.002	0.0	-0.002	0.003	-0.003	0.029	-0.017	0.0	0.0	0.0	0.0	0.0
	Z	0.0	0.0	0.002	-0.001	-0.001	-0.007	0.005	-0.034	-0.033	-0.045	0.0	0.0	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CH3-COBR

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	Q(14)	Q(15)
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	0.045	-0.143	0.209	-0.042
C	Y	0.008	-0.010	0.216	-0.033	0.073	-0.042	-0.061	-0.025	-0.079	-0.069	0.0	0.003	0.001	0.0	0.0
	Z	-0.009	0.002	-0.081	-0.095	0.176	-0.109	-0.003	0.133	0.013	0.0	0.003	-0.006	-0.006	-0.002	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.131	0.010	0.141	0.029	0.008
C	Y	-0.069	-0.063	-0.031	0.125	0.045	0.075	0.137	0.075	-0.066	0.014	0.0	0.0	0.0	0.0	0.0
	Z	0.114	-0.033	-0.005	0.129	-0.054	0.005	-0.077	0.107	-0.032	-0.143	0.0	0.0	0.0	0.0	0.0
	X	0.0	0.0	0.0	-0.001	0.0	0.0	0.001	0.0	0.0	0.0	0.059	-0.409	-0.286	-0.128	0.405
D	Y	0.116	-0.061	0.034	-0.307	-0.267	0.226	-0.192	0.368	-0.050	0.224	0.0	0.0	0.0	0.0	0.0
	Z	-0.521	0.359	0.041	0.052	-0.124	0.025	-0.160	0.168	-0.029	-0.104	0.0	0.0	0.0	0.0	0.0
	X	-0.183	-0.327	0.0	-0.006	-0.168	-0.279	-0.041	0.018	-0.015	0.013	0.364	0.045	-0.009	-0.105	-0.187
D	Y	0.139	0.233	-0.023	-0.002	-0.221	-0.246	0.197	0.017	-0.056	-0.017	-0.242	0.102	-0.288	-0.234	-0.169
	Z	-0.057	-0.079	-0.012	-0.253	-0.083	0.147	0.239	-0.027	-0.033	-0.255	0.062	0.385	-0.033	-0.071	0.296
	X	0.183	0.327	0.0	0.006	0.168	0.279	0.041	-0.018	0.015	-0.013	0.364	0.045	-0.009	-0.105	-0.187
D	Y	0.121	0.233	-0.052	-0.020	-0.178	-0.261	0.216	0.042	-0.068	0.010	0.244	-0.106	0.283	0.233	0.169
	Z	-0.058	-0.080	0.008	-0.277	-0.040	0.123	0.232	-0.003	-0.074	-0.259	-0.062	-0.385	0.033	0.071	-0.296
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	-0.002	0.029	-0.093	-0.041
O	Y	-0.002	0.004	-0.135	-0.026	-0.010	0.010	-0.097	-0.096	-0.007	-0.085	0.0	0.003	0.001	0.0	0.0
	Z	0.003	0.0	0.058	0.010	-0.026	0.008	0.024	-0.006	0.202	-0.029	0.0	0.003	0.001	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.002	-0.009	0.012
BR	Y	0.0	0.0	0.0	0.0	0.002	0.0	0.003	0.001	0.028	0.021	0.0	0.0	0.0	0.0	0.0
	Z	0.0	0.0	0.001	0.004	-0.007	0.007	-0.001	-0.038	-0.035	0.043	0.0	0.0	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CO3-COBR

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	Q(14)	Q(15)
	X	-0.033	-0.355	0.558	-0.119	-0.411	0.569	-0.051	-0.221	-0.208	-0.245	0.196	-0.135	0.246	0.094	-0.098
C	Y	-0.131	0.784	-1.632	-0.363	0.717	-0.712	-0.512	-0.378	0.375	-0.126	-0.310	0.344	-0.973	0.082	-0.009
	Z	0.033	0.107	0.088	-0.057	-0.048	-0.223	-0.020	-0.140	0.121	-0.032	-0.404	-0.195	-0.266	-0.124	0.002
	X	-0.106	0.280	-0.358	0.0	-0.196	0.183	0.019	-0.078	-0.447	0.216	0.011	-0.115	0.009	-0.010	-0.024
C	Y	-0.033	-0.923	1.523	-1.090	-1.644	1.211	-0.903	-0.948	-0.420	-0.031	0.591	0.203	0.517	0.152	-0.001
	Z	-0.072	-0.129	0.026	-0.716	-0.599	0.353	-0.638	-0.962	0.049	0.006	-0.237	-0.300	0.132	-0.140	0.005
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.097	-0.029	0.009	0.014	-0.045
F	Y	-0.013	-0.025	0.138	-0.215	0.145	-0.006	-0.155	-0.053	-0.020	0.040	0.0	0.0	0.0	0.0	0.0
	Z	-0.004	-0.082	0.327	0.045	0.313	0.008	-0.220	0.556	0.077	-0.087	0.0	0.0	0.0	0.0	0.0
	X	0.036	-0.061	0.103	0.114	0.035	0.042	-0.048	-0.097	0.061	-0.073	-0.021	0.111	-0.003	0.041	0.014
F	Y	0.047	-0.010	0.003	0.150	0.181	-0.166	0.046	0.218	0.179	-0.032	-0.309	-0.191	0.005	-0.128	-0.008
	Z	0.087	-0.260	0.453	0.140	0.317	-0.081	0.129	0.397	0.378	-0.260	0.188	0.042	0.012	-0.020	0.063
	X	0.018	0.009	-0.035	-0.080	-0.002	-0.075	0.084	0.130	0.007	0.047	-0.075	-0.002	0.097	-0.007	0.016
F	Y	0.017	0.069	-0.091	0.113	0.127	-0.129	0.006	0.188	0.074	0.030	-0.325	-0.259	-0.198	-0.118	0.014
	Z	0.036	-0.117	0.239	0.340	0.212	0.088	0.379	0.403	0.045	-0.157	-0.188	-0.042	-0.012	0.020	-0.063
	X	0.0	0.0	0.0	-0.003	0.0	-0.001	-0.004	0.0	0.002	0.0	0.008	0.028	0.0	-0.069	0.147
O	Y	-0.020	-0.260	0.792	-0.101	-0.253	0.490	-0.143	0.194	-0.181	-0.307	0.155	-0.172	0.486	-0.041	0.005
	Z	0.072	-0.325	0.344	-0.026	-0.126	-0.057	-0.058	0.039	-0.057	-0.061	-0.039	-0.091	0.086	-0.038	0.002
	X	0.0	0.0	0.001	-0.007	0.0	-0.003	-0.008	-0.002	0.004	0.0	0.091	0.264	0.007	-0.737	-0.565
H	Y	-1.273	0.305	-0.773	-0.154	-0.281	0.546	-0.123	-0.493	-0.669	-0.180	0.0	0.0	0.0	0.0	0.0
	Z	1.308	-0.376	-0.780	0.010	-3.144	-3.108	2.054	-3.615	1.640	4.234	-3.486	-3.001	-0.242	-1.545	0.045

CARTESIAN DISPLACEMENTS FOR --- CF3-COH

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	Q(14)	Q(15)
	X	0.000	0.007	0.020	-0.002	-0.002	-0.001	0.003	0.011	0.012	-0.008	-0.035	-0.235	-0.066	0.067	-0.071
C	Y	0.167	0.108	0.067	0.024	-0.183	-0.036	0.095	-0.013	0.066	0.057	-0.017	-0.015	0.001	-0.006	0.0
	Z	-0.056	-0.260	-0.036	0.025	-0.004	-0.255	0.036	0.019	0.011	0.032	0.008	0.007	0.0	0.003	0.0
	X	-0.003	-0.004	-0.011	0.018	0.005	0.007	0.019	-0.006	-0.015	0.004	0.220	0.043	-0.069	0.071	-0.019
C	Y	-0.017	-0.032	-0.223	0.103	0.027	0.017	0.055	-0.079	-0.079	0.070	0.025	0.013	-0.017	0.006	0.0
	Z	0.0	0.005	0.110	0.188	0.080	0.103	0.182	0.092	-0.049	0.008	-0.029	-0.036	-0.013	-0.013	0.0
	X	0.0	0.0	0.003	-0.005	-0.001	-0.002	-0.006	0.004	0.003	0.0	0.007	-0.007	0.150	0.014	-0.048
F	Y	-0.002	0.009	0.082	-0.106	0.094	-0.020	0.051	-0.059	-0.070	0.062	0.0	0.0	0.0	0.0	0.0
	Z	0.005	0.011	0.006	-0.028	0.002	0.017	-0.121	0.057	0.0	0.120	0.014	0.012	0.0	0.005	0.0
	X	0.002	-0.002	0.054	0.075	0.012	-0.013	-0.068	-0.116	0.028	0.009	-0.073	0.042	-0.031	0.009	0.019
F	Y	0.0	0.0	0.008	0.018	-0.001	0.006	-0.072	0.062	0.029	-0.018	-0.038	-0.012	-0.110	-0.028	-0.020
	Z	0.004	0.013	-0.036	-0.052	0.006	0.031	0.013	-0.057	0.095	-0.019	0.038	-0.088	0.0	-0.092	0.052
	X	-0.001	0.003	-0.050	-0.079	-0.013	0.012	0.064	0.118	-0.024	-0.010	-0.071	0.045	-0.029	0.010	0.019
F	Y	-0.002	-0.002	0.008	0.015	-0.002	0.005	-0.077	0.065	0.029	-0.017	0.026	0.006	0.119	0.025	0.020
	Z	0.002	0.011	-0.038	-0.048	0.008	0.032	0.016	-0.056	0.091	-0.017	-0.045	0.082	0.002	0.090	-0.052
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.008	0.027	0.0	-0.087	0.139
O	Y	-0.030	-0.084	0.0	-0.016	0.007	0.071	-0.010	-0.023	-0.008	-0.134	0.0	0.0	0.0	0.0	0.0
	Z	0.029	0.115	-0.026	0.012	0.020	-0.088	-0.042	-0.007	-0.118	-0.123	0.0	0.0	0.0	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.043	0.127	-0.003	-0.453	-0.475
O	Y	-0.594	0.231	0.005	0.053	-0.099	-0.184	0.095	0.011	0.125	0.060	0.0	0.0	0.0	0.0	0.0
	Z	0.032	0.287	0.393	-0.163	-0.733	0.725	-0.069	-0.160	-0.414	-0.100	0.0	0.0	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CF3-COD

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	Q(14)	Q(15)
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.024	-0.069	0.118	-0.212	0.081
C	Y	0.226	-0.011	-0.012	0.055	-0.073	-0.013	0.044	-0.092	-0.015	-0.054	0.0	0.0	0.0	0.0	0.0
	Z	-0.042	-0.053	-0.041	0.244	0.0	0.015	-0.076	0.034	0.0	-0.010	-0.002	0.0	0.003	-0.001	0.0
	X	0.0	0.0	0.0	0.001	0.0	0.0	0.0	0.0	0.0	0.0	0.227	-0.078	-0.121	0.018	0.009
C	Y	-0.016	0.035	0.231	0.048	0.085	-0.063	0.008	0.005	0.069	-0.034	0.0	0.0	0.0	0.0	0.0
	Z	0.008	0.221	-0.006	-0.004	-0.127	-0.024	-0.048	0.033	0.045	0.006	0.0	0.0	0.0	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.004	0.143	0.002	-0.044	-0.075
F	Y	0.003	-0.067	-0.021	-0.031	-0.059	-0.110	-0.079	0.059	-0.056	0.032	0.0	0.0	0.0	0.0	0.0
	Z	0.0	-0.090	-0.022	-0.063	-0.017	-0.038	0.016	0.030	0.159	-0.042	0.0	0.0	0.0	0.0	0.0
	X	0.0	0.045	-0.072	0.012	0.086	-0.098	0.006	-0.041	0.014	0.002	-0.078	-0.031	-0.027	0.016	0.038
F	Y	-0.003	0.023	-0.055	0.002	0.042	0.072	0.043	0.050	0.024	-0.014	-0.059	-0.076	-0.076	-0.025	-0.046
	Z	0.003	-0.008	0.010	-0.006	0.0	0.020	0.035	-0.061	-0.010	0.089	0.013	-0.076	0.098	0.041	-0.064
	X	0.0	-0.045	0.072	-0.012	-0.086	0.098	-0.006	0.041	-0.014	-0.002	-0.078	-0.031	-0.027	0.016	0.038
F	Y	-0.003	0.023	-0.055	0.003	0.042	0.072	0.042	0.049	0.024	-0.013	0.059	0.076	0.077	0.025	0.046
	Z	0.002	-0.009	0.010	-0.006	0.001	0.020	0.035	-0.061	-0.010	0.089	-0.013	0.076	-0.098	-0.041	0.064
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.005	0.010	0.050	0.141	0.096
O	Y	-0.149	0.001	-0.011	0.003	-0.088	-0.032	0.083	-0.090	-0.040	-0.052	0.0	0.0	0.0	0.0	0.0
	Z	0.027	0.014	0.024	-0.022	0.037	-0.045	0.090	0.129	-0.120	0.004	0.002	0.0	-0.002	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.003	0.004	0.012	0.015	-0.140
F	Y	-0.004	0.008	0.004	-0.044	0.042	0.038	-0.109	-0.026	0.007	0.095	0.0	0.0	0.0	0.0	0.0
	Z	-0.003	-0.012	0.012	-0.059	0.065	0.040	-0.083	-0.061	-0.068	-0.138	0.0	0.0	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CF3-COF

		Q(1)	Q(2)	Q(3)	Q(4)	Q(5)	Q(6)	Q(7)	Q(8)	Q(9)	Q(10)	Q(11)	Q(12)	Q(13)	Q(14)	Q(15)
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.020	-0.076	0.099	-0.207	0.114
C	Y	-0.230	-0.009	-0.007	-0.025	0.082	0.039	-0.105	-0.025	-0.002	-0.053	0.0	0.0	0.0	0.0	0.0
	Z	0.021	-0.032	-0.017	-0.266	0.032	-0.021	0.046	0.0	0.025	0.017	0.002	0.002	0.002	0.0	0.0
	X	-0.001	-0.001	0.0	0.001	0.0	0.0	-0.002	0.0	0.0	0.0	-0.224	-0.071	-0.130	0.018	0.007
C	Y	0.009	-0.004	0.224	-0.037	-0.074	-0.077	-0.045	0.005	0.065	-0.035	0.001	0.0	0.002	0.0	0.0
	Z	-0.001	0.212	0.059	0.054	0.110	-0.043	0.043	0.018	0.058	0.025	0.003	0.005	0.0	0.0	0.0
	X	0.0	0.0	0.0	-0.001	0.0	0.0	0.0	0.0	0.0	0.0	-0.009	0.140	0.023	-0.049	-0.079
F	Y	-0.001	-0.074	-0.029	0.020	0.068	-0.123	0.037	0.017	-0.063	0.039	0.0	0.0	0.0	0.0	0.0
	Z	0.0	-0.080	-0.048	0.067	0.027	-0.036	0.014	0.043	0.157	-0.023	0.0	0.0	0.0	0.0	0.0
	X	0.002	0.043	-0.064	-0.020	-0.074	-0.089	-0.078	-0.037	0.019	0.0	0.079	-0.025	-0.032	0.020	0.046
F	Y	0.004	0.034	-0.048	-0.011	-0.057	0.062	0.026	0.064	0.025	-0.016	0.062	-0.059	-0.089	-0.032	-0.051
	Z	-0.003	-0.035	0.017	0.004	-0.038	0.047	-0.068	-0.039	-0.009	0.100	-0.005	-0.093	0.088	0.028	-0.070
	X	0.0	-0.044	0.065	0.018	0.073	0.089	0.078	0.036	-0.018	0.001	0.079	-0.026	-0.032	0.020	0.046
F	Y	0.004	0.034	-0.048	-0.012	-0.057	0.061	0.027	0.063	0.025	-0.016	-0.063	0.058	0.089	0.032	0.051
	Z	-0.003	-0.035	0.016	0.005	-0.038	0.048	-0.067	-0.038	-0.009	0.099	0.006	0.094	-0.087	-0.029	0.070
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.005	0.004	0.049	0.148	0.081
O	Y	0.150	0.012	-0.019	0.004	0.114	0.041	-0.116	-0.012	-0.015	-0.052	0.0	0.0	0.0	0.0	0.0
	Z	-0.011	-0.020	0.028	0.017	-0.061	-0.035	-0.056	0.155	-0.115	-0.003	-0.001	-0.002	0.0	0.0	0.0
	X	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	0.0	0.012	0.001	-0.084
CL	Y	0.003	0.002	0.001	0.023	-0.029	-0.005	0.055	-0.063	-0.009	0.048	0.0	0.0	0.0	0.0	0.0
	Z	0.002	0.029	-0.015	0.024	0.004	0.003	0.058	-0.059	-0.050	-0.107	0.0	0.0	0.0	0.0	0.0

CARTESIAN DISPLACEMENTS FOR --- CF3-COCL

7. Significance Matrix

Each significance matrix requires three pages to complete. The columns correspond to each of the normal coordinates while the rows are the appropriately labeled force constants. The elements of the significance matrix are the changes (in wave numbers) of each normal coordinate for an increase of 0.01 millidynes/Å in the indicated force constant.

SIGNIFICANCE MATRIX ------- CH3-COH

1 K (C=O)	0.00	0.0	0.00	0.60	0.03	0.07	0.01	-0.00	0.02	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	0.00	0.01	3.24	-0.00	0.0	0.0	0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.00	0.00	0.00	0.17	0.0	0.05	0.07	0.61	0.24	0.08	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	0.89	2.10	0.00	-0.00	-0.00	0.0	0.00	-0.00	0.00	0.00	3.12	0.00	0.00	0.00	-0.00
5 K(C-X)*	2.30	0.74	0.00	0.0	0.0	-0.00	0.00	-0.00	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.01	0.0	0.03	0.04	0.01	0.03	0.01	0.82	0.00	1.42	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	-0.00	0.0	0.00	1.01	0.13	2.88	1.61	0.31	0.12	0.10	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.01	-0.00	0.01	1.47	0.05	2.31	1.35	0.12	0.11	0.75	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.02	0.01	0.0	0.08	5.62	0.11	2.46	0.05	0.56	0.00	0.06	12.78	0.77	0.06	0.00
10 H(XCX)*	0.04	0.01	-0.00	0.00	6.58	2.53	1.65	0.21	0.10	0.09	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.01	0.01	0.00	0.05	0.01	1.28	2.98	0.60	2.33	0.12	0.02	0.79	8.57	0.52	0.09
12 H(XCC)*	0.02	0.01	0.01	0.43	1.10	0.44	1.40	1.55	1.99	0.56	0.0	0.0	0.0	0.0	0.0
13 H (WAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.63	3.20	0.01
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02	1.41	24.68
15 F (X--X)	0.58	4.46	0.02	0.03	2.72	0.06	1.31	0.01	0.27	-0.00	1.58	6.22	0.34	0.03	0.00
16 F(X--X)*	0.95	2.58	0.00	0.00	3.02	1.38	0.89	0.12	0.04	0.04	-0.21	0.0	0.00	0.0	-0.00
17 F (X--C)	1.38	1.46	0.00	0.48	0.62	0.56	1.69	2.76	3.63	0.65	1.40	0.47	5.19	0.32	0.06
18 F (O--C)	0.00	0.01	0.01	0.01	0.01	0.11	0.06	0.19	0.36	1.28	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.01	0.02	1.73	0.41	0.03	0.99	1.14	0.73	0.37	0.21	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	0.00	0.00	1.93	0.17	0.12	1.68	0.89	0.11	0.03	0.03	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.42	0.96	0.03	0.26	1.35	0.63	2.12	2.03	4.25	6.87	1.43	0.51	5.30	-0.01	5.40
22 C(X--X')	0.29	0.24	1.65	0.91	0.05	6.47	0.79	0.54	5.11	0.96	0.45	0.61	7.17	1.13	2.07
23 MOL.TEN.	-0.05	-0.03	-0.00	-0.03	-0.27	-1.85	-5.01	-1.13	-2.39	-0.36	-0.05	-0.25	-4.12	0.01	-0.03
24 CC..CX*	-0.01	-0.13	-0.01	-0.01	0.0	-0.00	0.01	-0.03	0.01	-0.02	0.0	0.0	0.0	0.0	0.0
25 CC..CX	0.01	-0.31	-0.01	-0.02	0.00	0.02	0.02	-0.07	-0.03	0.02	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CH3-COH

26 CC..CO	0.0	0.00	0.01	-0.63	0.00	0.11	-0.05	0.02	0.16	0.04	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	0.00	0.01	-0.15	-0.02	-0.00	-0.02	-0.02	-0.12	-0.06	0.01	0.0	0.0	0.0	0.0	0.0
28 CC..XCX'	-0.00	0.02	-0.00	-0.04	-0.06	0.78	0.71	-0.79	0.29	-0.17	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	0.00	0.03	-0.00	0.36	0.30	0.19	1.22	0.39	-1.09	0.01	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	0.0	-0.02	-0.01	0.25	0.01	-0.67	-1.34	-1.74	2.14	-0.27	0.0	0.0	0.0	0.0	0.0
31 CC..CCX'	0.00	-0.02	0.01	-0.52	-0.04	-0.29	-0.66	1.93	-1.43	0.41	0.0	0.0	0.0	0.0	0.0
32 CC..OCZ	0.0	-0.00	0.00	0.83	0.02	0.76	-0.70	0.83	-0.36	-0.18	0.0	0.0	0.0	0.0	0.0
33 CC..OCC	0.0	0.00	-0.01	0.17	-0.00	-0.08	0.06	-1.41	0.03	0.64	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	0.0	0.0	0.01	-0.97	-0.01	-0.66	0.66	0.51	0.31	-0.49	0.0	0.0	0.0	0.0	0.0
35 CX'..CH	-3.51	3.23	0.01	0.00	-0.00	0.00	0.00	0.00	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
36 CX'.XCX'	0.63	-0.17	0.0	0.00	-0.17	-0.06	0.06	0.02	0.01	0.02	0.0	0.0	0.0	0.0	0.0
37 CX'..XCX	-0.58	-0.29	0.00	-0.01	0.08	-0.01	0.08	-0.01	-0.04	-0.00	0.0	0.0	0.0	0.0	0.0
38 CX'..CCX	0.48	0.29	0.01	-0.01	0.01	0.01	-0.18	0.03	0.03	0.03	0.0	0.0	0.0	0.0	0.0
39 CX'.CCX'	-0.38	0.20	-0.02	0.02	-0.06	0.01	-0.08	-0.06	-0.05	-0.05	0.0	0.0	0.0	0.0	0.0
40 CX..CX3	0.97	2.01	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	-3.12	-0.00	-0.00	-0.00	-0.00
41 CX..XCX'	-0.47	-0.39	0.00	0.00	-0.08	0.09	0.08	0.03	-0.02	-0.02	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	0.28	-0.33	0.00	-0.01	-0.05	0.02	0.07	-0.01	0.03	0.00	0.92	-0.29	0.07	-0.01	-0.00
43 CX4.XCX4	0.28	-0.33	0.00	-0.01	-0.05	0.02	0.07	-0.01	0.03	0.00	-0.82	0.08	-0.09	0.01	0.00
44 CX4.CCX3	-0.18	0.36	0.01	-0.00	-0.00	-0.07	-0.12	0.04	-0.09	-0.01	0.57	0.04	0.21	0.03	-0.00
45 CX4.CCX'	0.36	0.47	-0.02	0.02	-0.01	-0.06	-0.12	-0.12	0.06	0.04	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	-0.18	0.36	0.01	-0.00	-0.00	-0.07	-0.12	0.04	-0.09	-0.01	-0.53	-0.05	-0.32	-0.03	0.00
47 CO..CZ	0.0	0.0	-0.24	0.04	-0.01	-0.02	0.00	-0.00	-0.02	0.00	0.0	0.0	0.0	0.0	0.0
48 CO..OCZ	0.00	0.0	0.01	-1.54	0.13	0.86	0.20	0.01	-0.12	-0.04	0.0	0.0	0.0	0.0	0.0
49 CO..OCC	-0.00	0.0	-0.02	-0.32	-0.04	-0.09	-0.02	-0.03	0.01	0.15	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.00	0.0	0.01	1.89	-0.06	-0.78	-0.22	0.01	0.10	-0.12	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CH3-COH

51 CZ..OCZ	0.0	-0.00	-0.24	-0.07	-0.02	-0.15	0.06	-0.08	0.04	-0.02	0.0	0.0	0.0	0.0	0.0
52 CZ..OCC	-0.00	0.00	0.61	-0.01	0.01	0.01	-0.00	0.12	-0.00	0.05	0.0	0.0	0.0	C.0	0.0
53 CZ..ZCC	0.01	-0.00	-0.31	0.05	0.01	0.09	-0.08	-0.05	-0.04	-0.05	0.0	0.0	0.0	0.0	0.0
54 XCX*.XCX	-0.08	0.04	0.0	-0.04	-6.76	-6.24	4.52	-0.36	-0.81	-0.03	0.0	0.0	0.0	0.0	0.0
55 XCX*.CCX	0.06	-0.03	0.0	-0.03	1.04	-3.74	-10.23	0.95	1.01	0.28	0.0	0.0	0.0	0.0	0.0
56 XCX*CCX*	-0.05	-0.02	0.0	0.12	5.13	-1.78	-3.67	-1.35	-1.09	-0.50	0.0	0.0	0.0	0.0	0.0
57 XCX..XCX	0.02	0.01	0.0	0.09	5.91	0.09	2.15	0.05	0.54	0.00	-0.06	-12.96	-0.86	-0.07	-0.00
58 XCX..CCX	-0.03	-0.03	0.00	0.13	1.46	-0.90	-6.32	-0.42	-2.58	-0.02	0.08	-6.00	4.54	-0.43	0.02
59 XCX.CCX*	0.06	-0.03	-0.00	-0.45	-4.68	-1.12	-7.09	0.58	2.84	-0.01	0.0	0.0	0.0	0.0	0.0
60 XCX5CCX4	-0.03	-0.03	0.00	0.13	1.46	-0.90	-6.32	-0.42	-2.58	-0.02	-0.08	6.65	-5.82	0.32	-0.03
61 CCX.CCX*	-0.04	0.04	-0.01	-0.37	0.20	2.47	4.91	-2.57	-6.62	-0.83	0.0	0.0	0.0	0.0	0.0
62 CCX5CCX4	0.01	0.01	0.00	0.05	0.01	1.28	2.98	0.60	2.33	0.12	-0.02	-0.78	-8.55	-0.66	-0.09
63 CCX*.OCZ	-0.00	0.00	0.01	-1.26	-0.37	-2.44	3.06	1.31	0.90	-0.51	0.0	0.0	0.0	0.0	0.0
64 CCX*.OCC	-0.03	-0.00	-0.03	-0.27	0.27	0.23	-0.26	-2.26	-0.09	1.74	0.0	0.0	0.0	0.0	0.0
65 CCX*.ZCC	0.03	0.0	0.02	1.59	0.54	1.93	-2.84	0.83	-0.95	-1.34	0.0	0.0	0.0	0.0	0.0
66 OCZ..OCC	0.00	-0.00	-0.02	0.42	-0.08	-0.55	-0.30	-1.06	-0.02	-0.82	0.0	0.0	0.0	0.0	0.0
67 OCZ..ZCC	-0.00	0.0	0.01	-2.27	-0.09	-4.30	-4.16	0.38	-0.25	0.55	0.0	0.0	0.0	0.0	0.0
68 OCC..ZCC	-0.02	0.0	-0.03	-0.49	0.06	0.55	0.28	-0.66	0.02	-2.14	0.0	0.0	0.0	0.0	0.0
69 WAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	-0.02	-0.16	-4.22	-1.23
70 M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.02	-0.27	-5.80	3.13	-0.08
71 M.DF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.04	1.23	-1.90	-1.51	-0.01

SIGNIFICANCE MATRIX ------- CD3-COH

1 K (C=O)	0.00	0.0	0.0	0.63	0.08	0.01	0.00	0.00	0.02	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	3.25	0.0	0.00	0.0	0.0	0.01	-0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.00	0.0	0.02	0.17	0.01	0.71	0.00	0.13	0.12	0.06	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	0.00	0.75	1.40	0.0	0.0	0.00	0.00	0.01	0.00	0.00	2.31	0.00	0.0	0.00	0.00
5 K(C-X)'	0.0	1.56	0.66	0.00	-0.00	0.00	0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.03	0.03	0.0	0.04	0.07	0.23	0.03	0.74	0.10	1.08	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	0.01	0.00	0.0	1.00	4.73	0.00	0.00	0.27	0.11	0.06	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.01	0.06	0.0	1.43	3.62	0.26	0.02	0.11	0.00	0.63	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.0	0.05	0.05	0.01	0.00	2.13	2.61	1.09	0.72	0.00	0.16	9.03	0.73	0.12	0.00
10 H(XCX)'	0.0	0.12	0.03	0.00	0.01	0.59	6.90	0.47	0.01	0.15	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.00	0.03	0.05	0.03	0.00	2.15	0.21	0.19	2.77	0.19	0.07	0.42	0.88	6.17	0.08
12 H(XCC)'	0.01	0.07	0.03	0.19	0.00	0.52	0.10	2.68	1.10	0.96	0.0	0.0	0.0	0.0	0.0
13 H (WAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.08	3.62	0.13	0.01
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.04	1.07	0.48	19.69
15 F (X--X)	0.00	0.14	3.17	0.00	-0.00	1.21	1.28	0.60	0.36	-0.00	0.96	4.47	0.37	0.05	0.00
16 F(X--X)'	0.00	0.66	1.62	0.01	0.01	0.33	3.45	0.31	0.00	0.06	-0.16	-0.00	-0.00	-0.00	0.00
17 F (X--C)	0.01	0.84	0.93	0.42	0.01	0.53	0.15	2.97	3.22	0.91	0.88	0.23	0.55	3.79	0.05
18 F (O--C)	0.01	0.01	0.02	0.02	0.05	0.36	0.02	0.18	0.38	0.96	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	1.75	0.03	0.01	0.40	1.86	1.03	0.00	0.27	0.08	0.18	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	1.93	0.0	0.0	0.17	2.72	-0.00	0.00	0.09	0.03	0.01	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.02	0.28	0.55	0.11	0.15	0.80	0.37	2.01	3.97	6.58	0.94	0.32	1.42	2.58	4.38
22 C(X--X')	1.57	0.32	0.19	0.90	5.46	0.51	0.25	1.38	3.59	1.02	0.26	0.23	-0.05	6.93	1.57
23 MOL.TEN.	-0.00	-0.16	-0.08	-0.05	-0.01	-2.84	-0.74	-2.16	-2.00	-0.61	-0.14	-0.40	-0.98	-2.12	-0.03
24 CC..CX'	0.00	0.01	-0.26	-0.04	-0.01	0.10	-0.00	0.00	-0.01	-0.01	0.0	0.0	0.0	0.0	0.0
25 CC..CX	0.00	-0.00	-0.52	0.02	0.01	0.11	0.01	-0.07	0.00	0.02	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CD3-CDH

26 CC..CO	0.00	-0.00	0.00	-0.64	0.06	0.15	-0.00	-0.02	0.09	0.02	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	-0.13	-0.00	-0.01	-0.02	-0.00	-0.15	0.00	-0.03	-0.02	0.01	0.0	0.0	0.0	0.0	0.0
28 CC..XCX'	-0.00	0.00	0.05	0.05	0.02	1.37	0.15	-0.59	-0.08	-0.19	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	-0.00	0.0	0.10	0.13	0.02	3.49	-0.24	-1.15	-0.85	0.01	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	-0.00	0.00	-0.10	0.18	-0.02	-3.49	-0.06	0.45	1.60	-0.30	0.0	0.0	0.0	0.0	0.0
31 CC..CCX'	0.01	-0.00	-0.05	-0.35	-0.01	-1.18	0.03	1.15	-0.74	0.46	0.0	0.0	0.0	0.0	0.0
32 CC..OCZ	0.00	0.0	-0.00	0.82	0.47	-0.11	-0.00	0.36	-0.23	-0.12	0.0	0.0	0.0	0.0	0.0
33 CC..OCC	-0.01	0.0	0.0	0.16	-0.05	-0.79	0.01	-0.64	0.22	0.49	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	0.01	-0.00	0.01	-0.96	-0.36	0.83	-0.01	0.24	0.01	-0.39	0.0	0.0	0.0	0.0	0.0
35 CX'..CH	-0.00	-3.00	2.72	-0.00	-0.00	0.01	-0.01	-0.00	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
36 CX'.XCX'	-0.00	0.86	-0.26	-0.00	-0.00	0.09	-0.29	-0.01	0.00	0.02	0.0	0.0	0.0	0.0	0.0
37 CX'..XCX	-0.00	-0.77	-0.52	-0.01	-0.01	0.23	0.16	-0.03	0.02	-0.00	0.0	0.0	0.0	0.0	0.0
38 CX'..CCX	-0.00	0.64	0.52	-0.02	0.01	-0.30	0.06	0.00	-0.10	0.03	0.0	0.0	0.0	0.0	0.0
39 CX'.CCX'	0.00	-0.63	0.28	0.04	0.01	-0.10	-0.03	-0.01	0.02	-0.06	0.0	0.0	0.0	0.0	0.0
40 CX..CX5	-0.00	0.77	1.39	0.00	-0.00	0.00	0.00	0.00	-0.00	0.00	-2.32	-0.00	-0.00	-0.00	-0.00
41 CX..XCX'	-0.00	-0.79	-0.53	0.00	0.01	0.10	0.20	0.13	-0.00	-0.03	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	0.00	0.41	-0.52	0.00	0.00	0.13	-0.15	0.14	-0.02	0.00	1.26	-0.38	-0.03	0.01	0.00
43 CX4.XCX4	0.00	0.41	-0.52	0.00	0.00	0.13	-0.15	0.14	-0.02	0.00	-1.19	0.24	0.02	-0.02	0.00
44 CX4.CCX5	0.0	-0.29	0.54	0.01	-0.00	-0.17	-0.04	-0.06	0.00	-0.02	0.85	0.06	-0.03	0.07	-0.00
45 CX4.CCX'	0.00	0.65	0.58	-0.04	-0.01	-0.11	0.04	-0.36	-0.03	0.06	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	0.0	-0.29	0.54	0.01	-0.00	-0.17	-0.04	-0.06	0.00	-0.02	-0.81	-0.07	0.02	-0.15	0.00
47 CO..CZ	-0.25	0.00	0.0	0.03	-0.01	-0.02	-0.00	0.00	-0.01	0.00	0.0	0.0	0.0	0.0	0.0
48 CO..OCZ	0.01	-0.00	-0.00	-1.56	1.21	-0.01	0.00	-0.03	-0.09	-0.02	0.0	0.0	0.0	0.0	0.0
49 CO..OCC	-0.02	-0.00	0.0	-0.31	-0.16	-0.09	-0.00	0.05	0.08	0.09	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.01	0.01	0.0	1.89	-1.09	0.09	0.00	-0.02	0.00	-0.08	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CD3-CCH

51	CZ..OCZ	-0.25	0.00	0.00	-0.06	-0.15	C.01	0.00	-0.04	0.02	-0.01	0.0	0.0	0.0	C.0	0.0
52	CZ..OCC	0.60	0.00	0.0	-0.01	0.02	0.C8	0.00	0.05	-0.02	0.04	0.0	0.0	0.0	0.C	0.0
53	CZ..ZCC	-0.29	-0.01	-0.00	0.04	0.06	-0.05	-0.00	-0.02	-0.00	-0.04	0.0	0.0	0.C	C.0	0.0
54	XCX*.XCX	0.00	-0.22	0.11	0.02	0.02	3.40	-11.53	1.23	0.09	-0.05	0.0	0.0	0.0	0.0	0.0
55	XCX*.CCX	0.0	0.17	-0.10	0.03	-0.02	-2.17	-3.62	-1.33	-1.04	0.47	0.0	0.0	0.0	0.0	0.0
56	XCX*CCX*	-0.00	-0.17	-0.06	-0.04	-0.01	-0.95	2.44	-3.37	0.10	-0.85	C.0	0.C	0.0	0.0	0.0
57	XCX..XCX	0.00	0.05	0.05	0.01	0.00	2.25	2.62	0.95	0.69	0.00	-0.16	-9.09	-0.86	-0.14	-0.00
58	XCX..CCX	0.0	-0.08	-0.10	0.03	-0.01	-3.99	1.44	-1.00	-3.13	-0.03	0.22	-3.53	1.64	1.16	0.02
59	XCX.CCX*	-0.01	0.17	-0.10	-0.13	-0.01	-2.47	-0.49	-6.45	2.49	-0.03	0.0	0.0	0.0	C.0	0.0
60	XCX5CCX4	0.0	-0.08	-0.10	0.03	-0.01	-3.99	1.44	-1.00	-3.13	-0.03	-0.22	4.14	-1.54	-2.43	-0.03
61	CCX.CCX*	-0.01	-0.12	0.11	-0.19	0.02	3.18	-0.33	1.81	-5.15	-1.40	0.0	0.0	0.0	0.0	0.0
62	CCX5CCX4	0.00	0.03	0.05	0.03	0.00	2.15	0.21	0.19	2.77	0.19	-0.07	-0.41	-0.81	-6.33	-0.08
63	CCX*.OCZ	0.01	-0.03	0.01	-0.85	-0.2C	0.02	-0.03	1.58	0.65	-0.51	0.0	0.0	0.C	C.0	0.0
64	CCX*.OCC	-0.03	-0.09	0.00	-0.17	0.04	0.69	0.10	-2.81	-0.69	2.02	0.0	0.0	0.0	0.0	0.0
65	CCX*.ZCC	0.02	0.13	-0.00	1.04	0.31	-0.73	-0.08	1.08	-0.05	-1.60	0.0	0.0	0.0	0.0	0.0
66	CCZ..OCC	-0.03	0.02	0.00	0.39	-1.14	0.02	-0.01	-0.93	-0.21	-0.55	0.0	0.0	0.0	0.0	0.C
67	OCZ..ZCC	0.01	-0.03	0.0	-2.22	-8.56	-0.06	0.01	0.35	-0.02	0.38	0.0	0.0	0.C	0.0	0.0
68	OCC..ZCC	-0.03	-0.09	0.00	-0.46	1.06	-0.49	-0.04	-0.62	0.01	-1.72	0.C	0.0	0.0	0.0	0.0
69	WAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	-0.11	-3.88	-0.53	-0.96
70	M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	C.0	0.0	0.0	0.0	-0.07	-0.51	-4.73	2.26	-0.07
71	M.OF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.10	2.63	-4.97	C.36	-0.01

SIGNIFICANCE MATRIX ------- CH3-COD

1 K (C=O)	0.00	0.00	0.05	0.61	0.01	0.01	0.02	0.02	0.01	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	0.0	0.0	2.32	0.07	0.00	0.00	-0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.0	0.01	0.00	0.19	-0.00	0.14	0.52	0.05	0.25	0.07	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	0.90	2.09	-0.00	0.00	-0.00	0.00	0.00	0.00	-0.00	0.00	3.12	0.0	0.00	0.00	0.00
5 K(C-X)*	2.29	0.75	0.0	0.00	0.0	0.0	0.00	-0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.01	-0.00	0.10	0.02	0.01	0.00	0.70	0.10	0.01	1.41	0.0	0.0	0.0	0.0	0.0
7 H (CCZ)	0.0	0.0	0.01	0.45	-0.00	0.02	2.30	1.07	0.90	0.07	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.01	0.00	0.06	0.68	0.01	0.01	0.46	1.90	0.77	0.85	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.02	0.01	0.01	0.07	5.55	2.46	0.02	0.44	0.32	0.00	0.06	12.83	0.69	0.07	0.00
10 H(XCX)*	0.04	0.01	0.00	0.01	7.35	3.42	0.13	0.11	0.06	0.09	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.01	0.01	0.01	0.04	0.06	4.03	0.03	1.64	1.46	0.12	0.02	0.80	8.95	0.14	0.08
12 H(XCC)*	0.02	0.01	0.08	0.34	0.95	2.05	0.72	1.44	1.33	0.57	0.0	0.0	0.0	0.0	0.0
13 H (WAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.29	2.93	0.01
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.46	23.81
15 F (X--X)	0.57	4.49	0.01	0.02	2.68	1.32	0.02	0.20	0.15	0.00	1.58	6.24	0.30	0.04	0.00
16 F(X--X)*	0.96	2.57	0.00	0.01	3.45	1.82	0.08	0.06	0.02	0.04	-0.21	-0.00	-0.00	0.0	-0.00
17 F (X--C)	1.38	1.46	0.06	0.49	0.58	2.15	2.05	1.87	2.57	0.63	1.40	0.47	5.43	0.05	0.05
18 F (O--C)	0.00	0.01	0.02	0.01	0.00	0.16	0.22	0.03	0.34	1.24	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.01	0.01	1.06	0.20	0.00	0.05	0.13	1.49	1.05	0.26	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	0.0	0.0	1.04	0.37	0.00	0.02	1.24	0.65	0.35	0.02	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.42	0.60	0.10	0.20	1.22	2.67	1.28	2.50	2.82	6.74	1.43	0.49	5.19	-0.00	5.19
22 C(X--X')	0.24	0.32	1.02	0.26	0.12	2.41	0.14	1.38	7.09	1.15	0.45	0.65	7.67	0.39	2.01
23 MOL.TEN.	-0.05	-0.03	-0.01	-0.01	-0.25	-6.70	-0.40	-1.81	-1.50	-0.36	-0.05	-0.26	-4.15	0.04	-0.03
24 CC..CX*	-0.01	-0.14	-0.00	-0.01	0.00	0.01	-0.04	-0.00	0.01	-0.02	0.0	0.0	0.0	0.0	0.0
25 CC..CX	0.01	-0.32	0.00	-0.03	-0.00	0.04	-0.06	-0.00	-0.03	0.01	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CH3-CCD

26 CC..CO	0.00	0.0	0.01	-0.68	0.00	0.08	0.19	-0.07	0.11	0.03	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	0.00	0.00	-0.09	-0.24	0.00	-0.03	0.01	0.00	-0.05	0.00	0.0	0.0	0.0	0.0	0.0
28 CC..XCX'	-0.00	0.02	-0.00	-0.05	0.03	1.42	-0.58	-0.17	0.22	-0.16	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	0.00	0.03	-0.01	0.36	0.16	1.67	-0.37	0.40	-0.84	0.01	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	-0.00	-0.02	-0.01	0.25	0.00	-2.09	-0.33	-0.90	1.71	-0.26	0.0	0.0	0.0	0.0	0.0
31 CC..CCX'	0.00	-0.02	0.02	-0.49	-0.00	-1.07	1.27	0.49	-1.18	0.39	0.0	0.0	0.0	0.0	0.0
32 CC..OCZ	0.0	-0.00	0.00	0.58	-0.00	0.11	2.15	-0.50	-0.97	-0.14	0.0	0.0	0.0	0.0	0.0
33 CC..OCC	-0.00	0.00	-0.02	0.14	0.0	-0.03	-1.19	-0.17	0.07	0.61	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	0.00	0.0	0.02	-0.71	0.00	-0.08	-0.90	0.60	0.87	-0.49	0.0	0.0	0.0	0.0	0.0
35 CX'..CH	-3.54	3.27	0.00	-0.00	-0.00	0.0	0.00	0.00	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
36 CX'.XCX'	0.63	-0.17	-0.00	0.00	-0.21	0.03	0.01	0.00	0.01	0.02	0.0	0.0	0.0	0.0	0.0
37 CX'..XCX	-0.57	-0.30	0.00	-0.01	0.10	0.03	0.01	-0.01	-0.03	-0.00	0.0	0.0	0.0	0.0	0.0
38 CX'..CCX	0.48	0.30	0.00	-0.01	0.02	-0.16	0.01	-0.01	0.04	0.03	0.0	0.0	0.0	0.0	0.0
39 CX'.CCX'	-0.38	0.19	-0.01	0.01	-0.06	-0.07	-0.04	-0.02	-0.05	-0.05	0.0	0.0	0.0	0.0	0.0
40 CX..CX5	0.98	2.00	0.0	-0.00	0.0	0.00	0.00	-0.00	0.00	0.00	-3.12	-0.00	-0.00	0.0	-0.00
41 CX..XCX'	-0.48	-0.39	0.0	0.00	-0.07	0.15	0.02	0.00	-0.02	-0.02	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	0.28	-0.33	0.00	-0.01	-0.07	0.10	0.01	-0.01	0.02	0.00	0.92	-0.29	0.07	-0.01	-0.00
43 CX4.XCX4	0.28	-0.33	0.00	-0.01	-0.07	0.10	0.01	-0.01	0.02	0.00	-0.82	0.08	-0.08	0.01	0.00
44 CX4.CCX5	-0.18	0.36	0.00	-0.01	-0.00	-0.18	0.01	0.00	-0.06	-0.02	0.57	0.04	0.22	0.01	-0.00
45 CX4.CCX'	0.37	0.45	-0.01	0.03	0.0	-0.19	-0.07	-0.04	0.05	0.04	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	-0.18	0.36	0.00	-0.01	-0.00	-0.18	0.01	0.00	-0.06	-0.02	-0.53	-0.05	-0.34	-0.01	0.00
47 CO..CZ	0.00	0.0	-0.65	0.41	-0.00	-0.01	0.00	-0.00	-0.01	0.00	0.0	0.0	0.0	0.0	0.0
48 CO..OCZ	-0.00	0.00	0.03	-1.04	-0.00	0.03	0.39	0.32	-0.21	-0.03	0.0	0.0	0.0	0.0	0.0
49 CO..OCC	0.0	0.0	-0.14	-0.24	-0.02	-0.01	-0.22	0.10	0.02	0.15	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.00	0.0	0.11	1.29	0.03	-0.02	-0.17	-0.44	0.19	-0.12	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CH3-COO

51 CZ..OCZ	0.00	-0.00	-0.20	-0.37	0.00	-0.01	0.01	-0.03	0.07	-0.01	0.0	0.0	0.0	0.0	0.0
52 CZ..OCC	0.0	0.0	0.98	-0.08	0.00	0.00	-0.03	-0.01	-0.01	0.01	0.0	0.0	0.0	0.0	0.0
53 CZ..ZCC	0.00	-0.00	-0.72	0.43	-0.01	0.01	-0.02	0.01	-0.08	-0.02	0.0	0.0	0.0	0.0	0.0
54 XCX*.XCX	-0.08	0.03	-0.00	-0.04	-17.47	8.96	0.14	-0.80	-0.48	-0.03	0.0	0.0	0.0	0.0	0.0
55 XCX*.CCX	0.06	-0.03	0.00	-0.04	0.57	-13.30	0.22	0.90	0.63	0.28	0.0	0.0	0.0	0.0	0.0
56 XCX*CCX*	-0.05	-0.02	0.00	0.13	5.23	-5.61	-0.65	-1.03	-0.70	-0.50	0.0	0.0	0.0	0.0	0.0
57 XCX..XCX	0.02	0.01	0.01	0.08	5.92	2.08	0.02	0.42	0.31	0.00	-0.06	-13.02	-0.77	-0.08	-0.00
58 XCX..CCX	-0.03	-0.03	0.02	0.11	1.76	-7.09	0.05	-1.90	-1.58	-0.02	0.08	-6.03	4.37	-0.24	0.02
59 XCX.CCX*	0.06	-0.03	-0.06	-0.37	-4.16	-8.75	-0.53	2.21	1.73	0.00	0.0	0.0	0.0	0.0	0.0
60 XCX5CCX4	-0.03	-0.03	0.02	0.11	1.76	-7.09	0.05	-1.90	-1.58	-0.02	-0.08	6.67	-5.71	0.20	-0.03
61 CCX.CCX*	-0.04	0.04	-0.08	-0.30	-0.27	7.77	-0.25	-4.39	-4.44	-0.84	0.0	0.0	0.0	0.0	0.0
62 CCX5CCX4	0.01	0.01	0.01	0.04	0.06	4.03	0.03	1.64	1.46	0.12	-0.02	-0.78	-9.06	-0.16	-0.08
63 CCX*.OCZ	-0.00	0.00	0.04	-0.75	0.07	-0.36	2.54	-2.68	2.11	-0.42	0.0	0.0	0.0	0.0	0.0
64 CCX*.OCC	-0.03	-0.00	-0.18	-0.18	0.18	0.13	-1.30	-0.91	-0.18	1.74	0.0	0.0	0.0	0.0	0.0
65 CCX*.ZCC	0.03	0.0	0.14	0.96	-0.21	0.32	-1.10	3.32	-2.07	-1.43	0.0	0.0	0.0	0.0	0.0
66 OCZ..OCC	0.00	-0.00	-0.05	0.21	0.01	-0.01	-2.48	0.68	-0.15	-0.68	0.0	0.0	0.0	0.0	0.0
67 OCZ..ZCC	-0.00	-0.00	0.04	-1.08	-0.00	-0.03	-1.46	-3.39	-1.86	0.46	0.0	0.0	0.0	0.0	0.0
68 OCC..ZCC	-0.02	0.0	-0.15	-0.25	-0.02	0.01	1.16	-0.95	0.13	-2.26	0.0	0.0	0.0	0.0	0.0
69 HAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.00	0.07	-2.26	-1.50
70 M.RK.HAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.02	-0.16	-4.34	1.58	-0.10
71 M.DF.HAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.03	0.75	-1.27	-1.51	-0.01

SIGNIFICANCE MATRIX ------- CD3-COD

1 K (C=O)	0.0	0.0	0.05	0.63	0.03	0.00	0.00	0.00	0.01	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	0.0	0.04	2.28	0.06	0.00	0.00	-0.00	0.0	0.00	0.00	0.0	0.0	0.0	C.0	0.0
3 K (C-C)	0.00	0.02	0.00	0.19	0.65	0.00	0.01	0.16	0.13	0.05	C.0	0.0	0.0	0.0	0.0
4 K (C-X)	0.75	1.37	0.03	-0.CC	0.00	0.00	0.00	0.00	0.00	0.00	2.31	0.00	0.00	0.0C	-0.00
5 K(C-X)'	1.56	0.65	0.01	0.0C	0.00	0.00	-0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.03	0.00	0.10	0.02	0.27	0.01	0.09	0.62	0.11	1.07	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	0.00	0.00	0.01	0.45	1.03	2.21	0.77	0.01	0.30	0.04	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.04	0.0	0.06	0.67	0.24	1.74	0.43	0.78	0.05	0.71	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.05	0.05	0.0	0.01	1.58	3.64	0.18	0.49	0.66	0.00	0.16	9.26	0.61	0.0C	0.00
10 H(XCX)'	0.12	0.02	0.00	0.0	0.53	4.34	2.83	0.27	0.01	0.15	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.03	0.04	0.02	0.02	1.52	0.38	0.91	-0.00	2.50	0.20	0.07	0.40	4.01	3.06	0.07
12 H(XCC)'	0.06	0.04	0.04	0.16	0.53	0.49	0.03	2.40	0.95	0.96	0.0	0.0	0.0	0.0	0.0
13 H (HAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.02	2.09	1.11	0.01
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0C	0.11	0.45	18.66
15 F (X--X)	0.14	3.10	0.07	0.0	0.88	1.88	0.10	0.26	0.33	0.00	0.96	4.60	0.30	0.00	0.00
16 F(X--X)'	0.66	1.57	0.04	0.00	0.30	1.41	2.20	0.18	0.00	0.06	-0.16	0.00	0.00	0.00	-0.00
17 F (X--C)	0.84	0.94	0.04	0.43	0.43	0.38	0.43	2.60	3.00	0.89	0.88	0.22	2.46	1.89	0.04
18 F (O--C)	0.02	0.02	0.02	0.01	0.39	0.01	0.06	0.14	0.40	0.93	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.02	0.08	1.00	0.19	0.19	1.01	0.34	0.99	0.20	0.22	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	0.0	0.02	1.03	0.37	0.63	1.06	0.48	0.01	0.09	0.01	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.28	0.54	0.10	0.09	0.74	0.55	0.49	1.89	3.72	6.43	0.95	0.25	2.90	1.09	4.11
22 C(X--X')	0.28	-0.01	1.19	0.28	0.62	1.76	0.22	2.49	4.29	1.19	0.26	0.29	2.95	3.58	1.53
23 MOL.TEN.	-0.16	-0.09	-0.01	-0.04	-2.17	-1.21	-1.24	-1.32	-1.81	-0.61	-0.14	-0.45	-2.25	-0.80	-0.02
24 CC..CX'	0.01	-0.24	-0.01	-0.04	0.06	0.01	-0.00	0.02	-0.01	-0.01	0.0	0.0	0.0	0.0	0.0
25 CC..CX	0.00	-0.48	-0.03	0.01	0.12	-0.00	0.01	-0.07	0.00	0.02	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CD3-COD

26 CC..CO	0.0	-0.01	0.02	-0.69	0.25	-0.01	-0.01	-0.05	0.09	0.02	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	0.0	0.06	-0.17	-0.22	-0.05	-0.00	-0.00	0.02	-0.02	0.01	0.0	0.0	0.0	0.0	0.0
28 CC..XCX*	0.00	0.05	0.0	0.05	1.23	-0.15	0.37	-0.49	-0.09	-0.18	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	-0.00	0.10	0.0	0.14	2.90	0.28	-0.16	-0.87	-0.87	0.02	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	0.00	-0.09	-0.02	0.17	-2.77	-0.09	-0.27	0.00	1.62	-0.29	0.0	0.0	0.0	0.0	0.0
31 CC..CCX*	0.00	-0.06	0.02	-0.34	-1.13	-0.09	-0.04	1.25	-0.73	0.43	0.0	0.0	0.0	0.0	0.0
32 CC..OCZ	0.0	-0.00	0.01	0.58	1.64	-0.15	-0.22	-0.12	-0.41	-0.09	0.0	0.0	0.0	0.0	0.0
33 CC..OCC	0.00	0.01	-0.03	0.13	-0.83	0.01	0.05	-0.65	0.24	0.46	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	0.0	-0.01	0.03	-0.70	-0.75	0.16	0.12	0.71	0.16	-0.39	0.0	0.0	0.0	0.0	0.0
35 CX*..CH	-3.01	2.68	0.05	-0.00	0.01	0.00	-0.00	-0.00	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
36 CX*.XCX*	0.86	-0.26	-0.00	-0.00	0.05	-0.14	-0.10	-0.03	0.00	0.02	0.0	0.0	0.0	0.0	0.0
37 CX*..XCX	-0.78	-0.53	0.00	-0.01	0.12	0.30	0.00	-0.05	0.01	-0.00	0.0	0.0	0.0	0.0	0.0
38 CX*..CCX	0.64	0.48	0.04	-0.01	-0.17	-0.10	-0.00	-0.00	-0.08	0.04	0.0	0.0	0.0	0.0	0.0
39 CX*.CCX*	-0.02	0.33	-0.04	0.03	-0.06	-0.09	0.00	0.05	0.01	-0.06	0.0	0.0	0.0	0.0	0.0
40 CX..CX5	0.78	1.35	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-2.32	-0.00	-0.00	-0.00	0.00
41 CX..XCX*	-0.79	-0.53	-0.00	0.0	0.10	-0.02	0.28	0.08	-0.00	-0.03	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	0.41	-0.52	0.00	0.0	0.12	-0.01	-0.07	0.08	-0.01	0.00	1.26	-0.39	-0.00	0.00	-0.00
43 CX4.XCX4	0.41	-0.52	0.00	0.0	0.12	-0.01	-0.07	0.08	-0.01	0.00	-1.19	0.25	-0.01	-0.00	0.00
44 CX4.CCX5	-0.29	0.50	0.05	0.00	-0.15	-0.00	-0.12	0.00	-0.00	-0.02	0.85	0.06	-0.02	0.05	-0.00
45 CX4.CCX*	0.64	0.67	-0.10	-0.02	-0.12	-0.01	-0.03	-0.29	-0.03	0.06	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	-0.29	0.50	0.05	0.00	-0.15	-0.00	-0.12	0.00	-0.00	-0.02	-0.82	-0.07	-0.03	-0.10	0.00
47 CO..CZ	0.0	-0.01	-0.64	0.39	-0.01	0.00	0.00	-0.00	-0.01	0.00	0.0	0.0	0.0	0.0	0.0
48 CO..OCZ	0.0	0.00	0.03	-1.06	0.37	0.17	0.11	0.01	-0.13	-0.02	0.0	0.0	0.0	0.0	0.0
49 CO..OCC	-0.01	-0.00	-0.13	-0.23	-0.15	-0.01	-0.04	0.09	0.08	0.09	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.01	0.0	0.10	1.30	-0.17	-0.14	-0.11	-0.11	0.05	-0.08	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CD3-COD

51	CZ..OCZ	0.0	-0.01	-0.21	-0.35	-0.06	0.06	0.01	-0.00	0.03	-0.01	0.0	0.0	0.0	0.0	0.0
52	CZ..OCC	0.01	0.02	0.95	-0.08	0.02	-0.01	-0.01	-0.04	-0.02	0.02	0.0	0.0	0.0	0.0	0.0
53	CZ..ZCC	-0.00	-0.01	-0.69	0.40	0.02	-0.08	-0.03	0.03	-0.01	-0.03	0.0	0.0	0.0	0.0	0.0
54	XCX*.XCX	-0.22	0.11	0.00	0.02	2.75	2.12	-12.62	0.85	0.12	-0.06	0.0	0.0	0.0	0.0	0.0
55	XCX*.CCX	0.17	-0.09	-0.00	0.02	-1.87	1.83	-7.11	-0.05	-0.98	0.48	0.0	0.0	0.0	0.0	0.0
56	XCX*CCX*	-0.17	-0.06	0.00	-0.04	-0.92	2.44	-0.98	-2.46	0.11	-0.84	0.0	0.0	0.0	0.0	0.0
57	XCX..XCX	0.05	0.05	0.0	0.01	1.67	3.70	0.06	0.43	0.64	0.00	-0.16	-9.38	-0.70	-0.00	-0.00
58	XCX..CCX	-0.08	-0.09	0.00	0.03	-2.80	1.23	-2.21	-0.04	-2.87	-0.04	0.22	-3.49	2.84	-0.08	0.02
59	XCX.CCX*	0.17	-0.13	-0.00	-0.11	-2.18	-0.15	-2.35	-4.51	2.22	0.00	0.0	0.0	0.0	0.0	0.0
60	XCX5CCX4	-0.08	-0.09	0.00	0.03	-2.80	1.23	-2.21	-0.04	-2.87	-0.04	-0.22	4.14	-3.40	-0.56	-0.03
61	CCX.CCX*	-0.12	0.12	-0.07	-0.15	2.69	1.64	0.04	-0.21	-4.58	-1.42	0.0	0.0	0.0	0.0	0.0
62	CCX5CCX4	0.03	0.04	0.02	0.02	1.52	0.38	0.91	-0.00	2.50	0.20	-0.07	-0.39	-3.84	-3.33	-0.07
63	CCX*.OCZ	-0.01	0.01	0.03	-0.52	-1.41	2.44	0.08	-0.68	1.02	-0.41	0.0	0.0	0.0	0.0	0.0
64	CCX*.OCC	-0.09	-0.02	-0.12	-0.12	0.76	-0.10	-0.12	-2.48	-0.66	2.01	0.0	0.0	0.0	0.0	0.0
65	CCX*.ZCC	0.10	0.01	0.09	0.65	0.71	-1.50	-0.43	2.74	-0.45	-1.69	0.0	0.0	0.0	0.0	0.0
66	OCZ..OCC	0.01	-0.00	-0.05	0.20	-1.01	-0.11	-0.79	0.09	-0.37	-0.44	0.0	0.0	0.0	0.0	0.0
67	OCZ..ZCC	-0.01	0.00	0.04	-1.07	-0.87	-0.42	-4.65	-0.38	-0.27	0.30	0.0	0.0	0.0	0.0	0.0
68	OCC..ZCC	-0.08	-0.00	-0.14	-0.24	0.52	0.45	0.31	-1.45	0.14	-1.81	0.0	0.0	0.0	0.0	0.0
69	WAG.TURS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	-0.02	-0.91	-1.42	-1.14
70	M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.07	-0.25	-8.13	5.35	-0.08
71	M.DF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.10	1.37	-3.37	0.12	-0.01

SIGNIFICANCE MATRIX ------- CH3-COF

1 K (C=O)	0.0	0.0	0.64	0.0	0.00	0.00	0.02	0.01	0.00	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	-0.00	0.00	0.07	0.02	0.01	0.35	0.13	0.52	0.00	0.00	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.0	0.00	0.15	0.01	0.13	0.37	0.32	0.16	0.06	0.00	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	2.41	0.50	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	3.10	0.03	-0.00	0.00	0.00
5 K(C-X)*	0.60	2.45	0.00	0.01	-0.00	0.00	0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.01	0.00	0.07	0.02	0.00	0.80	0.05	0.03	0.15	1.58	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	-0.00	0.0	0.12	0.04	0.02	0.53	0.26	0.01	1.18	0.18	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.01	0.00	0.38	0.00	0.00	0.03	0.08	0.06	0.49	0.69	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.00	0.06	0.00	7.56	0.01	0.71	0.01	0.00	0.02	0.00	0.16	11.12	2.65	0.00	0.09
10 H(XCX)*	0.06	0.00	0.03	0.88	9.32	0.82	0.09	0.11	0.01	0.05	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.0	0.03	0.04	0.98	2.86	0.95	1.80	0.02	0.01	0.05	0.01	1.64	4.44	2.15	0.20
12 H(XCC)*	0.02	0.00	0.22	2.65	0.29	1.24	2.06	0.26	0.04	0.35	0.0	0.0	0.0	0.0	0.0
13 H (WAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.12	1.40	3.15	3.17
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.13	1.05	17.19
15 F (X--X)	-0.05	4.98	0.00	4.19	0.00	0.29	0.01	0.00	0.01	0.00	1.40	5.85	1.28	0.00	0.05
16 F(X--X)*	2.79	0.70	0.01	0.33	4.67	0.42	0.08	0.06	0.01	0.02	-0.20	-0.00	0.00	-0.00	-0.00
17 F (X--C)	1.37	1.54	0.37	1.78	0.98	1.91	3.32	0.63	0.24	0.23	1.41	0.86	2.86	1.33	0.12
18 F (O--C)	0.01	0.00	0.04	0.03	0.14	0.15	0.30	0.31	0.20	0.83	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.00	0.01	0.11	0.04	0.02	-0.01	-0.01	0.56	0.62	0.59	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	-0.00	0.0	0.07	0.01	0.00	0.11	0.05	0.61	0.63	0.10	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	1.00	0.42	0.19	2.59	1.05	1.68	4.09	1.68	1.01	4.56	1.39	0.90	2.43	2.48	1.79
22 C(X--X')	0.37	0.01	0.22	0.42	1.65	0.21	1.47	0.44	1.88	2.00	0.26	1.37	4.76	0.20	7.46
23 MOL.TEN.	-0.04	-0.05	-0.11	-3.17	-3.82	-2.21	-0.55	-0.22	-0.04	-0.19	-0.07	0.81	-4.24	-0.43	0.05
24 CC..CX*	0.05	-0.18	-0.02	0.02	-0.00	-0.05	0.00	-0.03	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
25 CC..CX	-0.13	-0.12	-0.04	0.02	0.06	-0.03	-0.12	-0.02	-0.01	0.00	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CH3-COF

26 CC..CO	0.0	0.00	-0.61	0.00	0.05	-0.05	0.17	0.09	-0.01	0.00	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	-0.00	0.00	0.20	0.02	-0.08	-0.71	-0.41	0.58	-0.01	-0.00	0.0	0.0	0.0	0.0	0.0
28 CC..XCX*	0.01	-0.00	0.13	-0.14	2.28	-1.14	-0.36	-0.28	-0.06	-0.01	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	-0.01	0.04	0.03	0.75	-0.16	1.39	-0.22	0.02	-0.10	-0.00	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	0.0	-0.03	0.22	-0.19	-1.72	-1.77	2.14	-0.20	0.05	-0.01	0.0	0.0	0.0	0.0	0.0
31 CC..CCX*	-0.01	-0.00	-0.35	-0.23	-0.41	1.34	-1.65	0.41	0.09	0.02	0.0	0.0	0.0	0.0	0.0
32 CC..OCZ	0.0	-0.00	0.26	-0.03	0.09	0.88	0.56	0.07	-0.54	-0.01	0.0	0.0	0.0	0.0	0.0
33 CC..OCC	0.00	-0.00	0.21	0.02	-0.04	-1.08	-0.25	0.14	0.19	0.03	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	-0.00	0.01	-0.47	0.01	-0.04	0.20	-0.32	-0.21	0.34	-0.03	0.0	0.0	0.0	0.0	0.0
35 CX*..CH	-3.30	3.09	0.00	0.02	-0.00	0.00	-0.00	0.00	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
36 CX*.XCX*	0.37	0.14	-0.01	-0.21	-0.10	0.07	-0.00	0.02	0.00	0.02	0.0	0.0	0.0	0.0	0.0
37 CX*..XCX	-0.11	-1.05	0.0	0.77	0.00	-0.11	-0.00	-0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
38 CX*..CCX	0.01	0.84	-0.01	-0.33	-0.03	0.10	-0.01	0.01	-0.00	0.02	0.0	0.0	0.0	0.0	0.0
39 CX*.CCX*	-0.23	0.19	0.02	-0.39	0.00	-0.10	-0.03	-0.03	-0.00	-0.05	0.0	0.0	0.0	0.0	0.0
40 CX..CX5	2.41	0.50	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	-3.10	-0.03	-0.00	-0.00	-0.00
41 CX..XCX*	-0.98	0.09	-0.02	-0.17	0.36	0.03	0.06	0.02	0.01	-0.01	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	0.19	-0.35	-0.00	0.34	-0.01	-0.03	0.02	-0.00	0.01	-0.00	1.41	-1.23	0.00	-0.00	-0.02
43 CX4.XCX4	0.21	-0.35	-0.00	0.30	-0.01	-0.03	0.02	-0.00	0.01	-0.00	-1.35	1.11	-0.03	0.00	0.02
44 CX4.CCX5	0.02	0.26	-0.01	-0.13	-0.21	0.03	-0.21	0.01	-0.00	-0.01	0.40	0.45	-0.02	0.18	0.03
45 CX4.CCX*	0.70	0.11	0.03	-0.33	-0.09	-0.07	0.27	-0.03	-0.01	0.03	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	0.02	0.26	-0.01	-0.13	-0.21	0.03	-0.21	0.01	-0.00	-0.01	-0.36	-0.47	-0.05	-0.21	-0.03
47 CO..CZ	-0.00	-0.00	-0.42	0.00	-0.02	0.04	-0.11	0.15	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
48 CO..OCZ	0.0	-0.00	-0.55	-0.01	0.02	-0.05	0.16	0.02	0.04	-0.04	0.0	0.0	0.0	0.0	0.0
49 CO..OCC	0.00	-0.00	-0.43	0.01	-0.01	0.06	-0.07	0.04	-0.02	0.11	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.0	0.00	0.99	0.0	-0.01	-0.01	-0.09	-0.06	-0.03	-0.08	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CH3-COF

51	CZ..OCZ	-0.00	0.0	0.18	-0.05	-0.03	-0.85	-0.36	0.13	0.03	0.05	0.0	0.0	0.0	0.0	0.0
52	CZ..OCC	0.0	0.0	0.14	0.03	0.01	1.06	0.15	0.25	-0.02	-0.17	0.0	0.0	0.0	0.0	0.0
53	CZ..ZCC	0.0	0.00	-0.32	0.01	0.02	-0.20	0.21	-0.37	-0.03	0.10	0.0	0.0	0.0	0.0	0.0
54	XCX'.XCX	-0.04	-0.02	0.01	-5.35	-2.35	-2.47	0.09	-0.04	0.05	0.02	0.0	0.0	0.0	0.0	0.0
55	XCX'.CCX	0.0	0.02	0.09	2.52	-14.67	2.55	-1.33	0.14	-0.03	0.14	0.0	0.0	0.0	0.0	0.0
56	XCX'CCX'	-0.07	0.00	-0.15	3.08	-3.37	-2.18	0.82	-0.36	-0.05	-0.28	0.0	0.0	0.0	0.0	0.0
57	XCX..XCX	0.00	0.06	0.00	7.56	0.01	0.71	0.01	0.00	0.02	0.00	-0.16	-11.06	-2.85	-0.00	-0.09
58	XCX..CCX	0.00	-0.09	0.00	-4.46	-0.39	-1.87	-0.45	-0.01	-0.02	0.01	0.09	-8.34	6.71	-0.25	-0.29
59	XCX.CCX'	0.02	-0.04	-0.00	-12.36	-0.01	2.63	0.17	0.02	-0.08	-0.10	0.0	0.0	0.0	0.0	0.0
60	XCX5CCX4	-0.00	-0.09	0.01	-5.07	0.10	-1.74	-0.35	-0.01	-0.02	0.02	-0.09	8.54	-7.09	0.03	0.26
61	CCX.CCX'	0.0	0.03	-0.24	5.04	2.02	-2.96	-5.87	-0.28	0.04	-0.41	0.0	0.0	0.0	0.0	0.0
62	CCX5CCX4	0.0	0.03	0.04	0.98	2.86	0.95	1.80	0.02	0.01	0.05	-0.01	-1.61	-4.48	-2.26	-0.21
63	CCX'.OCZ	0.00	0.00	-0.32	0.63	-0.13	1.61	-1.46	0.09	-0.43	-0.51	0.0	0.0	0.0	0.0	0.0
64	CCX'.OCC	-0.03	0.00	-0.25	-0.43	0.07	-2.02	0.62	0.18	0.14	1.44	0.0	0.0	0.0	0.0	0.0
65	CCX'.ZCC	0.02	-0.01	0.58	-0.15	0.07	0.37	0.84	-0.26	0.26	-1.01	0.0	0.0	0.0	0.0	0.0
66	OCZ..OCC	-0.00	0.00	0.19	-0.05	-0.01	-1.29	-0.22	0.03	-0.84	-1.09	0.0	0.0	0.0	0.0	0.0
67	OCZ..ZCC	0.0	-0.00	-0.42	-0.02	-0.02	0.24	-0.29	-0.04	-1.53	0.70	0.0	0.0	0.0	0.0	0.0
68	OCC..ZCC	-0.01	-0.00	-0.34	0.02	0.01	-0.30	0.12	-0.09	0.54	-2.14	0.0	0.0	0.0	0.0	0.0
69	HAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.04	0.87	3.62	-16.90
70	M.HK.HAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.03	-1.15	-7.15	7.31	1.84
71	M.DF.HAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.10	3.31	-5.58	-0.30	-1.70

SIGNIFICANCE MATRIX ------- CD3-COF

1 K (C=O)	0.0	0.0	0.64	0.00	0.00	0.01	0.02	0.00	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	-0.00	-0.00	0.07	0.40	0.13	0.05	0.02	0.42	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.00	0.01	0.15	0.73	0.03	0.00	0.16	0.04	0.08	0.00	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	1.27	0.83	-0.00	0.00	0.01	0.00	0.00	-0.00	0.00	0.00	2.29	0.02	0.01	0.00	0.00
5 K(C-X)'	0.99	1.24	0.00	0.00	0.01	0.01	0.00	-0.00	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.03	0.00	0.07	0.63	0.20	0.21	0.00	0.02	0.15	1.35	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	0.00	-0.00	0.12	0.60	0.16	0.03	0.22	0.02	1.01	0.15	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.03	0.00	0.37	0.00	0.00	0.09	0.26	0.00	0.38	0.60	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.03	0.11	0.00	0.23	3.30	2.47	0.01	0.00	0.09	0.00	0.27	5.32	4.65	0.00	0.07
10 H(XCX)'	0.15	0.00	0.01	0.74	0.24	5.98	1.09	0.03	0.07	0.07	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.01	0.08	0.02	1.25	1.08	0.00	2.04	0.42	0.10	0.10	0.06	1.94	1.60	2.67	0.14
12 H(XCC)'	0.07	0.01	0.15	0.00	2.42	0.08	0.66	1.38	0.06	0.52	0.0	0.0	0.0	0.0	0.0
13 H (WAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.03	0.84	1.76	2.33	2.31
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.03	0.13	0.47	12.97
15 F (X--X)	-0.19	3.42	0.00	0.12	2.03	1.28	0.02	0.00	0.05	0.00	0.86	2.80	2.46	0.00	0.04
16 F(X--X)'	1.22	1.05	0.00	0.36	0.19	2.97	0.60	0.01	0.04	0.03	-0.15	-0.00	-0.00	-0.00	-0.00
17 F (X--C)	0.83	1.05	0.34	0.88	1.45	0.09	2.57	1.25	0.48	0.35	0.86	1.08	1.16	1.64	0.08
18 F (O--C)	0.02	0.01	0.04	0.29	0.25	0.12	0.27	0.02	0.24	0.70	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.02	0.02	0.10	-0.02	0.16	0.02	0.07	0.46	0.57	0.49	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	0.00	0.00	0.07	0.10	0.05	0.04	0.29	0.44	0.50	0.07	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.44	0.41	0.16	0.68	1.44	0.29	3.13	1.85	1.48	4.46	0.90	1.01	0.86	2.47	1.37
22 C(X--X')	0.29	0.01	0.21	0.20	0.31	0.08	1.62	0.03	2.24	1.93	0.14	1.88	2.02	0.94	5.57
23 MOL.TEN.	-0.14	-0.12	-0.06	-0.75	-3.55	-2.29	-0.21	-0.51	-0.20	-0.29	-0.17	1.06	-3.50	-0.59	0.03
24 CC..CX'	0.08	-0.27	-0.06	-0.01	0.04	0.00	-0.02	-0.01	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
25 CC..CX	-0.11	-0.31	-0.01	0.04	0.05	-0.00	-0.06	-0.01	-0.02	0.00	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CD3-COF

26 CC..CO	-0.00	0.01	-0.62	0.12	0.02	-0.00	0.12	0.01	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	0.00	0.0	0.20	-1.08	0.12	-0.01	0.11	0.24	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
28 CC..XCX'	0.03	0.01	0.08	1.46	0.16	-0.13	-0.86	-0.07	-0.15	-0.01	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	-0.02	0.11	0.06	1.42	0.64	0.03	-0.15	-0.03	-0.25	0.00	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	0.01	-0.10	0.16	-2.54	-0.63	-0.00	1.61	-0.37	0.24	-0.01	0.0	0.0	0.0	0.0	0.0
31 CC..CCX'	-0.02	-0.03	-0.29	0.18	-0.61	0.01	-0.65	0.43	0.14	0.01	0.0	0.0	0.0	0.0	0.0
32 CC..OCZ	0.0	-0.01	0.27	1.32	-0.14	0.01	0.37	0.05	-0.57	-0.01	0.0	0.0	0.0	0.0	0.0
33 CC..OCC	0.01	-0.01	0.20	-1.34	0.15	-0.02	0.03	-0.05	0.22	0.03	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	-0.01	0.02	-0.47	0.03	-0.02	0.01	-0.41	-0.00	0.34	-0.02	0.0	0.0	0.0	0.0	0.0
35 CX'..CH	-3.15	2.88	0.00	-0.00	0.03	-0.01	0.00	0.00	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
36 CX'.XCX'	0.77	-0.11	-0.01	-0.01	0.10	-0.41	0.04	0.00	0.00	0.02	0.0	0.0	0.0	0.0	0.0
37 CX'..XCX	-0.49	-1.02	-0.01	-0.00	0.50	0.30	0.01	0.00	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
38 CX'..CCX	0.32	0.91	-0.03	-0.02	-0.34	-0.02	-0.12	0.02	-0.01	0.04	0.0	0.0	0.0	0.0	0.0
39 CX'.CCX'	-0.52	0.27	0.05	0.00	-0.36	0.04	0.03	-0.04	-0.00	-0.07	0.0	0.0	0.0	0.0	0.0
40 CX..CX5	1.27	0.83	0.0	0.00	0.01	0.00	0.00	-0.00	0.00	0.00	-2.30	-0.02	-0.01	-0.00	-0.00
41 CX..XCX'	-1.18	-0.12	-0.00	0.03	0.14	0.19	0.14	0.00	0.02	-0.02	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	0.43	-0.60	0.0	0.02	0.37	-0.14	0.01	0.00	0.02	-0.00	1.60	-0.63	-0.47	0.00	-0.01
43 CX4.XCX4	0.43	-0.59	-0.00	0.02	0.36	-0.15	0.01	0.00	0.02	-0.00	-1.55	0.58	0.42	-0.00	0.01
44 CX4.CCX5	-0.23	0.53	-0.00	-0.05	-0.23	0.01	-0.17	0.01	-0.02	-0.02	0.76	0.36	-0.28	0.18	0.02
45 CX4.CCX'	0.87	0.31	0.00	0.00	-0.50	-0.04	0.11	-0.05	-0.02	0.05	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	-0.23	0.53	-0.00	-0.05	-0.23	0.01	-0.17	0.01	-0.02	-0.02	-0.73	-0.39	0.25	-0.22	-0.02
47 CO..CZ	-0.00	0.00	-0.42	-0.09	0.05	0.04	0.04	0.03	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
48 CO..OCZ	-0.00	-0.00	-0.56	0.11	-0.06	-0.02	0.14	0.01	0.01	-0.03	0.0	0.0	0.0	0.0	0.0
49 CO..OCC	-0.01	-0.00	-0.41	-0.12	0.06	0.07	0.01	-0.01	-0.00	0.08	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.01	0.00	0.97	0.00	-0.01	-0.05	-0.15	-0.00	-0.01	-0.06	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CO3-COF

51 CZ..OCZ	-0.00	0.00	0.18	-0.97	-0.31	-0.08	0.13	0.16	-0.03	0.02	0.0	0.0	0.0	0.0	0.0
52 CZ..OCC	0.00	0.0	0.14	1.02	0.32	0.20	0.01	-0.16	0.01	-0.08	0.0	0.0	0.0	0.0	0.0
53 CZ..ZCC	-0.00	0.0	-0.32	-0.02	-0.03	-0.14	-0.13	-0.01	0.01	0.04	0.0	0.0	0.0	0.0	0.0
54 XCX*.XCX	-0.20	0.05	0.01	1.21	2.56	-11.34	0.27	0.03	0.23	0.00	0.0	0.0	0.0	0.0	0.0
55 XCX*.CCX	0.11	-0.04	0.04	-2.48	-1.34	0.42	-4.49	0.28	-0.25	0.24	0.0	0.0	0.0	0.0	0.0
56 XCX*CCX*	-0.20	-0.01	-0.08	0.12	-1.37	-1.53	1.71	-0.48	-0.14	-0.41	0.0	0.0	0.0	0.0	0.0
57 XCX..XCX	0.03	0.11	0.00	0.23	3.30	2.47	0.01	0.00	0.09	0.00	-0.27	-5.06	-5.02	-0.00	-0.07
58 XCX..CCX	-0.04	-0.19	0.02	-0.74	-3.88	-0.30	-0.49	0.04	-0.20	-0.00	0.26	-6.32	5.58	-0.14	-0.21
59 XCX.CCX*	0.14	-0.10	-0.05	0.11	-7.68	1.20	0.14	-0.39	-0.24	-0.06	0.0	0.0	0.0	0.0	0.0
60 XCX5CCX4	-0.04	-0.18	0.01	-0.93	-3.81	-0.25	-0.37	0.06	-0.19	0.00	-0.26	6.31	-5.58	-0.15	0.19
61 CCX.CCX*	-0.08	0.09	-0.15	0.15	4.28	-0.06	-2.67	-2.97	0.22	-0.70	0.0	0.0	0.0	0.0	0.0
62 CCX5CCX4	0.01	0.08	0.02	1.25	1.08	0.00	2.04	0.42	0.10	0.10	-0.06	-1.90	-1.63	-2.74	-0.15
63 CCX*.OCZ	-0.00	0.01	-0.27	0.11	1.24	0.09	-0.75	0.30	-0.53	-0.57	0.0	0.0	0.0	0.0	0.0
64 CCX*.OCC	-0.09	0.01	-0.20	-0.01	-1.45	-0.28	-0.06	-0.31	0.20	1.63	0.0	0.0	0.0	0.0	0.0
65 CCX*.ZCC	0.09	-0.02	0.47	0.00	0.15	0.17	0.82	-0.01	0.31	-1.14	0.0	0.0	0.0	0.0	0.0
66 OCZ..OCC	0.0	0.00	0.18	-1.21	-0.38	-0.15	0.03	-0.03	-0.79	-0.91	0.0	0.0	0.0	0.0	0.0
67 OCZ..ZCC	-0.00	-0.00	-0.42	0.03	0.04	0.09	-0.47	0.00	-1.25	0.59	0.0	0.0	0.0	0.0	0.0
68 OCC..ZCC	-0.06	-0.01	-0.31	-0.02	-0.04	-0.27	-0.04	-0.00	0.48	-1.84	0.0	0.0	0.0	0.0	0.0
69 WAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.33	0.94	2.09	-12.56
70 M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.11	-3.26	-5.17	7.01	1.33
71 M.DF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.23	5.88	-8.26	-0.03	-1.25

SIGNIFICANCE MATRIX ------- CH3-COCL

1 K (C=O)	0.0	-0.00	0.65	0.01	0.00	0.00	0.03	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	0.0	-0.00	0.06	0.00	0.0	0.25	0.11	0.71	0.00	0.03	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.0	0.00	0.13	0.00	0.07	0.34	0.65	0.08	0.02	0.0	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	0.93	2.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.03	0.11	0.01	0.00	0.0
5 K(C-X)*	2.20	0.84	0.00	0.00	0.0	0.00	0.01	0.00	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.01	0.0	0.08	0.00	0.00	0.84	0.09	0.31	0.69	0.84	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	-0.00	0.0	0.06	0.02	0.0	0.41	0.25	0.06	1.46	0.00	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.01	-0.00	0.28	0.01	0.00	0.08	0.04	0.10	0.14	0.94	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.01	0.00	0.02	7.29	0.84	0.43	0.02	0.00	0.00	0.01	0.30	10.63	2.83	0.33	0.0
10 H(XCX)*	0.05	0.01	0.01	3.54	6.59	0.92	0.41	0.08	0.02	0.11	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.01	0.02	0.09	0.16	5.15	1.00	0.34	0.09	0.01	0.01	0.01	2.15	5.29	0.20	0.12
12 H(XCC)*	0.04	0.0	0.27	2.05	0.53	2.16	1.67	0.48	0.14	0.31	0.0	0.0	0.0	0.0	0.0
13 H (HAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.00	0.71	4.93	0.15
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.06	0.40	17.39
15 F (X--X)	0.45	4.81	0.00	3.26	0.43	0.22	0.04	0.00	0.00	0.00	1.17	6.12	1.49	0.17	-0.00
16 F(X--X)*	0.96	2.52	0.01	1.72	3.41	0.49	0.16	0.04	0.01	0.04	-0.21	-0.01	-0.00	-0.00	0.0
17 F (X--C)	1.30	1.49	0.45	1.34	2.35	2.83	2.18	0.62	0.18	0.19	1.45	0.94	3.43	0.13	0.07
18 F (O--C)	0.01	0.00	0.05	0.01	0.05	0.15	0.55	0.44	0.48	0.43	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.01	0.00	0.10	0.02	0.03	0.05	0.02	0.50	0.19	1.21	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	0.0	-0.00	0.07	0.01	0.0	0.09	0.06	0.45	1.02	0.01	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.43	0.99	0.22	1.98	2.65	2.46	2.56	3.01	2.55	2.86	1.44	1.02	3.07	0.38	3.89
22 C(X--X*)	0.15	0.05	0.23	0.03	3.21	0.18	0.66	0.26	0.51	3.61	0.11	1.72	5.22	-0.11	4.50
23 MOL.TEN.	-0.07	-0.02	-0.01	-1.13	-5.39	-2.67	-1.31	-0.30	-0.07	-0.24	-0.10	1.21	-4.99	-0.33	-0.03
24 CC..CX*	0.01	-0.12	-0.04	0.0	-0.02	0.05	-0.13	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
25 CC..CX	-0.01	-0.26	-0.03	-0.00	0.05	-0.06	-0.12	-0.01	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CH3-CCCL

26	CC..CO	-0.00	0.00	-0.58	0.01	-0.02	-0.06	0.27	0.04	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
27	CC..CZ	-0.00	0.0	0.18	0.00	0.00	-0.57	-0.54	0.47	-0.01	0.00	0.0	0.0	0.0	0.0	0.0
28	CC..XCX'	0.00	0.01	-0.07	-0.11	1.37	-1.15	1.03	-0.16	-0.04	0.01	0.0	0.0	0.0	0.0	0.0
29	CC..XCX	0.0	0.01	0.14	0.27	0.69	1.08	-0.33	0.01	-0.03	0.00	0.0	0.0	0.0	0.0	0.0
30	CC..CCX	0.00	-0.03	0.31	-0.03	-1.64	-1.70	1.33	-0.24	-0.04	0.00	0.0	0.0	0.0	0.0	0.0
31	CC..CCX'	-0.00	-0.00	-0.37	-0.08	-0.38	1.71	-2.15	0.38	0.10	-0.01	0.0	0.0	0.0	0.0	0.0
32	CC..OCZ	0.0	-0.00	0.18	-0.01	-0.00	0.76	0.79	-0.13	-0.36	-0.00	0.0	0.0	0.0	0.0	0.0
33	CC..OCC	0.00	0.0	0.20	0.00	0.02	-1.06	-0.48	0.31	0.24	-0.02	0.0	0.0	0.0	0.0	0.0
34	CC..ZCC	0.00	0.0	-0.38	0.00	-0.02	0.32	-0.32	-0.18	0.11	0.01	0.0	0.0	0.0	0.0	0.0
35	CX'..CH	-3.88	3.69	0.00	0.00	-0.00	-0.01	0.01	-0.00	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
36	CX'.XCX'	0.71	-0.22	0.01	0.11	-0.22	-0.09	-0.11	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0	0.0
37	CX'..XCX	-0.44	-0.17	-0.02	-0.39	-0.10	0.07	0.03	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0	0.0
38	CX'..CCX	0.42	0.36	-0.05	0.04	0.13	-0.14	-0.14	-0.01	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
39	CX'.CCX'	-0.57	0.08	0.06	0.09	0.04	0.11	0.20	0.01	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
40	CX..CX5	0.93	2.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-3.04	-0.11	-0.01	-0.00	-0.00
41	CX..XCX'	-0.59	-0.47	0.01	0.10	0.39	0.08	-0.10	0.01	0.00	-0.02	0.0	0.0	0.0	0.0	0.0
42	CX..XCX	0.23	-0.21	-0.01	-0.18	0.12	-0.05	0.01	-0.00	0.00	-0.00	1.91	-2.17	-0.27	-0.02	-0.00
43	CX4.XCX4	0.23	-0.19	-0.01	-0.22	0.12	-0.05	0.01	0.00	0.00	-0.00	-1.85	2.07	0.23	0.01	0.00
44	CX4.CCX5	-0.17	0.40	-0.02	0.02	-0.34	0.06	-0.06	0.01	0.00	-0.00	0.34	0.95	-0.39	-0.01	0.00
45	CX4.CCX'	0.55	0.19	0.04	0.09	-0.15	-0.18	0.16	-0.02	-0.01	0.03	0.0	0.0	0.0	0.0	0.0
46	CX4.CCX4	-0.17	0.40	-0.02	0.02	-0.34	0.06	-0.06	0.01	0.00	-0.00	-0.30	-0.98	0.31	0.01	-0.01
47	CO..CZ	-0.00	0.0	-0.40	0.01	0.0	0.05	-0.11	0.11	0.00	-0.01	0.0	0.0	0.0	0.0	0.0
48	CO..OCZ	0.0	0.0	-0.40	-0.02	0.0	-0.07	0.17	-0.03	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
49	CO..OCC	-0.00	-0.00	-0.45	0.01	-0.00	0.09	-0.10	0.07	-0.00	0.06	0.0	0.0	0.0	0.0	0.0
50	CO..ZCC	0.00	0.0	0.85	0.01	0.00	-0.03	-0.07	-0.04	-0.00	-0.07	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CH3-COCL

51 CZ..OCZ	0.00	-0.00	0.12	-0.01	0.00	-0.64	-0.33	-0.40	0.09	-0.02	0.0	0.0	0.0	0.0	0.0
52 CZ..OCC	0.00	0.00	0.14	0.01	0.00	0.92	0.19	0.94	-0.08	-0.33	0.0	0.0	0.0	0.0	0.0
53 CZ..ZCC	-0.00	0.0	-0.26	0.01	0.0	-0.28	0.13	-0.54	-0.03	0.32	0.0	0.0	0.0	0.0	0.0
54 XCX*.XCX	-0.07	0.03	-0.03	-11.82	4.72	-2.15	-0.32	-0.02	0.02	0.06	0.0	0.0	0.0	0.0	0.0
55 XCX*.CCX	0.06	-0.05	-0.08	2.18	-16.95	2.78	1.06	0.24	0.04	0.08	0.0	0.0	0.0	0.0	0.0
56 XCX*CCX*	-0.09	-0.01	0.10	5.26	-3.74	-2.92	-1.80	-0.41	-0.10	-0.39	0.0	0.0	0.0	0.0	0.0
57 XCX..XCX	0.01	0.00	0.02	7.29	0.84	0.43	0.02	0.00	0.00	0.01	-0.29	-10.58	-3.02	-0.35	-0.00
58 XCX..CCX	-0.02	-0.02	0.08	-1.11	-5.23	-1.52	-0.19	-0.01	0.01	0.01	0.10	-9.42	7.59	0.49	-0.00
59 XCX.CCX*	0.07	-0.01	-0.18	-10.63	-2.13	2.71	0.40	0.01	-0.07	-0.13	0.0	0.0	0.0	0.0	0.0
60 XCX5CCX4	-0.02	-0.02	0.08	-1.75	-4.60	-1.40	-0.17	-0.01	0.01	0.01	-0.10	9.53	-8.00	-0.54	-0.01
61 CCX.CCX*	-0.05	0.01	-0.43	1.77	4.53	-4.19	-2.32	-0.62	-0.11	-0.14	0.0	0.0	0.0	0.0	0.0
62 CCX5CCX4	0.01	0.02	0.09	0.16	5.15	1.00	0.34	0.09	0.01	0.01	-0.01	-2.11	-5.38	-0.20	-0.12
63 CCX*.OCZ	0.00	0.0	-0.26	0.35	0.01	1.87	-1.30	-0.33	-0.92	0.05	0.0	0.0	0.0	0.0	0.0
64 CCX*.OCC	-0.05	-0.00	-0.29	-0.13	-0.04	-2.71	0.77	0.78	0.60	0.97	0.0	0.0	0.0	0.0	0.0
65 CCX*.ZCC	0.04	-0.00	0.55	-0.21	0.04	0.81	0.52	-0.44	0.28	-1.10	0.0	0.0	0.0	0.0	0.0
66 OCZ..OCC	-0.00	0.0	0.14	-0.01	-0.00	-1.15	-0.30	-0.26	-2.03	0.04	0.0	0.0	0.0	0.0	0.0
67 OCZ..ZCC	0.00	0.0	-0.26	-0.02	0.0	0.35	-0.20	0.15	-0.88	-0.15	0.0	0.0	0.0	0.0	0.0
68 OCC..ZCC	-0.02	0.0	-0.29	0.01	-0.00	-0.50	0.12	-0.35	0.63	-1.83	0.0	0.0	0.0	0.0	0.0
69 WAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.00	0.42	2.88	-3.74
70 M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.33	5.58	-3.28	0.35
71 M.OF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.15	-0.51	4.04	-3.93	0.00

SIGNIFICANCE MATRIX ------- CD3-COCL

1 K (C=O)	0.00	C.00	0.66	0.00	-0.00	-0.00	0.02	0.00	0.00	0.00	0.0	0.0	0.C	0.0	0.0
2 K (C-Z)	0.00	0.00	0.06	0.01	0.28	C.16	0.00	0.64	0.00	0.01	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.00	0.01	0.14	0.35	C.48	0.05	C.19	0.05	0.03	-0.00	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	0.73	1.45	0.0	0.00	-0.00	0.01	-0.00	0.0	-0.00	0.00	2.23	0.08	0.01	0.CC	0.00
5 K(C-X)'	1.55	0.66	0.01	-0.00	-0.00	0.00	0.01	0.00	0.0	-0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.04	0.00	0.07	0.04	0.56	0.53	0.07	0.06	0.64	0.79	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	0.0	0.00	0.06	0.02	0.46	0.26	0.03	0.00	1.40	-0.00	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.04	0.00	0.27	0.00	0.00	0.05	0.19	0.04	0.15	0.81	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.05	0.03	0.01	5.42	0.49	0.14	0.30	0.00	0.02	0.00	0.40	7.49	1.92	0.52	-0.00
10 H(XCX)'	0.13	0.03	0.00	0.00	2.36	5.79	0.05	0.11	0.04	0.15	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.03	0.05	0.03	2.13	0.67	0.64	1.56	0.10	0.00	0.03	0.06	1.62	3.63	0.53	0.09
12 H(XCC)'	0.10	0.01	0.15	1.49	0.58	0.58	1.46	0.72	0.24	0.44	0.0	0.0	0.C	0.0	0.0
13 H (WAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.02	1.65	3.92	0.10
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.10	0.25	12.57
15 F (X--X)	0.17	3.31	0.01	2.57	0.23	0.06	0.24	0.0	0.01	0.00	0.72	4.33	1.09	0.27	-0.00
16 F(X--X)'	0.62	1.66	0.00	0.00	1.11	3.14	0.02	0.06	0.02	0.06	-0.15	-0.01	-0.00	-0.0C	-0.00
17 F (X--C)	0.78	1.02	0.34	0.72	1.60	1.31	2.63	0.75	0.30	0.28	0.88	0.71	2.46	0.34	0.05
18 F (O--C)	0.02	0.02	0.05	0.25	0.16	0.14	0.46	0.15	0.48	0.41	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.03	0.01	0.10	0.16	-0.03	-0.00	0.07	0.50	0.27	0.97	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	-0.00	0.0	0.08	0.00	0.09	0.05	0.07	0.54	0.87	0.01	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.29	0.58	0.19	1.29	1.05	0.73	3.34	2.03	2.91	3.08	0.92	0.75	2.05	0.63	2.81
22 C(X--X')	0.20	-0.02	0.21	0.48	0.1C	0.91	1.12	0.24	0.72	3.22	0.07	1.32	3.93	-0.01	3.26
23 MOL.TEN.	-0.18	-0.06	-0.03	-3.97	0.59	-2.65	-1.53	-0.43	-0.13	-0.34	-0.22	0.92	-3.43	-0.67	-C.02
24 CC..CX'	0.04	-0.19	-0.09	-0.01	0.02	0.03	-0.09	0.01	0.00	0.00	0.0	0.0	0.0	0.0	0.0
25 CC..CX	-0.04	-0.40	-0.02	0.02	0.02	-0.07	-0.01	-0.01	-0.00	0.00	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CO3-CCCL

26	CC..CO	-0.00	0.01	-0.60	0.08	0.02	-0.00	0.13	0.02	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
27	CC..CZ	0.0	-0.00	0.18	-0.11	-0.75	-0.19	0.02	0.35	0.01	-0.00	0.0	0.0	0.C	0.0	0.0
28	CC..XCX'	0.01	0.04	0.02	0.00	2.06	-1.15	0.18	-0.15	-0.07	-0.00	0.0	0.0	0.0	0.0	0.0
29	CC..XCX	-0.01	0.06	0.09	3.91	-1.56	0.24	-0.69	-0.02	-0.07	-0.00	0.0	0.0	0.0	0.0	0.0
30	CC..CCX	0.01	-0.07	0.19	-2.25	-1.75	0.52	1.53	-0.21	-0.03	-0.00	0.0	0.0	0.0	0.0	0.0
31	CC..CCX'	-0.01	-0.02	-0.28	-1.38	1.08	0.33	-1.08	0.37	0.16	-0.00	0.0	0.0	0.0	0.0	0.0
32	CC..OCZ	0.0	-0.00	0.19	0.18	0.93	0.22	0.15	-0.02	-0.41	-0.00	0.0	0.0	0.0	0.0	0.0
33	CC..OCC	0.01	-0.00	0.19	-0.22	-1.04	-0.34	0.22	0.11	0.27	-0.00	0.0	0.0	0.0	0.0	0.0
34	CC..ZCC	-0.01	0.00	-0.38	0.07	0.10	0.10	-0.38	-0.09	0.13	-0.01	0.0	0.0	0.0	0.0	0.0
35	CX'..CH	-2.97	2.76	0.00	-0.00	0.0	-0.02	0.00	-0.00	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
36	CX'.XCX'	0.92	-0.27	-0.00	0.00	0.03	-0.32	-0.05	-0.02	-0.01	0.00	0.0	0.0	0.0	0.0	0.0
37	CX'..XCX	-0.71	-0.38	-0.02	-0.14	-0.04	0.06	0.15	-0.00	-0.01	-0.00	0.0	0.0	0.0	0.0	0.0
38	CX'..CCX	0.05	0.52	-0.06	0.00	-0.05	0.12	-0.38	-0.03	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
39	CX'.CCX'	-0.76	0.17	0.09	0.01	0.02	0.08	0.23	0.05	0.01	-0.01	0.0	0.0	0.0	0.0	0.0
40	CX..CX5	0.73	1.45	0.0	0.00	-0.00	0.01	-0.00	0.0	-0.00	0.00	-2.24	-0.08	-0.01	-0.00	-0.00
41	CX..XCX'	-0.84	-0.56	-0.00	-0.00	0.02	0.62	-0.00	0.01	0.00	-0.03	0.0	0.C	0.0	0.0	0.0
42	CX..XCX	0.36	-0.41	-0.00	0.07	-0.02	-0.08	0.01	0.00	0.00	-0.00	1.89	-1.56	-0.34	-0.04	0.0
43	CX4.XCX4	0.37	-0.40	0.0	0.04	-0.02	-0.08	0.01	0.00	0.00	-0.00	-1.86	1.50	0.31	0.03	-0.00
44	CX4.CCX5	-0.29	0.55	-0.00	-0.07	-0.03	-0.17	-0.03	0.01	0.00	-0.01	0.74	0.70	-0.48	-0.04	0.00
45	CX4.CCX'	0.77	0.36	0.00	-0.08	0.02	-0.23	0.00	-0.04	-0.01	0.04	0.0	0.0	0.0	0.0	0.0
46	CX4.CCX4	-0.29	0.55	-0.00	-0.07	-0.03	-0.17	-0.03	0.01	0.00	-0.01	-0.71	-0.72	0.42	0.03	-0.00
47	CO..CZ	-0.00	0.00	-0.39	-0.01	-0.01	0.00	0.01	0.06	0.0	-0.01	0.0	0.0	0.0	0.0	0.0
48	CO..OCZ	-0.00	-0.00	-0.41	0.02	0.02	-0.01	0.06	-0.00	-0.01	0.00	0.0	0.0	0.0	0.0	0.0
49	CO..OCC	-0.01	0.00	-0.42	-0.03	-0.02	0.01	0.08	0.02	0.00	0.05	0.0	0.0	0.0	0.0	0.0
50	CO..ZCC	0.01	0.0	0.84	0.01	0.00	-0.00	-0.14	-0.02	0.00	-0.05	0.0	0.0	0.C	0.0	0.0

SIGNIFICANCE MATRIX ------- CD3-CCCL

51	CZ..OCZ	0.0	0.00	0.13	-0.03	-0.72	-0.41	0.01	-0.06	-0.08	-0.00	0.0	0.0	0.0	C.0	0.0
52	CZ..OCC	0.01	0.00	0.13	0.05	0.81	0.56	0.01	0.39	0.04	-0.22	0.0	0.0	0.0	0.0	0.0
53	CZ..ZCC	-0.01	-0.00	-0.25	-0.01	-0.07	-0.18	-0.03	-0.32	0.02	0.21	0.0	0.0	0.0	0.0	0.0
54	XCX*.XCX	-0.21	0.08	0.01	2.54	-3.90	-4.88	-0.51	0.02	0.08	0.02	0.0	0.0	0.0	0.0	0.0
55	XCX*.CCX	0.18	-0.11	0.01	0.54	-3.48	-5.95	0.63	0.31	0.03	0.18	0.0	0.0	0.0	0.0	0.0
56	XCX*CCX*	-0.23	-0.03	-0.02	0.26	2.20	-3.75	-0.63	-0.60	-0.21	-0.55	0.0	0.0	0.0	0.0	0.0
57	XCX..XCX	0.05	0.03	0.01	5.42	0.49	0.14	0.30	0.00	0.02	0.00	-0.40	-7.39	-2.12	-0.55	-0.00
58	XCX..CCX	-0.07	-0.08	0.03	-6.36	1.14	0.53	-1.61	0.02	0.02	0.01	0.31	-6.71	5.15	1.00	-0.00
59	XCX.CCX*	0.19	-0.05	-0.09	-7.27	-2.21	0.80	1.86	-0.11	-0.20	-0.06	0.0	0.0	0.0	0.0	0.0
60	XCX5CCX4	-0.07	-0.08	0.03	-6.58	1.25	0.59	-1.47	0.02	0.02	0.01	-0.30	6.91	-5.52	-1.10	-0.01
61	CCX.CCX*	-0.15	0.06	-0.20	4.95	-1.80	1.66	-4.37	-0.82	-0.09	-0.33	0.0	0.0	0.0	0.0	0.0
62	CCX5CCX4	0.03	0.05	0.03	2.13	0.67	0.64	1.56	0.10	0.00	0.03	-0.06	-1.56	-3.71	-0.55	-0.09
63	CCX*.OCZ	-0.00	0.00	-0.20	-0.30	1.04	0.76	-0.43	-0.07	-1.18	0.00	0.0	0.0	0.0	0.0	0.0
64	CCX*.OCC	-0.12	0.00	-0.20	0.53	-1.14	-1.16	-0.67	0.43	0.77	1.13	0.0	0.0	0.0	0.0	0.0
65	CCX*.ZCC	0.13	-0.00	0.40	-0.14	0.11	0.34	1.05	-0.34	0.37	-1.22	0.0	0.0	0.0	0.0	0.0
66	OCZ..OCC	0.0	0.0	0.13	-0.05	-0.99	-0.77	0.09	-0.02	-1.92	-0.03	0.0	0.0	0.0	0.0	0.0
67	OCZ..ZCC	0.0	-0.00	-0.26	0.02	0.10	0.23	-0.15	0.02	-0.89	-0.05	0.0	0.0	0.0	0.0	0.0
68	OCC..ZCC	-0.08	-0.00	-0.27	-0.02	-0.10	-0.32	-0.23	-0.10	0.61	-1.65	C.0	0.0	0.0	C.0	0.0
69	WAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	C.0	0.0	0.0	0.0	0.01	0.01	0.81	2.02	-2.63
70	M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.12	0.71	6.80	-4.43	0.25
71	M.DF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.30	-0.98	5.00	-4.31	0.00

SIGNIFICANCE MATRIX ------- CH3-COBR

1 K (C=O)	0.0	0.0	0.66	0.00	0.01	0.00	0.02	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	0.00	0.0	0.06	0.0	0.01	0.23	0.10	0.52	0.09	0.06	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.00	0.00	0.14	0.05	0.00	0.42	0.61	0.10	0.00	0.00	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	0.75	2.25	0.00	0.00	0.01	0.00	0.00	-0.00	0.00	0.00	3.05	0.08	0.00	-0.00	0.00
5 K(C-X)*	2.37	0.67	0.00	0.00	0.00	0.00	0.00	-0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.01	0.0	0.08	0.00	0.05	0.78	0.07	0.85	0.35	0.67	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	0.0	0.0	0.05	0.00	0.01	0.39	0.23	0.35	1.23	0.00	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.01	0.0	0.25	0.01	0.01	0.07	0.04	0.11	0.28	0.76	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.02	0.01	0.04	8.13	0.29	0.04	0.15	0.01	0.00	0.00	0.25	10.54	3.00	0.24	-0.00
10 H(XCX)*	0.05	0.01	0.04	0.24	10.58	0.01	0.98	0.00	0.00	0.06	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.01	0.02	0.09	2.14	2.34	1.85	0.38	0.13	0.00	0.01	0.01	2.19	5.12	0.31	0.11
12 H(XCC)*	0.03	0.00	0.27	2.37	0.08	2.47	1.76	0.47	0.00	0.20	0.0	0.0	0.0	0.0	0.0
13 H (WAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.01	0.70	4.89	0.37
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.07	0.68	17.01
15 F (X--X)	0.74	4.41	0.01	3.89	0.13	0.02	0.13	0.00	0.00	0.00	1.23	5.91	1.55	0.12	0.0
16 F(X--X)*	0.77	2.74	0.03	0.08	5.36	0.00	0.41	0.00	0.00	0.02	-0.21	-0.01	-0.00	-0.00	0.00
17 F (X--C)	1.31	1.52	0.45	1.93	1.37	3.39	2.20	0.66	0.00	0.11	1.44	1.01	3.29	0.19	0.06
18 F (O--C)	0.01	0.01	0.05	0.06	0.02	0.14	0.51	0.90	0.18	0.32	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.01	0.00	0.10	0.05	0.00	0.06	0.02	0.40	0.13	1.24	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	0.0	-0.00	0.07	0.0	0.00	0.10	0.06	0.18	1.43	0.03	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.38	1.06	0.22	2.74	1.42	3.27	2.58	4.99	0.72	2.07	1.43	1.07	2.92	0.60	3.76
22 C(X--X')	0.12	0.00	0.23	0.92	2.10	0.41	0.61	0.19	0.63	3.59	0.05	1.80	5.12	-0.19	5.07
23 MOL.TEN.	-0.06	-0.03	0.04	-4.71	-2.62	-1.06	-2.03	-0.14	-0.00	-0.14	-0.09	1.23	-5.02	-0.35	-0.02
24 CC..CX*	-0.01	-0.11	-0.03	-0.01	-0.00	0.03	-0.10	-0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
25 CC..CX	0.01	-0.28	-0.03	0.03	0.00	-0.03	-0.12	-0.01	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CH3-CCBR

26 CC..CO	0.0	0.00	-0.59	0.03	0.0	-0.07	0.24	0.05	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	0.0	0.0	0.18	0.00	0.00	-0.61	-0.50	0.46	-0.03	0.01	0.0	0.0	0.0	0.0	0.0
28 CC..XCX'	-0.00	0.02	-0.13	-0.19	0.17	0.05	1.50	-0.04	0.00	0.01	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	0.00	0.02	0.21	1.79	-0.02	0.35	-0.88	-0.08	-0.00	0.01	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	0.00	-0.03	0.31	-0.88	-0.07	-2.51	1.37	-0.33	-0.00	0.01	0.0	0.0	0.0	0.0	0.0
31 CC..CCX'	0.00	-0.01	-0.37	-0.66	-0.01	2.02	-2.14	0.43	-0.00	-0.03	0.0	0.0	0.0	0.0	0.0
32 CC..OCZ	-0.00	-0.00	0.17	-0.02	-0.00	0.82	0.74	-0.38	-0.11	-0.00	0.0	0.0	0.0	0.0	0.0
33 CC..OCC	0.00	0.00	0.20	-0.01	0.01	-1.13	-0.43	0.58	0.05	-0.05	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	-0.00	0.0	-0.36	0.03	-0.00	0.33	-0.33	-0.21	0.04	0.04	0.0	0.0	0.0	0.0	0.0
35 CX'..CH	-3.52	3.31	0.00	-0.00	-0.00	-0.00	0.01	0.00	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
36 CX'.XCX'	0.09	-0.20	0.02	0.02	-0.21	0.00	-0.13	-0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
37 CX'..XCX	-0.46	-0.24	-0.03	-0.31	0.03	0.01	0.07	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
38 CX'..CCX	0.45	0.33	-0.04	0.06	0.05	-0.12	-0.12	0.00	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
39 CX'.CCX'	-0.54	0.14	0.04	0.05	0.01	0.06	0.16	-0.01	0.0	-0.01	0.0	0.0	0.0	0.0	0.0
40 CX..CX5	0.75	2.25	0.00	0.00	0.01	0.00	0.00	-0.00	0.00	0.00	-3.05	-0.08	-0.00	-0.00	-0.00
41 CX..XCX'	-0.49	-0.48	0.01	-0.06	0.49	-0.00	-0.16	0.00	-0.00	-0.02	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	0.21	-0.31	-0.01	0.22	-0.08	-0.00	0.04	0.00	0.0	-0.00	1.75	-1.86	-0.23	-0.00	-0.00
43 CX4.XCX4	0.21	-0.29	-0.01	0.18	-0.08	-0.01	0.04	0.00	0.00	-0.00	-1.70	1.75	0.19	-0.00	0.00
44 CX4.CCX5	-0.16	0.43	-0.02	-0.14	-0.24	0.03	-0.07	0.00	0.00	-0.00	0.37	0.81	-0.32	-0.00	0.01
45 CX4.CCX'	0.46	0.36	0.04	-0.22	-0.06	-0.10	0.17	-0.02	0.00	0.02	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	-0.16	0.43	-0.02	-0.14	-0.24	0.03	-0.07	0.00	0.00	-0.00	-0.33	-0.85	0.24	-0.00	-0.01
47 CO..CZ	0.00	0.00	-0.39	0.00	-0.01	0.05	-0.10	0.11	0.02	-0.01	0.0	0.0	0.0	0.0	0.0
48 CO..OCZ	0.0	0.0	-0.37	-0.01	0.02	-0.07	0.15	-0.09	0.06	0.00	0.0	0.0	0.0	0.0	0.0
49 CO..OCC	0.0	0.0	-0.44	-0.00	-0.04	0.09	-0.08	0.14	-0.03	0.03	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.00	0.0	0.81	0.01	0.02	-0.03	-0.06	-0.05	-0.03	-0.04	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CH3-CBBR

51 CZ..OCZ	0.00	-0.00	0.11	0.0	-0.02	-0.59	-0.31	-0.86	0.67	-0.03	0.0	0.0	0.0	0.0	0.0
52 CZ..OCC	0.0	0.0	0.13	0.0	0.04	0.85	0.17	1.32	-0.35	-0.42	0.0	0.0	0.0	0.0	0.0
53 CZ..ZCC	-0.00	0.0	-0.24	0.0	-0.02	-0.25	0.13	-0.48	-0.32	0.42	0.0	0.0	0.0	0.0	0.0
54 XCX'.XCX	-0.07	0.04	-0.09	1.47	-10.68	0.04	-1.32	0.01	-0.00	0.04	0.0	0.0	0.0	0.0	0.0
55 XCX'.CCX	0.06	-0.05	-0.15	2.17	-14.47	-0.47	1.74	0.05	-0.00	0.05	0.0	0.0	0.0	0.0	0.0
56 XCX'CCX'	-0.08	-0.02	0.21	2.10	-2.17	-0.04	-2.96	-0.11	0.00	-0.25	0.0	0.0	0.0	0.0	0.0
57 XCX..XCX	0.02	0.01	0.04	8.13	0.29	0.04	0.15	0.01	0.00	0.00	-0.25	-10.49	-3.20	-0.25	-0.00
58 XCX..CCX	-0.02	-0.03	0.12	-7.57	1.16	-0.74	-0.54	0.06	0.00	0.01	0.10	-9.48	7.70	0.52	-0.01
59 XCX.CCX'	0.06	-0.02	-0.28	-12.29	0.46	0.80	1.40	-0.19	-0.00	-0.09	0.0	0.0	0.0	0.0	0.0
60 XCX5CCX4	-0.02	-0.03	0.12	-8.03	1.58	-0.62	-0.50	0.06	0.00	0.01	-0.10	9.56	-8.09	-0.57	0.00
61 CCX.CCX'	-0.05	0.03	-0.42	6.39	1.10	-6.03	-2.54	-0.72	0.00	-0.10	0.0	0.0	0.0	0.0	0.0
62 CCX5CCX4	0.01	0.02	0.09	2.14	2.34	1.85	0.38	0.13	0.00	0.01	-0.01	-2.15	-5.20	-0.32	-0.11
63 CCX'.OCZ	0.00	0.00	-0.23	0.13	0.06	1.96	-1.29	-0.83	-0.03	0.02	0.0	0.0	0.0	0.0	0.0
64 CCX'.OCC	-0.04	-0.00	-0.27	0.12	-0.12	-2.80	0.73	1.24	-0.02	0.70	0.0	0.0	0.0	0.0	0.0
65 CCX'.ZCC	0.04	0.0	0.52	-0.21	0.07	0.81	0.56	-0.46	-0.01	-0.81	0.0	0.0	0.0	0.0	0.0
66 OCZ..OCC	-0.00	0.0	0.12	0.00	-0.04	-1.10	-0.27	-1.09	-1.30	0.00	0.0	0.0	0.0	0.0	0.0
67 OCZ..ZCC	0.0	0.0	-0.23	-0.00	0.02	0.32	-0.20	0.39	-1.08	-0.20	0.0	0.0	0.0	0.0	0.0
68 OCC..ZCC	-0.02	0.00	-0.27	-0.00	-0.05	-0.45	0.11	-0.60	0.61	-1.48	0.0	0.0	0.0	0.0	0.0
69 WAG.TURS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.45	3.71	-5.75
70 M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.03	0.45	5.38	-3.69	0.57
71 M.DF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.14	-0.87	4.14	-3.35	-0.03

SIGNIFICANCE MATRIX ------- CD3-COBR

1 K (C=O)	0.00	-0.00	0.67	0.01	-0.00	0.00	0.02	0.00	0.00	C.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	0.00	-0.00	0.06	0.05	0.25	C.1C	0.00	0.47	0.10	0.03	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.00	0.01	0.14	0.49	0.17	0.23	0.18	0.08	0.00	0.00	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	0.66	1.51	0.0	0.00	0.01	0.00	0.00	-0.00	0.00	0.00	2.25	0.06	0.01	-0.0C	0.00
5 K(C-X)*	1.63	0.59	0.01	0.00	0.00	0.00	0.01	0.00	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.04	-0.00	0.07	0.16	0.77	0.16	0.10	0.50	0.48	0.54	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	0.0	0.0	0.05	0.08	0.45	0.17	0.02	0.27	1.20	0.02	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.04	-0.00	0.24	0.01	0.04	0.00	0.20	0.04	0.17	0.75	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.05	0.04	0.01	4.67	0.20	1.16	0.32	0.03	0.00	0.00	0.35	7.23	2.35	0.36	0.00
10 H(XCX)*	0.13	0.03	0.00	0.01	2.40	6.03	0.17	0.01	0.0	0.08	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.03	0.05	0.03	2.08	0.44	1.03	1.47	0.15	0.00	0.02	0.06	1.75	3.38	0.61	0.08
12 H(XCC)*	0.09	0.02	0.16	0.90	1.42	0.24	1.79	0.86	0.00	0.28	0.0	0.0	0.0	0.0	0.0
13 H (WAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.03	0.06	1.50	4.02	0.25
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0C	0.11	0.41	12.29
15 F (X--X)	0.25	3.13	0.00	2.36	0.11	0.56	0.23	0.01	0.00	-0.00	0.75	4.07	1.31	0.18	0.00
16 F(X--X)*	0.56	1.74	0.00	0.00	1.30	3.02	0.08	0.01	0.0	0.03	-0.15	-0.00	-0.00	-0.0C	0.0
17 F (X--C)	0.00	1.03	0.34	0.48	2.54	0.76	2.66	0.95	0.01	0.17	0.88	0.82	2.29	0.39	0.05
18 F (O--C)	0.02	0.02	0.05	0.27	0.15	0.07	0.49	0.58	0.25	0.26	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.03	0.01	0.10	0.16	-0.02	-0.01	0.08	0.44	0.06	1.09	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	0.00	-0.00	0.08	0.02	0.10	0.04	0.05	0.16	1.42	0.01	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.27	0.61	0.19	1.04	1.45	0.77	3.39	4.56	1.08	1.95	0.92	0.83	1.88	0.78	2.72
22 C(X--X*)	0.18	-0.06	0.21	0.39	0.79	0.49	0.94	0.19	0.33	3.55	0.05	1.52	3.74	-0.11	3.67
23 MOL.TEN.	-0.17	-0.08	-0.02	-3.57	-2.36	0.11	-1.87	-0.25	-0.00	-0.21	-0.21	1.01	-3.62	-0.61	-0.02
24 CC..CX*	0.01	-0.19	-0.06	0.03	0.04	-0.02	-0.07	0.01	0.00	0.00	0.0	0.0	0.0	0.0	0.0
25 CC..CX	-0.01	-0.43	-0.02	0.07	-0.12	0.04	-0.02	-0.00	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CD3-COBR

26 CC..CO	0.00	0.00	-0.60	0.11	0.00	-0.02	0.13	0.03	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	0.00	-0.00	0.18	-0.30	-0.42	-0.32	0.02	0.38	-0.03	0.01	0.0	0.0	0.0	0.0	0.0
28 CC..XCX*	0.00	0.04	-0.01	-0.03	-1.28	2.37	0.32	-0.07	-0.00	0.02	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	-0.00	0.07	0.11	4.25	-0.53	-1.51	-0.70	-0.15	-0.01	0.00	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	0.00	-0.08	0.19	-2.81	0.79	-1.42	1.46	-0.32	0.00	0.01	0.0	0.0	0.0	0.0	0.0
31 CC..CCX*	0.0	-0.03	-0.29	-1.30	1.02	0.46	-1.17	0.52	0.01	-0.03	0.0	0.0	0.0	0.0	0.0
32 CC..OCZ	0.0	-0.00	0.17	0.42	0.56	0.39	0.11	-0.29	-0.12	-0.01	0.0	0.0	0.0	0.0	0.0
33 CC..OCC	0.00	0.00	0.19	-0.55	-0.74	-0.39	0.26	0.40	0.07	-0.04	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	0.0	0.00	-0.36	0.15	0.17	-0.02	-0.38	-0.11	0.04	0.04	0.0	0.0	0.0	0.0	0.0
35 CX*..CH	-2.88	2.64	0.00	0.00	-0.01	-0.00	0.00	-0.00	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
36 CX*.XCX*	0.91	-0.25	0.0	-0.00	-0.15	-0.14	-0.08	-0.00	0.0	0.01	0.0	0.0	0.0	0.0	0.0
37 CX*..XCX	-0.73	-0.44	-0.02	0.06	-0.06	0.04	0.13	-0.01	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
38 CX*..CCX	0.66	0.50	-0.04	-0.12	0.08	0.04	-0.32	-0.02	0.0	0.00	0.0	0.0	0.0	0.0	0.0
39 CX*.CCX*	-0.73	0.22	0.06	-0.05	0.10	-0.02	0.22	0.03	0.00	-0.01	0.0	0.0	0.0	0.0	0.0
40 CX..CX5	0.66	1.51	0.0	0.00	0.01	0.00	0.00	-0.00	0.00	0.00	-2.25	-0.06	-0.01	-0.00	-0.00
41 CX..XCX*	-0.77	-0.56	0.0	-0.01	0.38	0.11	-0.02	0.00	0.0	-0.02	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	0.35	-0.50	-0.00	0.15	0.09	-0.07	0.01	0.00	-0.00	-0.00	1.79	-1.30	-0.37	-0.01	-0.00
43 CX4.XCX4	0.35	-0.48	-0.00	0.12	0.08	-0.08	0.01	0.00	0.00	-0.00	-1.76	1.24	0.34	0.01	0.0
44 CX4.CCX5	-0.28	0.58	-0.01	-0.12	-0.13	-0.07	-0.04	0.00	0.0	-0.01	0.76	0.62	-0.45	-0.01	0.00
45 CX4.CCX*	0.69	0.49	0.01	-0.11	-0.35	0.04	0.02	-0.03	-0.00	0.03	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	-0.28	0.58	-0.01	-0.12	-0.13	-0.07	-0.04	0.00	0.0	-0.01	-0.73	-0.64	0.40	0.01	-0.01
47 CO..CZ	0.0	0.0	-0.40	-0.03	-0.01	0.01	0.01	0.07	0.01	-0.01	0.0	0.0	0.0	0.0	0.0
48 CO..OCZ	0.00	-0.00	-0.38	0.04	0.01	-0.01	0.04	-0.06	0.04	0.00	0.0	0.0	0.0	0.0	0.0
49 CO..OCC	-0.01	0.0	-0.43	-0.06	-0.01	0.01	0.09	0.08	-0.03	0.03	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.01	0.00	0.80	0.02	0.00	0.00	-0.13	-0.02	-0.02	-0.03	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CD3-CGBR

51 CZ..OCZ	0.0	-0.00	0.11	-0.13	-0.67	-0.28	0.01	-0.71	0.69	-0.04	0.0	0.0	0.0	0.0	0.0
52 CZ..OCC	0.01	0.0	0.13	0.18	0.89	0.25	0.01	0.96	-0.44	-0.26	0.0	0.0	0.0	0.0	0.0
53 CZ..ZCC	-0.01	0.0	-0.24	-0.05	-0.21	0.01	-0.02	-0.26	-0.26	0.28	0.0	0.0	0.0	0.0	0.0
54 XCX'.XCX	-0.21	0.10	-0.00	1.02	1.30	-8.78	-0.92	0.06	0.00	0.00	0.0	0.0	0.0	0.0	0.0
55 XCX'.CCX	0.17	-0.11	-0.01	0.52	-2.59	-7.59	1.33	0.12	-0.00	0.13	0.0	0.0	0.0	0.0	0.0
56 XCX'CCX'	-0.20	-0.05	0.01	0.28	-3.29	2.30	-1.47	-0.29	-0.00	-0.34	0.0	0.0	0.0	0.0	0.0
57 XCX..XCX	0.05	0.04	0.01	4.67	0.20	1.16	0.32	0.03	0.00	0.00	-0.35	-7.10	-2.57	-0.38	0.0
58 XCX..CCX	-0.07	-0.09	0.04	-5.97	-0.75	2.23	-1.57	0.14	-0.00	0.00	0.30	-6.93	5.57	0.85	-0.01
59 XCX.CCX'	0.18	-0.08	-0.11	-5.48	-1.67	-1.64	2.11	-0.52	-0.01	-0.03	0.0	0.0	0.0	0.0	0.0
60 XCX5CCX4	-0.07	-0.09	0.04	-6.11	-0.65	2.24	-1.45	0.14	-0.00	0.00	-0.30	7.04	-5.86	-0.98	0.00
61 CCX.CCX'	-0.14	0.09	-0.20	3.92	2.13	-1.40	-4.71	-1.08	0.00	-0.25	0.0	0.0	0.0	0.0	0.0
62 CCX5CCX4	0.03	0.05	0.03	2.08	0.44	1.03	1.47	0.15	0.00	0.02	-0.06	-1.69	-3.46	-0.64	-0.08
63 CCX'.OCZ	0.00	0.00	-0.18	-0.54	1.63	0.39	-0.37	-0.96	-0.19	0.11	0.0	0.0	0.0	0.0	0.0
64 CCX'.OCC	-0.11	-0.00	-0.20	0.76	-2.04	-0.42	-0.87	1.32	0.07	0.75	0.0	0.0	0.0	0.0	0.0
65 CCX'.ZCC	0.11	-0.00	0.39	-0.20	0.49	-0.02	1.19	-0.36	0.05	-0.94	0.0	0.0	0.0	0.0	0.0
66 OCZ..OCC	0.0	-0.00	0.12	-0.22	-1.16	-0.35	0.08	-0.73	-1.55	0.15	0.0	0.0	0.0	0.0	0.0
67 OCZ..ZCC	0.00	0.0	-0.23	0.06	0.28	-0.01	-0.12	0.20	-0.86	-0.28	0.0	0.0	0.0	0.0	0.0
68 OCC..ZCC	-0.07	0.00	-0.26	-0.08	-0.36	0.01	-0.28	-0.27	0.57	-1.32	0.0	0.0	0.0	0.0	0.0
69 WAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.03	0.82	2.60	-4.02
70 M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.12	0.94	6.34	-4.61	0.39
71 M.DF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.28	-1.64	5.31	-3.66	-0.02

SIGNIFICANCE MATRIX ------- CF3-COH

1 K (C=O)	0.01	0.65	0.01	0.00	0.00	0.01	0.00	0.00	0.01	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	3.16	0.01	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.00	0.09	0.04	0.15	0.02	0.97	0.15	0.03	0.03	0.00	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	0.0	-0.00	0.09	0.52	0.10	0.00	0.02	0.01	-0.00	0.01	1.09	0.05	0.02	0.01	0.00
5 K(C-X)*	-0.00	0.00	0.30	0.04	0.56	0.03	0.00	0.00	0.00	0.01	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.04	0.07	0.21	0.04	0.00	0.58	0.18	0.11	0.81	0.90	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	0.01	0.41	1.87	0.13	1.11	3.41	0.17	0.17	1.66	1.45	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.01	0.82	3.33	0.03	1.15	1.18	0.00	0.01	0.16	0.07	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.0	-0.00	0.13	0.17	0.08	0.08	0.82	0.37	0.23	0.02	0.48	0.00	2.03	0.04	-0.00
10 H(XCX)*	0.0	0.0	0.11	0.20	0.13	0.01	0.16	1.44	0.08	0.07	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.00	0.05	0.14	0.13	0.04	0.14	0.38	0.00	1.08	0.17	0.66	0.69	0.01	0.44	0.00
12 H(XCC)*	0.01	0.09	0.13	0.26	0.06	0.00	0.64	0.10	0.26	0.42	0.0	0.0	0.0	0.0	0.0
13 H (HAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.20	1.54	0.00	3.14	0.93
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.15	0.00	2.87	19.02
15 F (X--X)	0.0	-0.00	0.01	0.31	0.13	0.02	0.72	0.26	0.13	0.01	0.21	0.04	1.24	0.01	0.00
16 F(X--X)*	0.0	-0.00	0.04	0.32	0.04	0.00	0.22	0.87	0.06	0.03	-0.07	-0.00	-0.00	-0.00	-0.00
17 F (X--C)	0.02	0.30	0.11	0.19	0.31	1.20	0.33	0.04	0.87	0.39	0.21	0.81	0.00	0.28	0.00
18 F (O--C)	0.01	0.06	0.07	0.20	0.02	0.38	0.46	0.15	0.37	0.53	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	1.65	0.27	2.24	0.19	0.83	0.26	0.10	0.04	0.03	0.04	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	1.79	0.28	0.98	0.08	0.48	1.71	0.06	0.07	0.63	0.60	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.03	0.12	0.23	0.04	0.07	0.66	0.53	0.21	2.22	3.99	0.37	1.14	0.01	0.09	5.15
22 C(X--X')	1.19	0.42	5.46	-0.08	2.34	0.49	0.10	0.05	1.75	0.06	0.27	0.56	0.00	2.37	3.83
23 MOL.TEN.	-0.00	-0.04	-0.30	-0.43	-0.18	-0.13	-1.05	-0.68	-0.61	-0.34	-0.68	-0.16	-0.51	-0.20	-0.00
24 CC..CX*	0.0	0.03	-0.23	-0.15	0.24	-0.34	-0.01	0.02	-0.02	0.00	0.0	0.0	0.0	0.0	0.0
25 CC..CX	-0.00	-0.01	0.19	-0.79	-0.14	-0.16	0.15	-0.04	0.01	-0.00	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CF3-COH

26 CC..CO	0.01	-0.48	-0.05	-0.03	-0.00	0.21	0.04	0.00	-0.03	-0.00	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	-0.19	-0.07	-0.01	-0.02	0.00	0.07	-0.02	-0.00	0.01	0.00	0.0	0.0	0.0	0.0	0.0
28 CC..XCX*	0.0	0.02	-0.14	0.35	0.11	0.16	0.31	0.36	0.09	0.01	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	-0.00	-0.03	0.22	0.46	-0.12	0.85	0.95	-0.29	0.23	-0.01	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	-0.01	0.18	-0.22	-0.40	0.09	-1.03	-0.70	-0.01	-0.55	0.01	0.0	0.0	0.0	0.0	0.0
31 CC..CCX*	0.01	-0.18	0.16	-0.39	-0.08	0.10	-0.64	-0.11	0.18	-0.02	0.0	0.0	0.0	0.0	0.0
32 CC..OCZ	0.01	0.38	-0.58	-0.28	-0.34	3.63	-0.33	-0.14	0.42	0.02	0.0	0.0	0.0	0.0	0.0
33 CC..OCC	-0.02	0.16	-0.20	0.16	-0.01	-1.50	0.33	0.11	-0.32	-0.03	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	0.01	-0.54	0.80	0.12	0.34	-2.17	-0.01	0.03	-0.14	-0.01	0.0	0.0	0.0	0.0	0.0
35 CX*..CH	0.0	-0.00	-0.47	0.39	-0.66	0.03	-0.01	-0.02	-0.00	-0.02	0.0	0.0	0.0	0.0	0.0
36 CX*.XCX*	-0.00	0.00	0.37	-0.17	0.53	-0.03	-0.01	0.14	-0.03	0.05	0.0	0.0	0.0	0.0	0.0
37 CX*..XCX	-0.00	-0.00	-0.54	-0.22	-0.59	-0.14	-0.04	-0.11	-0.09	-0.04	0.0	0.0	0.0	0.0	0.0
38 CX*..CCX	-0.00	0.03	0.57	0.20	0.42	0.18	0.02	-0.00	0.17	0.10	0.0	0.0	0.0	0.0	0.0
39 CX*.CCX*	0.00	-0.03	-0.38	0.20	-0.37	-0.02	0.02	-0.04	-0.06	-0.12	0.0	0.0	0.0	0.0	0.0
40 CX..CX5	0.0	-0.00	0.09	0.52	0.10	0.00	0.02	0.01	-0.00	0.01	-1.09	-0.05	-0.02	-0.01	-0.00
41 CX..XCX*	0.00	-0.00	-0.28	-0.90	-0.32	-0.01	0.15	-0.31	0.02	-0.07	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	0.00	0.00	0.22	-0.59	0.17	-0.03	0.25	0.10	0.02	0.03	1.46	-0.01	0.39	0.04	-0.00
43 CX4.XCX4	0.00	0.00	0.22	-0.59	0.17	-0.03	0.25	0.10	0.02	0.03	-1.45	0.02	-0.42	-0.04	-0.00
44 CX4.CCX5	0.0	-0.00	-0.23	0.52	-0.12	0.04	-0.17	0.00	-0.04	-0.07	1.69	-0.38	0.02	0.14	-0.00
45 CX4.CCX*	0.0	0.01	0.31	1.03	0.22	-0.01	-0.31	0.08	0.03	0.16	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	0.0	-0.00	-0.23	0.53	-0.12	0.04	-0.17	0.00	-0.04	-0.07	-1.69	0.38	-0.02	-0.14	0.00
47 CO..CZ	-0.36	0.18	0.01	0.00	0.00	0.01	-0.00	0.00	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
48 CO..OCZ	0.02	-1.03	0.30	0.03	0.01	0.40	-0.04	-0.01	-0.25	-0.06	0.0	0.0	0.0	0.0	0.0
49 CO..OCC	-0.04	-0.43	0.10	-0.02	-0.00	-0.17	0.04	0.01	0.17	0.04	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.02	1.47	-0.43	-0.01	-0.01	-0.24	-0.00	0.00	0.07	0.01	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CF3-COH

51 CZ..OCZ	-0.34	-0.15	0.07	0.02	-0.01	0.12	0.02	0.00	0.05	-0.02	0.0	0.0	0.0	0.0	0.0
52 CZ..OCC	0.09	-0.06	0.03	-0.01	-0.00	-0.06	-0.02	-0.00	-0.05	0.00	0.0	0.0	0.0	0.0	0.0
53 CZ..ZCC	-0.29	0.20	-0.15	-0.01	-0.01	-0.09	0.00	-0.00	-0.02	0.00	0.0	0.0	0.0	0.0	0.0
54 XCX'.XCX	0.0	-0.00	-0.34	0.52	-0.28	0.06	1.02	-2.08	0.38	-0.12	0.0	0.0	0.0	0.0	0.0
55 XCX'.CCX	0.0	0.02	0.35	-0.46	0.20	-0.08	-0.68	-0.05	-0.86	0.32	0.0	0.0	0.0	0.0	0.0
56 XCX'CCX'	0.0	-0.02	-0.24	-0.45	-0.18	0.01	-0.62	-0.78	0.28	-0.36	0.0	0.0	0.0	0.0	0.0
57 XCX..XCX	0.0	-0.00	0.13	0.17	0.08	0.08	0.82	0.37	0.23	0.02	-0.48	-0.00	-2.04	-0.04	-0.00
58 XCX..CCX	0.0	-0.01	-0.26	-0.30	-0.11	-0.22	-1.12	0.02	-1.01	-0.13	1.13	0.06	0.24	0.24	-0.00
59 XCX.CCX'	-0.00	0.02	0.35	-0.59	0.19	0.04	-2.05	0.55	0.69	0.27	0.0	0.0	0.0	0.0	0.0
60 XCX3CCX4	0.0	-0.01	-0.26	-0.30	-0.11	-0.22	-1.12	0.02	-1.01	-0.13	-1.13	-0.06	-0.25	-0.26	0.00
61 CCX.CCX'	-0.02	-0.19	-0.37	0.52	-0.14	-0.05	1.40	0.02	-1.50	-0.79	0.0	0.0	0.0	0.0	0.0
62 CCX3CCX4	0.00	0.05	0.14	0.13	0.04	0.14	0.38	0.00	1.07	0.17	-0.66	-0.70	-0.01	-0.44	-0.00
63 CCX'.OCZ	0.02	-0.38	-0.95	0.38	0.52	0.21	0.62	0.26	1.27	-1.64	0.0	0.0	0.0	0.0	0.0
64 CCX'.OCC	-0.04	-0.16	-0.33	-0.20	0.01	-0.06	-0.68	-0.21	-0.94	1.23	0.0	0.0	0.0	0.0	0.0
65 CCX'.ZCC	0.02	0.55	1.30	-0.17	-0.54	-0.09	-0.02	-0.06	-0.42	0.33	0.0	0.0	0.0	0.0	0.0
66 OCZ..OCC	-0.04	0.34	1.26	-0.14	0.05	-2.80	-0.36	-0.27	-2.35	-2.42	0.0	0.0	0.0	0.0	0.0
67 OCZ..ZCC	0.02	-1.13	-4.90	-0.12	-2.30	-4.15	0.00	-0.07	-1.07	-0.68	0.0	0.0	0.0	0.0	0.0
68 OCC..ZCC	-0.03	-0.47	-1.68	0.06	-0.05	1.66	-0.02	0.05	0.68	0.47	0.0	0.0	0.0	0.0	0.0
69 WAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.09	-0.93	0.00	-5.96	-10.95
70 M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.01	-2.97	0.01	3.26	-0.16
71 M.OF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.87	-0.09	0.25	0.65	-0.01

SIGNIFICANCE MATRIX ------- CF3-COD

1 K (C=O)	0.09	0.58	0.00	0.00	0.00	0.02	0.00	0.00	0.01	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	2.12	0.19	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.00	0.11	0.00	0.18	0.31	0.71	0.12	0.02	0.04	-0.00	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	0.0	-0.00	0.42	0.26	0.03	0.00	0.02	0.01	0.00	0.01	1.10	0.04	0.02	0.01	-0.00
5 K(C-X)'	0.00	-0.00	0.53	0.27	0.08	0.04	0.00	0.00	0.01	0.01	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.13	0.02	0.27	0.00	0.29	0.21	0.19	0.08	0.80	0.92	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	0.00	0.31	0.09	0.08	0.39	3.61	0.24	0.21	2.02	1.50	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.09	0.48	0.67	0.07	1.35	2.06	0.00	0.03	0.29	0.08	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.00	-0.00	0.10	0.32	0.02	0.05	0.82	0.33	0.24	0.02	0.49	0.00	2.03	0.03	-0.00
10 H(XCX)'	0.0	-0.00	0.36	0.05	0.03	0.01	0.15	1.47	0.05	0.07	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.02	0.03	0.10	0.27	0.06	0.06	0.39	0.01	1.03	0.17	0.65	0.78	0.01	0.34	-0.00
12 H(XCC)'	0.04	0.05	0.38	0.09	0.00	0.01	0.62	0.09	0.28	0.41	0.0	0.0	0.0	0.0	0.0
13 H (WAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.15	1.16	0.00	2.41	0.88
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.03	0.0	1.01	16.95
15 F (X--X)	0.0	0.0	-0.06	0.46	0.06	0.02	0.73	0.23	0.13	0.01	0.21	0.04	1.24	0.01	-0.00
16 F(X--X)'	0.00	-0.00	0.19	0.20	0.02	0.01	0.22	0.89	0.04	0.02	-0.07	-0.00	-0.00	-0.00	-0.00
17 F (X--C)	0.05	0.33	0.21	0.16	0.57	0.85	0.34	0.03	0.84	0.38	0.21	0.86	0.00	0.22	-0.00
18 F (O--C)	0.04	0.04	0.17	0.11	0.09	0.38	0.40	0.11	0.35	0.53	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.88	0.25	0.39	0.25	1.84	0.36	0.10	0.06	0.07	0.04	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	0.81	0.62	0.05	0.07	0.13	1.88	0.10	0.09	0.80	0.62	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.13	0.04	0.27	0.09	0.22	0.59	0.49	0.13	2.08	4.00	0.36	0.97	0.01	0.0	4.53
22 C(X--X')	0.70	0.17	1.22	-0.03	3.27	1.17	0.10	0.07	2.06	0.06	0.30	0.89	0.00	1.26	3.46
23 MOL.TEN.	-0.01	-0.03	-0.55	-0.41	-0.04	-0.07	-1.04	-0.63	-0.62	-0.33	-0.68	-0.20	-0.52	-0.15	-0.00
24 CC..CX'	0.00	0.03	-0.01	-0.44	0.31	-0.34	-0.00	0.02	-0.03	0.00	0.0	0.0	0.0	0.0	0.0
25 CC..CX	0.0	0.01	0.04	-0.61	-0.30	-0.03	0.13	-0.04	0.01	-0.00	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CF3-COD

26 CC..CO	0.02	-0.52	-0.00	-0.05	0.01	0.21	0.03	-0.00	-0.03	-0.00	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	-0.10	-0.30	0.00	-0.04	0.08	0.10	-0.03	-0.00	0.01	-0.00	0.0	0.0	0.0	0.0	0.0
28 CC..XCX'	0.0	0.01	-0.01	0.19	0.19	0.20	0.26	0.34	0.08	0.01	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	0.0	-0.02	0.01	0.67	0.21	0.55	0.82	-0.26	0.25	-0.01	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	-0.01	0.17	-0.01	-0.61	-0.38	-0.55	-0.63	-0.03	-0.57	0.01	0.0	0.0	0.0	0.0	0.0
31 CC..CCX'	0.02	-0.16	0.02	-0.25	-0.01	-0.12	-0.56	-0.09	0.19	-0.03	0.0	0.0	0.0	0.0	0.0
32 CC..OCZ	0.00	0.39	-0.01	-0.23	-0.69	3.18	-0.34	-0.14	0.50	0.02	0.0	0.0	0.0	0.0	0.0
33 CC..OCC	-0.03	0.09	-0.01	0.01	-0.60	-0.77	0.29	0.09	-0.34	-0.04	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	0.02	-0.48	0.03	0.21	1.29	-2.43	0.04	0.05	-0.20	-0.01	0.0	0.0	0.0	0.0	0.0
35 CX'..CH	0.0	-0.00	-1.32	0.76	-0.15	0.01	-0.00	-0.02	-0.01	-0.02	0.0	0.0	0.0	0.0	0.0
36 CX'.XCX'	0.0	0.00	0.87	-0.24	0.09	-0.04	-0.01	0.16	-0.03	0.05	0.0	0.0	0.0	0.0	0.0
37 CX'..XCX	-0.00	-0.00	-0.58	-0.88	0.11	-0.12	-0.03	-0.12	-0.11	-0.04	0.0	0.0	0.0	0.0	0.0
38 CX'..CCX	0.00	0.02	0.67	0.75	-0.19	0.13	0.01	-0.01	0.22	0.10	0.0	0.0	0.0	0.0	0.0
39 CX'.CCX'	-0.00	-0.02	-0.88	0.31	-0.01	0.03	0.00	-0.04	-0.08	-0.11	0.0	0.0	0.0	0.0	0.0
40 CX..CX5	0.0	-0.00	0.42	0.26	0.03	0.00	0.02	0.01	0.00	0.01	-1.10	-0.04	-0.02	-0.01	-0.00
41 CX..XCX'	0.0	0.0	-1.04	-0.36	-0.09	-0.00	0.15	-0.31	0.02	-0.07	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	0.00	0.0	0.40	-0.58	-0.05	-0.00	0.25	0.10	0.02	0.02	1.47	-0.02	0.39	0.03	0.00
43 CX4.XCX4	0.00	0.0	0.40	-0.58	-0.05	-0.00	0.25	0.10	0.02	0.02	-1.46	0.02	-0.42	-0.03	0.00
44 CX4.CCX5	-0.00	0.0	-0.40	0.53	0.09	0.00	-0.17	0.01	-0.05	-0.07	1.69	-0.36	0.02	0.11	-0.00
45 CX4.CCX'	0.00	-0.01	1.12	0.42	0.01	0.00	-0.31	0.07	0.04	0.15	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	-0.00	0.0	-0.40	0.53	0.09	0.00	-0.17	0.01	-0.05	-0.07	-1.69	0.36	-0.03	-0.11	-0.00
47 CO..CZ	-0.88	0.66	-0.00	0.01	0.00	0.02	-0.00	0.00	-0.01	0.00	0.0	0.0	0.0	0.0	0.0
48 CO..OCZ	0.03	-0.85	0.02	0.03	-0.01	0.47	-0.04	-0.00	-0.24	-0.06	0.0	0.0	0.0	0.0	0.0
49 CO..OCC	-0.22	-0.21	0.04	-0.00	-0.01	-0.11	0.03	0.00	0.15	0.04	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.19	1.06	-0.07	-0.03	0.02	-0.37	0.00	-0.00	0.09	0.01	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CF3-COD

51 CZ..OCZ	-0.14	-0.50	-0.01	0.03	-0.09	0.22	0.04	0.00	0.08	-0.02	0.0	0.0	0.0	0.0	0.0
52 CZ..OCC	1.05	-0.12	-0.02	-0.00	-0.08	-0.06	-0.04	-0.00	-0.06	-0.00	0.0	0.0	0.0	0.0	0.0
53 CZ..ZCC	-0.36	0.61	0.02	-0.03	0.16	-0.20	-0.00	-0.00	-0.04	0.00	0.0	0.0	0.0	0.0	0.0
54 XCX'.XCX	0.0	-0.00	-0.51	0.37	0.06	0.07	0.99	-2.00	0.30	-0.12	0.0	0.0	0.0	0.0	0.0
55 XCX'.CCX	0.00	0.01	0.54	-0.34	-0.11	-0.07	-0.66	-0.25	-0.66	0.31	0.0	0.0	0.0	0.0	0.0
56 XCX'CCX'	-0.00	-0.01	-0.72	-0.14	-0.00	-0.02	-0.59	-0.73	0.23	-0.36	0.0	0.0	0.0	0.0	0.0
57 XCX..XCX	0.00	-0.00	0.10	0.32	0.02	0.05	0.82	0.33	0.24	0.02	-0.49	-0.00	-2.04	-0.03	-0.00
58 XCX..CCX	0.0	-0.01	-0.19	-0.58	-0.06	-0.10	-1.12	0.09	-1.01	-0.12	1.13	0.10	0.25	0.19	-0.00
59 XCX.CCX'	0.0	0.01	0.53	-0.48	-0.00	-0.05	-2.02	0.48	0.73	0.26	0.0	0.0	0.0	0.0	0.0
60 XCX5CCX4	0.0	-0.01	-0.19	-0.58	-0.06	-0.10	-1.12	0.09	-1.01	-0.12	-1.13	-0.10	-0.26	-0.20	-0.00
61 CCX.CCX'	-0.08	-0.12	-0.54	0.44	0.01	0.06	1.38	0.06	-1.52	-0.76	0.0	0.0	0.0	0.0	0.0
62 CCX5CCX4	0.02	0.03	0.10	0.27	0.00	0.06	0.39	0.01	1.03	0.16	-0.65	-0.79	-0.01	-0.34	0.00
63 CCX'.OCZ	0.02	-0.26	-0.36	0.17	0.01	-0.25	0.73	0.26	1.45	-1.65	0.0	0.0	0.0	0.0	0.0
64 CCX'.OCC	-0.15	-0.06	-0.62	-0.01	0.01	0.08	-0.68	-0.17	-0.96	1.23	0.0	0.0	0.0	0.0	0.0
65 CCX'.ZCC	0.12	0.33	1.00	-0.15	-0.02	0.26	-0.15	-0.10	-0.58	0.34	0.0	0.0	0.0	0.0	0.0
66 OCZ..OCC	-0.04	0.15	0.31	-0.01	0.67	-1.71	-0.43	-0.26	-2.56	-2.48	0.0	0.0	0.0	0.0	0.0
67 OCZ..ZCC	0.03	-0.77	-0.47	-0.14	-1.40	-5.52	-0.07	-0.16	-1.59	-0.73	0.0	0.0	0.0	0.0	0.0
68 OCC..ZCC	-0.22	-0.19	-0.82	0.01	-1.26	1.34	0.04	0.09	0.93	0.49	0.0	0.0	0.0	0.0	0.0
69 WAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.02	-0.34	-0.00	-3.05	-9.88
70 M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.86	-2.74	0.01	2.51	-0.12
71 M.DF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.75	-0.15	0.19	0.54	-0.00

SIGNIFICANCE MATRIX ------- CF3-COF

1 K (C=O)	0.66	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	0.04	0.02	0.01	0.73	0.11	0.03	0.12	0.02	0.05	0.02	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.10	0.33	0.04	0.36	0.37	0.00	0.02	0.02	0.00	0.00	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	0.00	0.04	0.68	0.00	0.02	0.00	0.00	0.00	0.00	0.00	1.13	0.0	0.02	0.03	0.01
5 K(C-X)*	0.00	0.56	0.22	0.07	0.00	0.02	0.00	0.02	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.09	0.18	0.27	0.73	0.06	0.10	0.22	0.28	0.04	0.03	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	0.06	0.03	0.02	0.61	0.00	0.05	0.59	0.01	0.40	0.35	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.28	0.06	0.13	0.01	0.08	0.01	0.09	0.20	0.19	0.59	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.00	0.54	0.01	0.01	0.29	0.27	0.31	0.07	0.01	0.04	0.48	1.59	0.17	0.20	0.03
10 H(XCX)*	0.00	0.0	0.51	0.03	0.27	0.64	0.00	0.19	0.05	0.00	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.03	0.56	0.01	0.03	0.22	0.00	0.12	0.41	0.14	0.14	0.40	0.02	2.27	0.67	0.04
12 H(XCC)*	0.09	0.00	0.53	0.03	0.38	0.01	0.06	0.01	0.75	0.08	0.0	0.0	0.0	0.0	0.0
13 H (WAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.08	0.16	1.62	11.44	2.89
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.00	0.81	2.66
15 F (X--X)	0.00	0.35	-0.04	0.04	0.37	0.33	0.31	0.12	0.00	0.02	0.21	1.16	0.08	0.08	0.01
16 F(X--X)*	0.00	0.05	0.30	0.01	0.33	0.52	0.00	0.12	0.02	0.00	-0.08	0.00	-0.00	-0.00	-0.00
17 F (X--C)	0.27	0.05	0.23	1.02	0.38	0.04	0.24	0.56	0.69	0.17	0.24	0.02	1.57	0.38	0.02
18 F (O--C)	0.07	0.12	0.30	0.14	0.60	0.03	0.06	0.29	0.03	0.01	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.10	0.29	0.05	-0.01	0.38	0.07	0.07	0.17	0.36	0.75	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	0.06	0.01	0.01	0.15	0.14	0.13	0.91	0.02	0.16	0.17	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.20	0.26	0.18	0.48	0.71	0.09	0.23	1.60	1.77	0.33	0.34	0.01	1.63	0.07	0.78
22 C(X--X*)	0.22	0.09	0.29	-0.05	0.22	0.11	0.25	0.15	0.42	3.39	0.28	0.05	2.93	2.23	0.42
23 MOL.TEN.	-0.03	-0.59	-0.64	0.01	-0.56	-0.26	-0.21	-0.19	-0.35	-0.12	-0.57	-0.22	-1.09	-0.52	-0.05
24 CC..CX*	0.01	-0.86	0.19	0.32	0.06	0.01	-0.01	-0.04	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
25 CC..CX	-0.02	-0.31	-0.47	-0.12	0.22	-0.00	-0.02	0.01	0.00	-0.00	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CF3-CDF

26 CC..CD	-0.50	-0.01	0.02	-0.02	0.10	0.00	0.00	0.02	0.00	0.0	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	0.12	-0.16	0.04	-1.03	0.40	0.01	0.09	-0.04	0.01	0.01	0.0	0.0	0.0	0.0	0.0
28 CC..XCX*	0.02	0.02	0.29	0.20	0.63	-0.08	0.01	-0.14	-0.02	0.00	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	0.00	1.21	-0.04	-0.12	0.93	0.05	-0.20	-0.12	-0.01	-0.03	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	0.16	-1.21	0.04	-0.30	-0.81	-0.00	0.13	0.27	-0.04	0.05	0.0	0.0	0.0	0.0	0.0
31 CC..CCX*	-0.19	0.02	-0.29	0.21	-0.76	0.01	0.06	-0.03	0.05	-0.03	0.0	0.0	0.0	0.0	0.0
32 CC..DCZ	0.15	0.19	-0.06	0.94	0.05	0.02	0.18	-0.03	-0.04	-0.06	0.0	0.0	0.0	0.0	0.0
33 CC..DCC	0.18	-0.48	0.21	-1.03	0.31	-0.03	-0.12	0.16	0.01	-0.02	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	-0.33	0.29	-0.15	0.09	-0.35	0.01	-0.07	-0.14	0.03	0.07	0.0	0.0	0.0	0.0	0.0
35 CX*..CH	0.0	0.44	-1.10	-0.05	0.02	-0.01	0.01	-0.01	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
36 CX*.XCX*	0.00	-0.00	0.66	0.09	0.05	-0.24	-0.00	0.11	0.00	0.00	0.0	0.0	0.0	0.0	0.0
37 CX*..XCX	0.00	-1.54	-0.10	-0.05	0.08	0.21	0.04	0.09	0.00	-0.03	0.0	0.0	0.0	0.0	0.0
38 CX*..CCX	0.01	1.59	0.10	-0.13	-0.07	-0.00	-0.03	-0.23	0.01	0.05	0.0	0.0	0.0	0.0	0.0
39 CX*.CCX*	-0.01	-0.01	-0.69	0.10	-0.07	0.02	-0.01	0.03	-0.02	-0.03	0.0	0.0	0.0	0.0	0.0
40 CX..CX5	0.00	0.04	0.68	0.00	0.02	0.00	0.00	0.00	0.00	0.00	-1.13	-0.00	-0.02	-0.03	-0.01
41 CX..XCX*	-0.00	-0.00	-1.66	-0.03	0.19	0.06	-0.01	-0.03	-0.03	-0.00	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	0.00	-0.29	0.11	0.01	0.14	-0.03	0.08	-0.01	-0.01	0.01	1.47	0.04	0.10	0.15	0.03
43 CX4.XCX4	0.00	-0.29	0.11	0.01	0.14	-0.03	0.08	-0.01	-0.01	0.01	-1.47	-0.06	-0.11	-0.16	-0.03
44 CX4.CCX5	-0.01	0.31	-0.13	0.02	-0.12	0.00	-0.05	0.03	-0.04	-0.02	1.34	-0.01	0.37	0.28	0.03
45 CX4.CCX*	0.02	-0.00	1.69	-0.03	-0.23	-0.01	-0.05	-0.01	0.13	0.02	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	-0.01	0.31	-0.13	0.02	-0.12	0.00	-0.05	0.03	-0.04	-0.02	-1.34	0.00	-0.38	-0.29	-0.03
47 CO..CZ	-0.32	0.00	0.01	0.02	0.05	0.00	0.01	-0.02	-0.00	0.00	0.0	0.0	0.0	0.0	0.0
48 CO..DCZ	-0.38	-0.00	-0.01	-0.02	0.01	0.01	0.02	-0.01	0.01	-0.00	0.0	0.0	0.0	0.0	0.0
49 CO..DCC	-0.47	0.01	0.04	0.02	0.04	-0.01	-0.02	0.07	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.85	-0.01	-0.03	-0.00	-0.04	0.00	-0.01	-0.06	-0.01	-0.00	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CF3-COF

51 CZ..OCZ	0.10	-0.05	-0.03	-1.33	0.02	0.08	0.53	0.02	-0.28	-0.18	0.0	0.0	0.0	0.0	0.0
52 CZ..OCC	0.12	0.12	0.11	1.45	0.16	-0.11	-0.33	-0.14	0.09	-0.05	0.0	0.0	0.0	0.0	0.0
53 CZ..ZCC	-0.21	-0.07	-0.08	-0.13	-0.19	0.03	-0.20	0.12	0.19	0.23	0.0	0.0	0.0	0.0	0.0
54 XCX'.XCX	0.0	0.04	-0.16	-0.03	0.79	-1.17	-0.09	0.32	0.05	-0.02	0.0	0.0	0.0	0.0	0.0
55 XCX'.CCX	0.01	0.00	0.14	-0.08	-0.67	0.01	0.03	-0.82	0.24	0.02	0.0	0.0	0.0	0.0	0.0
56 XCX'CCX'	-0.02	0.00	-1.04	0.06	-0.64	-0.12	0.02	0.09	-0.40	-0.01	0.0	0.0	0.0	0.0	0.0
57 XCX..XCX	0.00	0.54	0.01	0.01	0.29	0.27	0.31	0.07	0.01	0.04	-0.48	-1.60	-0.18	-0.21	-0.03
58 XCX..CCX	0.00	-1.10	-0.01	0.02	-0.50	-0.00	-0.39	-0.35	0.06	-0.15	0.88	-0.29	1.23	0.73	0.07
59 XCX.CCX'	-0.00	0.04	0.14	-0.03	-0.93	0.11	-0.40	0.07	-0.19	0.16	0.0	0.0	0.0	0.0	0.0
60 XCX5CCX4	0.00	-1.10	-0.01	0.02	-0.50	-0.00	-0.39	-0.35	0.06	-0.15	-0.87	0.34	-1.30	-0.76	-0.07
61 CCX.CCX'	-0.15	-0.02	-0.17	-0.09	0.81	-0.00	0.25	-0.18	-0.93	-0.30	0.0	0.0	0.0	0.0	0.0
62 CCX5CCX4	0.03	0.56	0.01	0.03	0.22	0.00	0.12	0.41	0.14	0.14	-0.40	-0.01	-2.28	-0.72	-0.05
63 CCX'.OCZ	-0.14	0.00	0.22	0.28	-0.04	0.03	0.38	0.02	-1.10	0.33	0.0	0.0	0.0	0.0	0.0
64 CCX'.OCC	-0.17	-0.00	-0.74	-0.31	-0.31	-0.05	-0.24	-0.11	0.34	0.10	0.0	0.0	0.0	0.0	0.0
65 CCX'.ZCC	0.31	0.00	0.53	0.03	0.35	0.01	-0.15	0.09	0.74	-0.45	0.0	0.0	0.0	0.0	0.0
66 OCZ..OCC	0.14	-0.14	-0.15	-1.33	0.02	-0.14	-0.73	-0.09	-0.26	0.21	0.0	0.0	0.0	0.0	0.0
67 OCZ..ZCC	-0.25	0.09	0.11	0.11	-0.02	0.04	-0.45	0.08	-0.54	-0.93	0.0	0.0	0.0	0.0	0.0
68 OCC..ZCC	-0.30	-0.21	-0.38	-0.13	-0.15	-0.05	0.28	-0.49	0.17	-0.28	0.0	0.0	0.0	0.0	0.0
69 WAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.06	0.17	6.11	-6.52
70 M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.49	-0.13	-5.04	-8.69	-1.30
71 M.DF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.54	1.52	-1.49	-4.66	-0.96

SIGNIFICANCE MATRIX ------- CF3-COCL

1 K (C=O)	0.68	0.0	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
2 K (C-Z)	0.09	0.00	0.00	0.52	0.18	0.0C	0.11	0.10	0.08	0.03	0.0	0.0	0.0	0.0	0.0
3 K (C-C)	0.09	0.28	0.03	0.65	C.27	0.03	0.01	-0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
4 K (C-X)	-0.00	0.10	0.63	0.00	0.01	-0.00	0.00	0.00	0.00	0.00	1.16	0.00	0.02	C.03	0.02
5 K(C-X)*	0.00	0.51	0.36	0.02	0.00	0.01	0.00	0.01	0.00	0.00	0.0	0.0	0.0	0.0	0.0
6 H(CCO)	0.08	0.06	0.22	1.0C	0.20	0.08	0.03	0.41	0.12	0.00	0.0	0.0	0.0	0.0	0.0
7 H (OCZ)	0.05	0.00	0.01	0.93	0.02	0.00	0.32	0.26	0.48	0.47	0.0	0.0	0.0	0.0	0.0
8 H (CCZ)	0.25	0.03	0.15	0.00	0.10	0.11	0.14	0.02	0.12	0.44	0.0	0.0	0.0	0.0	0.0
9 H (XCX)	0.0	0.52	0.03	0.01	0.47	0.43	0.12	0.00	0.00	0.03	0.46	1.64	0.34	0.17	0.09
10 H(XCX)*	0.0	0.01	0.47	0.02	0.13	0.68	0.40	0.18	0.06	0.01	0.0	0.0	0.0	0.0	0.0
11 H (XCC)	0.03	0.49	0.03	0.12	0.18	0.03	0.43	0.16	0.17	0.13	0.40	0.05	2.22	0.67	0.40
12 H(XCC)*	0.08	0.01	0.47	0.04	0.53	0.02	0.04	0.01	0.71	0.12	0.0	0.0	0.C	0.0	0.0
13 H (HAG)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.05	0.19	0.95	9.88	5.63
14 H (TORS)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00	0.01	0.02	1.12	1.88
15 F (X--X)	0.0	0.42	-0.08	0.05	0.50	0.46	0.14	0.00	0.00	0.01	0.22	1.1C	0.18	0.07	0.03
16 F(X--X)*	0.00	0.09	0.29	0.01	0.18	0.48	0.31	0.10	0.03	0.0C	-0.08	-0.0C	-0.0C	-0.0C	-0.00
17 F (X--C)	0.27	0.08	0.21	1.4C	0.33	0.11	0.48	0.19	0.66	0.16	0.24	0.06	1.57	0.4C	0.24
18 F (O--C)	0.08	0.13	0.24	0.22	0.68	0.12	0.01	0.24	0.06	0.00	0.0	0.0	0.0	0.0	0.0
19 F(C-Z)	0.09	0.29	0.08	-0.08	0.28	0.06	0.05	0.15	0.33	0.66	0.0	0.0	0.0	0.0	0.0
20 F(O--Z)	0.08	0.00	0.00	0.20	0.15	0.01	0.56	0.40	0.12	0.16	0.0	0.0	0.0	0.0	0.0
21 C (X--O)	0.20	0.15	0.21	0.68	0.86	0.35	0.48	1.13	2.08	0.25	0.35	0.04	1.51	0.03	1.29
22 C(X--X')	0.21	0.01	0.42	-0.05	0.18	0.10	0.35	-0.01	0.24	2.72	0.27	0.12	2.87	2.76	-0.28
23 MOL.TEN.	-0.03	-0.53	-0.63	-0.04	-0.56	-0.45	-0.39	-0.03	-0.37	-0.14	-0.55	-0.13	-1.33	-0.49	-0.28
24 CC..CX*	0.01	-0.75	0.20	0.22	0.05	-0.04	-0.01	-0.00	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
25 CC..CX	-0.01	-0.46	-0.38	-0.05	0.16	-0.00	-0.00	0.00	-0.00	0.00	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CF3-CCCL

26 CC..CO	-0.50	-0.00	0.01	-0.01	0.08	0.01	0.01	0.00	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
27 CC..CZ	0.18	-0.05	0.02	-1.17	0.44	0.01	0.05	-0.01	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
28 CC..XCX'	0.01	0.11	0.22	0.22	0.38	0.26	-0.11	-0.01	0.00	-0.00	0.0	0.0	0.0	0.0	0.0
29 CC..XCX	0.01	1.09	-0.08	0.27	0.95	-0.32	-0.09	-0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0
30 CC..CCX	0.16	-1.05	0.09	-0.80	-0.62	0.08	0.14	0.01	0.00	-0.01	0.0	0.0	0.0	0.0	0.0
31 CC..CCX'	-0.17	-0.12	-0.23	0.33	-0.77	-0.05	0.03	-0.00	-0.02	0.00	0.0	0.0	0.0	0.0	0.0
32 CC..OCZ	0.13	0.07	-0.03	1.56	-0.15	0.02	0.09	-0.01	0.00	0.00	0.0	0.0	0.0	0.0	0.0
33 CC..OCC	0.17	-0.25	0.15	-1.62	0.47	0.09	-0.03	0.01	-0.00	-0.00	0.0	0.0	0.0	0.0	0.0
34 CC..ZCC	-0.30	0.19	-0.13	0.06	-0.32	-0.11	-0.07	-0.00	-0.00	-0.01	0.0	0.0	0.0	0.0	0.0
35 CX'..CH	0.0	0.65	-1.36	-0.01	0.01	0.00	0.00	-0.02	-0.00	-0.01	0.0	0.0	0.0	0.0	0.0
36 CX'.XCX'	0.00	-0.12	0.81	0.04	0.03	-0.19	0.08	0.08	0.01	0.01	0.0	0.0	0.0	0.0	0.0
37 CX'..XCX	-0.00	-1.42	-0.34	0.05	0.08	0.20	0.06	0.01	0.00	-0.03	0.0	0.0	0.0	0.0	0.0
38 CX'..CCX	0.00	1.42	0.30	-0.14	-0.05	-0.05	-0.12	-0.11	0.02	0.07	0.0	0.0	0.0	0.0	0.0
39 CX'.CCX'	-0.01	0.17	-0.83	0.06	-0.07	0.03	-0.03	0.02	-0.03	-0.04	0.0	0.0	0.0	0.0	0.0
40 CX..CX5	-0.00	0.10	0.63	0.00	0.01	-0.00	0.00	0.00	0.00	0.00	-1.16	-0.01	-0.02	-0.03	-0.02
41 CX..XCX'	0.00	-0.08	-1.54	-0.01	0.11	-0.03	0.03	-0.08	-0.03	-0.01	0.0	0.0	0.0	0.0	0.0
42 CX..XCX	-0.00	-0.45	0.28	-0.00	0.15	0.01	0.01	-0.00	-0.00	0.01	1.46	0.17	0.15	0.13	0.08
43 CX4.XCX4	-0.00	-0.45	0.28	-0.00	0.15	0.01	0.01	-0.00	-0.00	0.01	-1.45	-0.19	-0.15	-0.14	-0.09
44 CX4.CCX5	-0.01	0.45	-0.30	0.01	-0.09	-0.00	-0.02	0.05	-0.03	-0.03	1.37	-0.03	0.37	0.27	0.18
45 CX4.CCX'	0.01	0.11	1.55	-0.01	-0.23	0.00	-0.01	-0.02	0.09	0.04	0.0	0.0	0.0	0.0	0.0
46 CX4.CCX4	-0.01	0.45	-0.30	0.01	-0.09	-0.00	-0.02	0.05	-0.03	-0.03	-1.37	0.03	-0.38	-0.27	-0.18
47 CO..CZ	-0.49	-0.00	0.00	0.00	0.07	0.00	0.04	-0.02	0.00	0.01	0.0	0.0	0.0	0.0	0.0
48 CO..OCZ	-0.36	0.00	-0.00	-0.01	-0.02	0.00	0.07	-0.03	-0.01	-0.03	0.0	0.0	0.0	0.0	0.0
49 CO..OCC	-0.46	0.00	0.03	0.01	0.07	0.01	-0.02	0.04	0.00	0.00	0.0	0.0	0.0	0.0	0.0
50 CO..ZCC	0.82	0.0	-0.02	0.00	-0.05	-0.02	-0.05	-0.01	0.00	0.03	0.0	0.0	0.0	0.0	0.0

SIGNIFICANCE MATRIX ------- CF3-CCCL

51 CZ..CCZ	0.13	-0.01	-0.01	-1.40	-0.12	0.00	0.38	0.33	-0.40	-0.23	0.0	0.0	0.0	0.0	0.0
52 CZ..CCC	0.17	0.02	0.04	1.45	0.37	0.01	-0.12	-0.42	0.20	0.01	0.0	0.0	0.0	0.0	0.0
53 CZ..ZCC	-0.30	-0.02	-0.04	-0.05	-0.26	-0.02	-0.25	0.08	0.20	0.22	0.0	0.0	0.0	0.0	0.0
54 XCX*.XCX	0.0	0.22	-0.37	0.04	0.71	-1.55	0.62	0.03	0.01	-0.04	0.0	0.0	0.0	0.0	0.0
55 XCX*.CCX	0.01	-0.16	0.34	-0.13	-0.41	0.41	-1.21	-0.51	0.27	0.08	0.0	0.0	0.0	0.0	0.0
56 XCX*CCX*	-0.01	-0.02	-0.94	0.05	-0.51	-0.23	-0.26	0.08	-0.42	-0.06	0.0	0.0	0.0	0.0	0.0
57 XCX..XCX	0.00	0.52	0.03	0.01	0.47	0.43	0.12	0.00	0.00	0.03	-0.46	-1.64	-0.36	-0.18	-0.09
58 XCX..CCX	0.00	-1.00	-0.07	-0.08	-0.56	-0.22	-0.49	-0.03	0.01	-0.13	0.86	-0.52	1.67	0.65	0.36
59 XCX.CCX*	-0.00	-0.23	0.34	0.07	-1.40	0.24	-0.21	0.01	-0.05	0.17	0.0	0.0	0.0	0.0	0.0
60 XCX5CCX4	0.00	-1.01	-0.07	-0.08	-0.57	-0.23	-0.48	-0.02	0.01	-0.13	-0.86	0.61	-1.80	-0.71	-0.40
61 CCX.CCX*	-0.15	0.24	-0.36	-0.20	0.87	-0.07	0.37	-0.10	-0.98	-0.36	0.0	0.0	0.0	0.0	0.0
62 CCX5CCX4	0.04	0.50	0.03	0.12	0.18	0.03	0.43	0.16	0.16	0.13	-0.40	-0.05	-2.23	-0.72	-0.44
63 CCX*.CCZ	-0.13	-0.01	0.12	0.39	0.20	-0.02	0.22	0.09	-1.19	0.46	0.0	0.0	0.0	0.0	0.0
64 CCX*.CCC	-0.16	0.06	-0.64	-0.40	-0.67	-0.08	-0.08	-0.12	0.58	-0.02	0.0	0.0	0.0	0.0	0.0
65 CCX*.ZCC	0.29	-0.04	0.53	0.01	0.45	0.09	-0.15	0.02	0.58	-0.47	0.0	0.0	0.0	0.0	0.0
66 CCZ..CCC	0.12	-0.03	-0.08	-1.93	-0.13	0.03	-0.21	-0.67	-0.50	-0.04	0.0	0.0	0.0	0.0	0.0
67 CCZ..ZCC	-0.22	0.02	0.07	0.07	0.09	-0.04	-0.43	0.13	-0.48	-0.93	0.0	0.0	0.0	0.0	0.0
68 CCC..ZCC	-0.28	-0.08	-0.36	-0.07	-0.28	-0.19	0.14	-0.17	0.24	0.02	0.0	0.0	0.0	0.0	0.0
69 WAG.TORS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.02	0.07	0.25	6.59	-7.85
70 M.RK.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.39	-0.27	-3.83	-7.99	-5.58
71 M.OF.WAG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.41	1.64	-1.59	-4.03	-2.46

BIBLIOGRAPHY

1. M. Davies, Infrared Spectroscopy and Molecular Structure, Elsevier Publishing Company, New York, 1963.
2. H. C. Urey and C. A. Bradley, Phys. Rev., 38, 1969 (1931).
3. J. H. Schachtschneider, Vibrational Analysis of Polyatomic Molecules. V, Technical Report No. 231-64, Shell Development Company, Emeryville, California, 1964.
4. E. B. Wilson, J. C. Decius, and P. C. Cross, Molecular Vibrations, McGraw-Hill, 1955.
5. E. B. Wilson, J. Chem. Phys., 7, 1047(1939); 9, 76 (1941).
6. J. C. Decius, J. Chem. Phys., 16, 1025(1948).
7. R. M. Badger and L. R. Zumwalt, J. Chem. Phys., 6, 711 (1938).
8. F. A. Cotton, Chemical Applications of Group Theory, Wiley-Interscience, New York, 1963.
9. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules, Van Nostrand Company, Inc., Princeton, N. J., 1945.
10. C. E. Sun, R. G. Parr, and B. L. Crawford, Jr., J. Chem. Phys., 17, 840(1949).
11. T. Shimanouchi, J. Chem. Phys., 17, 245(1949); 17, 734 (1949); 17, 848(1949).
12. R. L. Redington and A. L. K. Aljibury, J. Mol. Spectry, 37, 494(1971).

13. G. A. Segal, R. E. Burns, and W. B. Person, J. Chem. Phys., 50, 3811(1969).

14. I. W. Levin, and T. P. Lewis, J. Chem. Phys., 52, 1608(1970).

15. J. H. Schachtschneider and R. G. Snyder, Spectrochim. Acta, 19, 117(1963).

16. D. E. Mann, T. Shimanouchi, J. H. Meal, and L. Fano, J. Chem. Phys., 27, 43(1957).

17. K. Nakamoto, Infrared Spectra of Inorganic and Coordination Compounds, Wiley-Interscience, New York, 1970.

18. J. Overend and J. R. Scherer, J. Chem. Phys., 32, 1289 (1960).

19. D. Steele, Theory of Vibrational Spectroscopy, W. B. Saunders Company, Philadelphia, 1971.

20. P. Cossee and J. H. Schachtschneider, J. Chem. Phys., 44, 97(1966).

21. L. Pierce and L. C. Krisher, J. Chem. Phys., 31, 875 (1959).

22. R. C. Weast, Ed., Handbook of Chemistry and Physics, 50th Edition, The Chemical Rubber Company, Cleveland, Ohio, 1970.

23. Y. Morino, K. Kuchitso, and T. Shimanouchi, J. Chem. Phys., 20, 726(1952).

24. T. Shimanouchi, I. Nakagawa, J. Hiraishi, and M. Ishii, J. Mol. Spect., 19, 78(1966).

25. R. W. Kilb, C. C. Lin, and E. B. Wilson, J. Chem. Phys., 26, 1695(1957).

26. K. M. Sinnott, J. Chem. Phys., 34, 851(1961).

27. L. C. Krisher, J. Chem. Phys., 38, 1237(1960).

28. R. C. Woods III, Ph.D. Thesis, Harvard University (1965); J. Chem. Phys., 46, 4789(1967).

29. R. H. Schwendeman, Ph.D. Thesis, University of Michigan, (1956); Diss. Abs., 18, 1645(1956).

30. G. A. Boulet, Ph.D. Thesis, University of Michigan, (1964); Diss. Abs., 25, 3283(1964).

31. J. N. Shoolery, R. G. Shulman, W. F. Sheehan, Jr., V. Schomaker, and D. M. Yost, J. Chem. Phys., 19, 1364(1951).

32. C. V. Berney, and A. D. Cormier, Spectrochim Acta, to be published.

33. J. Overend, R. A. Nyquist, J. C. Evans, and W. J. Potts, Spectrochim Acta, 17, 1205(1961).

34. L. C. Hall, and J. Overend, Spectrochim Acta, 23A, 2535(1967).

35. R. J. Capwell, Jr., J. Chem. Phys., 49, 1436(1968).

36. C. V. Berney, Spectrochim Acta, 25A, 793(1969).

37. C. V. Berney, Spectrochim Acta, 27A, 663(1971).

38. C. V. Berney, Spectrochim Acta, 20, 1437(1964).

39. C. B. Moore, and G. C. Pimentel, J. Chem. Phys., 40, 1529(1964).

40. J. A. Devore, and H. E. O'Neal, J. Phys. Chem., 73, 2644(1969).

41. E. J. Jacob, H. B. Thompson, and L. S. Bartell, J. of Chem. Phys., 47, 3736(1967).

42. P. v. R. Schleyer, J. E. Williams, and K. R. Blanchard, J. Amer. Chem. Soc., 92, 2377(1970).

43. N. L. Allinger, M. T. Tribble, M. A. Miller, and D. H. Wertz, J. Amer. Chem. Soc., 93, 1637(1971).

44. M. Bixson, and S. Lifson, Tetrahedron, 23, 769(1967).

45. K. B. Wiberg, J. Amer. Chem. Soc., 87, 1070(1965).

46. R. H. Boyd, S. N. Sanwal, S. Shary-Tehrany, and D. McNally, J. Phys. Chem., 75, 1264(1971).

47. R. H. Boyd, J. Chem. Phys., 49, 2574(1968).

48. S. Chang, D. McNally, S. Shary-Tehrany, S. M. J. Hickey, R. H. Boyd, J. Amer. Chem. Soc., 92, 3109 (1970).

49. L. B. Kier, J. of Med. Chem., 11, 441(1968).