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TEST DATA FOR NORMAL COORDINATE CALCULATIONS

Prepared for publication by

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in conjunction with

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Test data for normal coordinate calculations

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CONTENTS

A. ABSTRACT

Input data for testing normal coordinate analysis programs and the results of calculation (**G** and **F** matrices, eigenvalues, normal frequencies in cm^{-1}, eigenvectors, potential energy distributions and the Jacobian matrix) are given for four representative molecules, namely, H_2O, CH_4, CH_3CN and Cl_2CCH_2.

B. INTRODUCTION

Today normal coordinate analyses (NCA) are being carried out routinely in many laboratories all over the world. Various computer programs which have been developed independently are in use for this purpose. In 1979, however, no one seemed to be sure as to whether the different programs gave exactly the same results from the same input data. Therefore, it seemed desirable to develop a set of reference input data for testing independent programs. Publication of such input data and the results of calculation (normal frequencies, eigenvector matrices, potential energy distributions, etc.) must be of value for many investigators who wish to test their own programs.

In 1979 the late Professor T. Shimanouchi and one of the present authors (MT) submitted a proposal for developing test data for NCA programs to the Commission on Molecular Structure and Spectroscopy. This proposal was approved by the Commission at the Davos meeting in 1979. A working group consisting of J. Durig, R.N. Jones, C.J.H. Schutte and G. Zerbi was then formed to choose the most suitable molecules and input data and to compare the results which were calculated by their own programs. The following four molecules, namely, H_2O, CH_4, CH_3CN and Cl_2CCH_2 were chosen, so that the treatment of all kinds of internal coordinates (bond stretch, angle bend, linear bend, out-of-plane bend and torsion) could be tested. These molecules belong to different point groups having degenerate and nondegenerate symmetry species. The results calculated independently by the members of this working group agreed with each other satisfactorily.

We wish to dedicate this report to Professor Takehiko Shimanouchi who passed away in May, 1980.

C. DEFINITION OF TERMS

The normal coordinate calculations reported were carried out using the Wilson **GF** matrix method.[1-3] The internal coordinates were defined according to the IUPAC recommendations.[4,5]

The input and output data given in Section D for the four molecules are mostly self-explanatory, but some additional descriptions may be in order. Case I (H_2O) will be taken below as an example. The data neccessary for NCA are given in Sub-sections 1-6. In Sub-section 3 the three internal coordinates (R_1, R_2 and R_3) are defined for the H_2O molecule. R_1 and R_2 are the stretchings of the two OH bonds, and R_3 represents the bending of the HOH angle. In Sub-section 4 the symmetry coordinates are derived from the

internal coordinates; S_1 (symmetric stretch) and S_2 (bend) belong to the symmetry species a_1, and S_3 (antisymmetric stretch) to b_1. In Sub-section 5 the information on force constants is provided. For H_2O, the potential energy function V is expressed as

$$V = (1/2)F(R1R1)R_1^2 + (1/2)F(R2R2)R_2^2 + (1/2)F(R3R3)R_3^2 + F(R1R2)R_1R_2 + F(R1R3)R_1R_3 + F(R2R3)R_2R_3 \quad (1)$$

where F(R1R1), F(R2R2), etc correspond to the force constants given in Sub-section 7, and F(R1R1) = F(R2R2) and F(R1R3) = F(R2R3) by definition. The force constants are given in units of 10^2 N m^{-1} (= mdyn $Å^{-1}$) for stretch-stretch, 10^{-8} N (= mdyn) for stretch-bend, and 10^{-18} N m (= mdyn Å) for bend-bend. For the other three molecules, V is expressed as

$$V = (1/2)F(1,1)S_1^2 + (1/2)F(2,2)S_2^2 + \cdots\cdots + F(1,2)S_1S_2 + \cdots\cdots \quad (2)$$

using S_i's instead of R_i's. The force field of this type is called the symmetrized valence force field.

In Sub-section 7 the symmetrized **B**, **G** and **F** matrices (B_S, G_S and F_S) are given. These matrices are defined as follows. In the first place,

$$\mathbf{S} = \mathbf{B}_S\mathbf{X} \quad (3)$$

where **S** stands for a vector consisting of the symmetry coordinates and **X** a vector consisting of the Cartesian displacements of all the atoms. Using the B_S matrix the kinetic energy matrix G_S is derived as

$$\mathbf{G}_S = \mathbf{B}_S\mathbf{M}^{-1}\tilde{\mathbf{B}}_S \quad (4)$$

where **M** is a diagonal matrix whose elements consist of the atomic masses. The potential energy V is expressed as

$$V = (1/2)\tilde{\mathbf{S}}\mathbf{F}_S\mathbf{S}. \quad (5)$$

The matrices G_S, F_S, Λ(a diagonal matrix whose elements are the eigenvalues) and L_S (a matrix consisting of the eigenvectors) are related by the secular equation

$$\mathbf{L}_S^{-1}\mathbf{G}_S\mathbf{F}_S\mathbf{L}_S = \Lambda. \quad (6)$$

The vector (**Q**) consisting of normal coordinates (Q_i) and **S** are linked by L_S as

$$\mathbf{S} = \mathbf{L}_S\mathbf{Q}. \tag{7}$$

Likewise, **X** is linked with **Q** by a matrix called $\mathbf{L}_X$ as

$$\mathbf{X} = \mathbf{L}_X\mathbf{Q}. \tag{8}$$

In this report the transposed matrix $\tilde{\mathbf{L}}_X$ is given for each molecule. An eigenvalue λ_a (calculated using atomic weights in the atomic mass unit and force constants in the units described above) can be converted to a normal frequency ν_a (in cm^{-1}) by the relation

$$\nu_a = 1302.78\sqrt{\lambda_a} \tag{9}$$

(Avogadro constant $N_A = 6.022045 \times 10^{23}$ mol^{-1} and the speed of light in vacuum $c = 2.99792458 \times 10^8$ m s^{-1} were used to calculate the conversion coefficient.) The elements of potential energy distribution (PED) for the a-th normal frequency ν_a correspond to

$$[(\mathbf{F}_S)_{ii}(\mathbf{L}_S)^2_{ia}/\lambda_a] \times 100, \tag{10}$$

where i refers to the i-th symmetry coordinates. Summation of the PED elements over i usually gives a value close to 100. In this report this sum is not normalized to 100. In the last place the Jacobian matrix is given. Its element $\partial\nu_a/\partial F_{ij}$ gives the expected change of the normal frequency ν_a (in cm^{-1}) per unit change of the **F**-matrix element F_{ij} (the unit of $\partial\nu_a/\partial F_{ij}$ itself is variable according to the unit of F_{ij}).

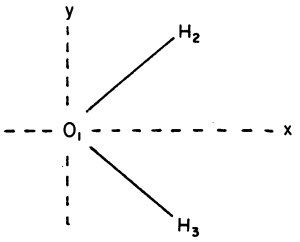
References

1. E.B. Wilson, Jr., J.C. Decius and P.C. Cross, "Molecular Vibrations," McGraw-Hill, New York (1955).
2. T. Shimanouchi, "Computer Programs for Normal Coordinate Treatment of Polyatomic Molecules," University of Tokyo (1968).
3. L.A. Woodward, "Introduction to the Theory of Molecular Vibrations and Vibrational Spectroscopy," Oxford University Press, Oxford (1972).
4. IUPAC Commission on Molecular Structure and Spectroscopy, Pure Appl. Chem. 50, 1707 (1978).
5. H. Matsuura and M. Tasumi, "Force Fields for Large Molecules," in "Vibrational Spectra and Structure," ed. by J.R. Durig, Vol. 12, Chapter 2, pp. 69-143, Elsevier, Amsterdam (1983).

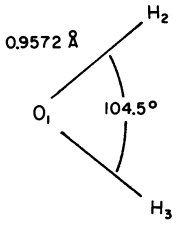
D. INPUT AND OUTPUT DATA

I. H_2O (Water)

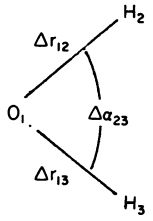
1. Numbering of atoms and the cartesian axes.



2. Structural parameters.



3. Internal coordinates.



$R_1 = \Delta r_{12}$
$R_2 = \Delta r_{13}$
$R_3 = \Delta \alpha_{23}$

4. Symmetry coordinates.

a_1: S_1 SYM STR = $(R_1 + R_2)/\sqrt{2}$
S_2 BEND = R_3
b_1: S_3 ANTI STR = $(R_1 - R_2)/\sqrt{2}$

5. Force constants.
Valence force field (VFF). See the output data.

6. Reference.
T. Oka and Y. Morino, J. Mol. Spectrosc., 8,9(1962).

7. Output data.

```
PROGRAM  NCTB      PROBLEM NO.   1

    **H2O**CALCULATION OF FREQUENCY
    REPORTED BY M. NAKATA AND M. TASUMI (THE UNIVERSITY OF TOKYO)

INTRAMOLECULAR PARAMETER

       LENGTH                                   ANGLE

            NO.  1       0.9572000                    NO.  2      104.500000
```

CARTESIAN COORDINATE

		X-	Y-	Z-
ATOM NO.	1	0.0	0.0	0.0
ATOM NO.	2	0.586014	0.756848	0.0
ATOM NO.	3	0.586014	-0.756848	0.0

ATOM DISTANCE CHECK

	ATOM 1	ATOM 2	ATOM 3
ATOM 1	0.0		
ATOM 2	0.957200	0.0	
ATOM 3	0.957200	1.513696	0.0

MASSES OF ATOMS

ATOM 1	15.994909
ATOM 2	1.007825
ATOM 3	1.007825

SYMMETRIZED B MATRIX

ROW 1	-0.865806	0.0	0.0	0.432903	0.559102	0.0
	0.432903	-0.559102	0.0			
ROW 2	1.652089	0.0	0.0	-0.826045	0.639592	0.0
	-0.826045	-0.639592	0.0			
ROW 3	0.0	-1.118204	0.0	0.432903	0.559102	0.0
	-0.432903	0.559102	0.0			

SYMMETRIZED G MATRIX

		S 1	S 2	S 3
S 1	SYM STR	1.039102		
S 2	BEND	-0.089428	2.336547	
S 3	ANTI STR	0.0	0.0	1.070409

FORCE CONSTANTS

1	F(R1R1)	8.4540	2	F(R1R2)	-0.1000
3	F(R1R3)	0.2240	4	F(R3R3)	0.6970

SYMMETRIZED F MATRIX

		S 1	S 2	S 3
S 1	SYM STR	8.35400		
S 2	BEND	0.31678	0.69700	
S 3	ANTI STR	0.0	0.0	8.55400

EIGENVALUES, EIGENVECTORS AND FREQUENCIES

	EIGENVALUE	8.652075	1.600506	9.156281
	FREQUENCY	3832.197	1648.225	3942.279
	ASSIGNMENT	SYM STR	BEND	ANTI STR
	PED	100	102	100
S 1	SYM STR	1.017721	-0.057841	0.0
S 2	BEND	-0.000996	1.528578	0.0
S 3	ANTI STR	0.0	0.0	1.034606

POTENTIAL ENERGY DISTRIBUTION

	FREQUENCY	3832.197	1648.225	3942.279
S 1	SYM STR	100.01	1.75	0.0
S 2	BEND	0.00	101.75	0.0
S 3	ANTI STR	0.0	0.0	100.00

TRANSPOSED LX MATRIX

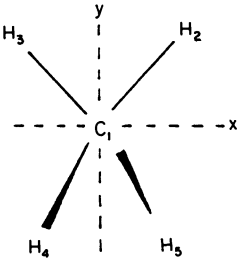
3832.20	1	-0.049349	0.0	0.0
	2	0.391602	0.568718	0.0
	3	0.391602	-0.568718	0.0
1648.22	1	0.067539	0.0	0.0
	2	-0.535950	0.415545	0.0
	3	-0.535950	-0.415545	0.0
3942.28	1	0.0	-0.067572	0.0
	2	0.415174	0.536205	0.0
	3	-0.415174	0.536205	0.0

JACOBIAN MATRIX(FREQUENCY)

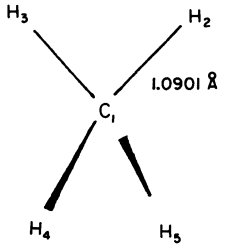
	FREQUENCY	3832.197	1648.225	3942.279
	ASSIGNMENT	SYM STR	BEND	ANTI STR
	PED	100	102	100
1	F(R1R1) 8.4540	229.381	1.723	230.435
2	F(R1R2) -0.1000	229.381	1.723	-230.435
3	F(R1R3) 0.2240	-0.635	-128.765	0.0
4	F(R3R3) 0.6970	0.000	1203.111	0.0

II. CH_4 (Methane)

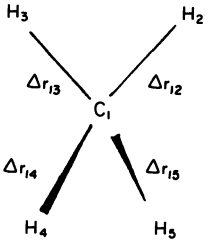
1. Numbering of atoms and the cartesian axes.

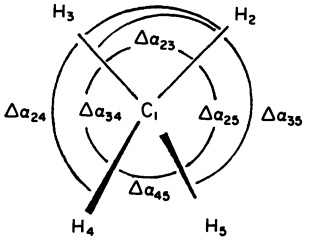


2. Structural parameters.



3. Internal coordinates.





$R_1 = \Delta r_{12}$ $R_3 = \Delta r_{14}$ $R_5 = \Delta\alpha_{23}$ $R_8 = \Delta\alpha_{34}$

$R_2 = \Delta r_{13}$ $R_4 = \Delta r_{15}$ $R_6 = \Delta\alpha_{24}$ $R_9 = \Delta\alpha_{35}$

$R_7 = \Delta\alpha_{25}$ $R_{10} = \Delta\alpha_{45}$

4. Symmetry coordinates.

a_1: S_1 SYM STR = $(R_1 + R_2 + R_3 + R_4)/2$

e : S_2 E BEND A = $(2R_5 - R_6 - R_7 - R_8 - R_9 + 2R_{10})/2\sqrt{3}$

S_3 E BEND B = $(R_6 - R_7 - R_8 + R_9)/2$

f_2: S_4 F STR X = $(R_1 - R_2 + R_3 - R_4)/2$

S_5 F STR Y = $(-R_1 + R_2 + R_3 - R_4)/2$

S_6 F STR Z = $(R_1 + R_2 - R_3 - R_4)/2$

S_7 F BEND X = $(R_6 - R_9)/\sqrt{2}$

S_8 F BEND Y = $(-R_7 + R_8)/\sqrt{2}$

S_9 F BEND Z = $(R_5 - R_{10})/\sqrt{2}$

5. Force constants.
Symmetrized valence force field. See the output data.

6. Reference.
P. Pulay, W. Meyer, and J.E. Boggs, J. Chem. Phys., 68,5077(1978).

7. Output data.

```
PROGRAM  NCTB     PROBLEM NO.   2

    **CH4**CALCULATION OF FREQUENCY
    REPORTED BY M. NAKATA AND M. TASUMI (THE UNIVERSITY OF TOKYO)


INTRAMOLECULAR PARAMETER

       LENGTH                                ANGLE

            NO.  1        1.090100                NO.  2      109.471222


CARTESIAN COORDINATE

                          X-             Y-             Z-

ATOM NO.    1            0.0            0.0            0.0
ATOM NO.    2            0.890063       0.629370       0.0
ATOM NO.    3           -0.890063       0.629370       0.0
ATOM NO.    4           -0.000000      -0.629369       0.890063
ATOM NO.    5           -0.000000      -0.629369      -0.890063
```

ATOM DISTANCE CHECK

	ATOM 1	ATOM 2	ATOM 3	ATOM 4	ATOM 5
ATOM 1	0.0				
ATOM 2	1.090100	0.0			
ATOM 3	1.090100	1.780126	0.0		
ATOM 4	1.090099	1.780125	1.780125	0.0	
ATOM 5	1.090099	1.780125	1.780125	1.780126	0.0

MASSES OF ATOMS

ATOM 1	12.000000
ATOM 2	1.007825
ATOM 3	1.007825
ATOM 4	1.007825
ATOM 5	1.007825

SYMMETRIZED B MATRIX

ROW 1	0.000000	-0.000000	0.0	0.408248	0.288675	0.0
	-0.408248	0.288675	0.0	-0.000000	-0.288675	0.408249
	-0.000000	-0.288675	-0.408249			
ROW 2	-0.000000	-0.000002	0.0	0.458674	-0.648662	0.0
	-0.458674	-0.648662	0.0	0.000000	0.648663	0.458674
	0.000000	0.648663	-0.458674			
ROW 3	0.0	0.0	0.0	0.0	0.0	-0.794447
	0.0	0.0	0.794447	-0.794447	0.0	0.0
	0.794447	0.0	0.0			
ROW 4	-0.816496	0.0	-0.816497	0.408248	0.288675	0.0
	0.408248	-0.288675	0.0	-0.000000	-0.288675	0.408249
	0.000000	0.288675	0.408249			
ROW 5	0.816496	0.0	-0.816497	-0.408248	-0.288675	0.0
	-0.408248	0.288675	0.0	-0.000000	-0.288675	0.408249
	0.000000	0.288675	0.408249			
ROW 6	-0.000000	-1.154700	0.0	0.408248	0.288675	0.0
	-0.408248	0.288675	0.0	0.000000	0.288675	-0.408249
	0.000000	0.288675	0.408249			
ROW 7	1.498022	0.0	1.498023	-0.187253	0.264815	-0.561759
	-0.187253	-0.264815	-0.561759	-0.561759	-0.264816	-0.187253
	-0.561759	0.264816	-0.187253			
ROW 8	-1.498022	0.0	1.498023	0.187253	-0.264815	-0.561759
	0.187253	0.264815	-0.561759	0.561759	-0.264816	-0.187253
	0.561759	0.264816	-0.187253			
ROW 9	0.000000	2.118523	0.0	0.374506	-0.529631	0.0
	-0.374506	-0.529631	0.0	-0.000000	-0.529632	-0.374506
	-0.000000	-0.529632	0.374506			

SYMMETRIZED G MATRIX

		S 1	S 2	S 3	S 4	S 5	S 6
S 1	SYM STR	0.992236					
S 2	E BEND A	0.0	2.504976				
S 3	E BEND B	0.0	0.0	2.504979			
S 4	F STR X	0.0	0.0	0.000000	1.103346		
S 5	F STR Y	0.0	0.0	0.000000	0.000001	1.103346	
S 6	F STR Z	-0.000000	0.000000	0.0	0.0	0.0	1.103346
S 7	F BEND X	0.0	0.0	0.0	-0.203855	-0.000000	0.0
S 8	F BEND Y	0.0	0.0	0.0	-0.000000	-0.203855	0.0
S 9	F BEND Z	0.000000	-0.000003	0.0	0.0	0.0	-0.203855

		S 7	S 8	S 9
S 7	F BEND X	2.043994		
S 8	F BEND Y	0.000001	2.043994	
S 9	F BEND Z	0.0	0.0	2.043997

FORCE CONSTANTS

1	F(1,1)	5.5029	2	F(2,2)	0.5775
3	F(4,4)	5.3845	4	F(7,7)	0.5443
5	F(4,7)	0.2246			

SYMMETRIZED F MATRIX

			S 1	S 2	S 3	S 4	S 5	S 6
S	1	SYM STR	5.50290					
S	2	E BEND A	0.0	0.57750				
S	3	E BEND B	0.0	0.0	0.57750			
S	4	F STR X	0.0	0.0	0.0	5.38450		
S	5	F STR Y	0.0	0.0	0.0	0.0	5.38450	
S	6	F STR Z	0.0	0.0	0.0	0.0	0.0	5.38450
S	7	F BEND X	0.0	0.0	0.0	0.22460	0.0	0.0
S	8	F BEND Y	0.0	0.0	0.0	0.0	0.22460	0.0
S	9	F BEND Z	0.0	0.0	0.0	0.0	0.0	0.22460

			S 7	S 8	S 9
S	7	F BEND X	0.54430		
S	8	F BEND Y	0.0	0.54430	
S	9	F BEND Z	0.0	0.0	0.54430

EIGENVALUES, EIGENVECTORS AND FREQUENCIES

		EIGENVALUE	5.460173	1.446624	1.446624	5.876997	5.876997
		FREQUENCY	3044.325	1566.988	1566.988	3158.388	3158.388
		ASSIGNMENT	SYM STR	E BEND A	E BEND B	F STR X	F STR Y
		PED	100	100	100	101	101
S	1	SYM STR	0.996110	0.0	0.0	0.0	0.0
S	2	E BEND A	0.0	1.582712	0.0	0.0	0.0
S	3	E BEND B	0.0	0.0	1.582712	0.0	0.0
S	4	F STR X	0.0	0.0	0.0	1.049621	0.0
S	5	F STR Y	0.0	0.0	0.0	0.0	1.049621
S	6	F STR Z	0.0	0.0	0.0	0.0	0.0
S	7	F BEND X	0.0	0.0	0.0	-0.139341	0.0
S	8	F BEND Y	0.0	0.0	0.0	0.0	-0.139341
S	9	F BEND Z	0.0	0.0	0.0	0.0	0.0

		EIGENVALUE	5.876985	1.084925	1.084925	1.084925
		FREQUENCY	3158.385	1357.024	1357.024	1357.024
		ASSIGNMENT	F STR Z	F BEND X	F BEND Y	F BEND Z
		PED	101	102	102	102
S	1	SYM STR	0.0	0.0	0.0	0.0
S	2	E BEND A	0.0	0.0	0.0	0.0
S	3	E BEND B	0.0	0.0	0.0	0.0
S	4	F STR X	0.0	-0.040481	0.0	0.0
S	5	F STR Y	0.0	0.0	-0.040481	0.0
S	6	F STR Z	1.049620	0.0	0.0	-0.040481
S	7	F BEND X	0.0	1.422875	0.0	0.0
S	8	F BEND Y	0.0	0.0	1.422875	0.0
S	9	F BEND Z	-0.139341	0.0	0.0	1.422876

POTENTIAL ENERGY DISTRIBUTION

		FREQUENCY	3044.325	1566.988	1566.988	3158.388	3158.388
S	1	SYM STR	100.00	0.0	0.0	0.0	0.0
S	2	E BEND A	0.0	100.00	0.0	0.0	0.0
S	3	E BEND B	0.0	0.0	100.00	0.0	0.0
S	4	F STR X	0.0	0.0	0.0	100.94	0.0
S	5	F STR Y	0.0	0.0	0.0	0.0	100.94
S	6	F STR Z	0.0	0.0	0.0	0.0	0.0
S	7	F BEND X	0.0	0.0	0.0	0.18	0.0
S	8	F BEND Y	0.0	0.0	0.0	0.0	0.18
S	9	F BEND Z	0.0	0.0	0.0	0.0	0.0

	FREQUENCY	3158.385	1357.024	1357.024	1357.024
S 1	SYM STR	0.0	0.0	0.0	0.0
S 2	E BEND A	0.0	0.0	0.0	0.0
S 3	E BEND B	0.0	0.0	0.0	0.0
S 4	F STR X	0.0	0.81	0.0	0.0
S 5	F STR Y	0.0	0.0	0.81	0.0
S 6	F STR Z	100.94	0.0	0.0	0.81
S 7	F BEND X	0.0	101.57	0.0	0.0
S 8	F BEND Y	0.0	0.0	101.57	0.0
S 9	F BEND Z	0.18	0.0	0.0	101.57

TRANSPOSED LX MATRIX

3044.32	1	0.000000	-0.000000	0.0
	2	0.406660	0.287552	0.0
	3	-0.406660	0.287552	0.0
	4	-0.000000	-0.287552	0.406660
	5	-0.000000	-0.287552	-0.406660
1566.99	1	-0.000000	-0.000000	0.0
	2	0.287552	-0.406660	0.0
	3	-0.287552	-0.406660	0.0
	4	0.000000	0.406661	0.287552
	5	0.000000	0.406661	-0.287552
1566.99	1	0.0	0.0	0.0
	2	0.0	0.0	-0.498056
	3	0.0	0.0	0.498056
	4	-0.498056	0.0	0.0
	5	0.498056	0.0	0.0
3158.39	1	-0.061674	0.0	-0.061674
	2	0.382336	0.281076	-0.015166
	3	0.382336	-0.281076	-0.015166
	4	-0.015166	-0.281076	0.382336
	5	-0.015166	0.281076	0.382336
3158.39	1	0.061674	0.0	-0.061674
	2	-0.382336	-0.281076	-0.015166
	3	-0.382336	0.281076	-0.015166
	4	0.015166	-0.281076	0.382336
	5	0.015166	0.281076	0.382336
3158.39	1	-0.000000	-0.087220	0.0
	2	0.397502	0.259629	0.0
	3	-0.397502	0.259629	0.0
	4	0.000000	0.259629	-0.397502
	5	0.000000	0.259629	0.397502
1357.02	1	0.081695	0.0	0.081695
	2	-0.093138	0.212193	-0.393225
	3	-0.093138	-0.212193	-0.393225
	4	-0.393225	-0.212194	-0.093139
	5	-0.393225	0.212194	-0.093139
1357.02	1	-0.081695	0.0	0.081695
	2	0.093138	-0.212193	-0.393225
	3	0.093138	0.212193	-0.393225
	4	0.393225	-0.212194	-0.093139
	5	0.393225	0.212194	-0.093139
1357.02	1	0.000000	0.115534	0.0
	2	0.300087	-0.343911	0.0
	3	-0.300087	-0.343911	0.0
	4	-0.000000	-0.343912	-0.300087
	5	-0.000000	-0.343912	0.300087

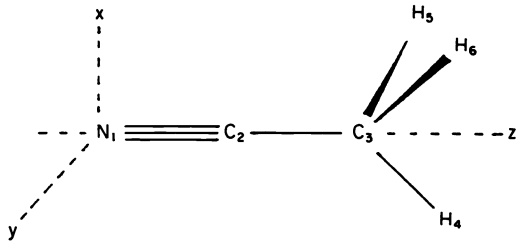
JACOBIAN MATRIX(FREQUENCY)

	FREQUENCY	3044.325	1566.988	1566.988	3158.388	3158.388
	ASSIGNMENT	SYM STR	E BEND A	E BEND B	F STR X	F STR Y
	PED	100	100	100	101	101
1	F(1,1) 5.5029	276.612	0.0	0.0	0.0	0.0
2	F(2,2) 0.5775	0.0	1356.704	1356.704	0.0	0.0
3	F(4,4) 5.3845	0.0	0.0	0.0	296.037	296.037
4	F(7,7) 0.5443	0.0	0.0	0.0	5.217	5.217
5	F(4,7) 0.2246	0.0	0.0	0.0	-78.600	-78.600

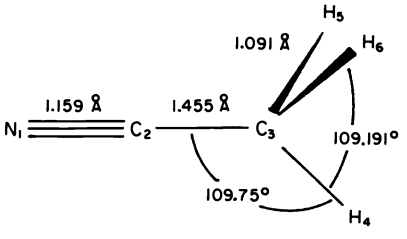
	FREQUENCY	3158.385	1357.024	1357.024	1357.024
	ASSIGNMENT	F STR Z	F BEND X	F BEND Y	F BEND Z
	PED	101	102	102	102
1	F(1,1) 5.5029	0.0	0.0	0.0	0.0
2	F(2,2) 0.5775	0.0	0.0	0.0	0.0
3	F(4,4) 5.3845	296.036	1.025	1.025	1.025
4	F(7,7) 0.5443	5.217	1266.173	1266.173	1266.174
5	F(4,7) 0.2246	-78.600	-72.046	-72.046	-72.046

III. CH_3CN (Methyl cyanide)

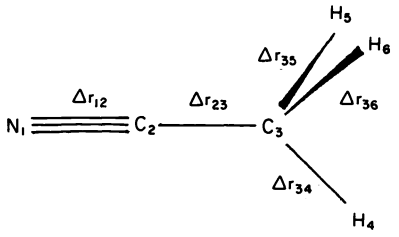
1. Numbering of atoms and the cartesian axes.

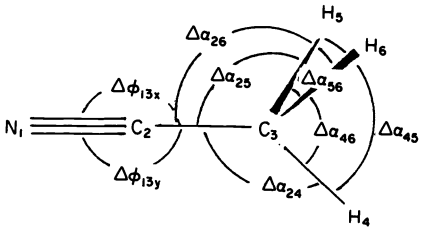


2. Structural parameters.



3. Internal coordinates.





$R_1 = \Delta r_{34}$ $R_4 = \Delta r_{23}$ $R_6 = \Delta\alpha_{56}$ $R_9 = \Delta\alpha_{24}$ $R_{12} = \Delta\phi_{13x}$
$R_2 = \Delta r_{35}$ $R_5 = \Delta r_{12}$ $R_7 = \Delta\alpha_{46}$ $R_{10} = \Delta\alpha_{25}$ $R_{13} = \Delta\phi_{13y}$
$R_3 = \Delta r_{36}$ $R_8 = \Delta\alpha_{45}$ $R_{11} = \Delta\alpha_{26}$

4. Symmetry coordinates.

a_1: S_1 ME S STR = $(R_1 + R_2 + R_3)/\sqrt{3}$
S_2 ME BEND = $-\{K(R_6 + R_7 + R_8) + (R_9 + R_{10} + R_{11})\}/\sqrt{3(1 + K^2)}$
; K = -1.010259452
S_3 CC STR = R_4
S_4 CN STR = R_5

e : S_5 ME STR A = $(2R_1 - R_2 - R_3)/\sqrt{6}$
S_6 ME STR B = $(R_2 - R_3)/\sqrt{2}$
S_7 ME BND A = $(2R_6 - R_7 - R_8)/\sqrt{6}$
S_8 ME BND B = $(R_7 - R_8)/\sqrt{2}$
S_9 ME RCK A = $(2R_9 - R_{10} - R_{11})/\sqrt{6}$
S_{10} ME RCK B = $(R_{10} - R_{11})/\sqrt{2}$
S_{11} CCN A = R_{12}
S_{12} CCN B = R_{13}

5. Force constants.
Symmetrized valence force field. See the output data.

6. Reference.
L. Halonen and I.M. Mills, J. Mol. Spectrosc., 73,494(1978).

7. Output data.

PROGRAM NCTB PROBLEM NO. 3

CH3CN CALCULATION OF FREQUENCY
REPORTED BY M. NAKATA AND M. TASUMI (THE UNIVERSITY OF TOKYO)

INTRAMOLECULAR PARAMETER

LENGTH		ANGLE	
NO. 1	1.091000	NO. 4	180.000000
NO. 2	1.455000	NO. 5	0.0
NO. 3	1.159000	NO. 6	109.750000

CARTESIAN COORDINATE

	X-	Y-	Z-
ATOM NO. 1	0.000000	0.0	0.0
ATOM NO. 2	0.0	0.0	1.159000
ATOM NO. 3	0.0	0.0	2.614000
ATOM NO. 4	-1.026823	0.0	2.982667
ATOM NO. 5	0.513411	-0.889255	2.982667
ATOM NO. 6	0.513411	0.889255	2.982667

ATOM DISTANCE CHECK

	ATOM 1	ATOM 2	ATOM 3	ATOM 4	ATOM 5	ATOM 6
ATOM 1	0.0					
ATOM 2	1.158999	0.0				
ATOM 3	2.613999	1.455000	0.0			
ATOM 4	3.154468	2.092875	1.090999	0.0		
ATOM 5	3.154468	2.092875	1.091000	1.778508	0.0	
ATOM 6	3.154468	2.092875	1.091000	1.778508	1.778509	0.0

MASSES OF ATOMS

ATOM 1	14.003075
ATOM 2	12.000000
ATOM 3	12.000000
ATOM 4	1.007825
ATOM 5	1.007825
ATOM 6	1.007825

SYMMETRIZED B MATRIX

ROW 1	0.0	0.0	0.0	0.0	0.0	0.0
	0.000000	0.0	-0.585290	-0.543388	0.0	0.195097
	0.271694	-0.470588	0.195097	0.271694	0.470588	0.195097
ROW 2	0.0	0.0	0.0	-0.000000	0.0	0.0
	0.000001	0.0	2.123978	-0.254196	0.0	-0.707993
	0.127098	-0.220140	-0.707993	0.127098	0.220140	-0.707993
ROW 3	0.0	0.0	0.0	0.0	0.0	-1.000000
	0.0	0.0	1.000000	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0
ROW 4	0.000000	0.0	-1.000000	-0.000000	0.0	1.000000
	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0
ROW 5	0.0	0.0	0.0	0.0	0.0	0.0
	1.152700	0.0	-0.000000	-0.768467	0.0	0.275908
	-0.192117	0.332756	-0.137954	-0.192117	-0.332756	-0.137954
ROW 6	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	1.152700	0.0	0.0	0.0	0.0
	0.332756	-0.576351	0.238944	-0.332756	-0.576351	-0.238944
ROW 7	0.0	0.0	0.0	0.0	0.0	0.0
	1.486469	0.0	0.000000	0.127745	0.0	0.355799
	-0.807108	-0.539737	-0.177900	-0.807108	0.539737	-0.177900
ROW 8	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	1.486470	0.0	0.0	-1.118725	0.0
	-0.539737	-0.183872	0.308131	0.539737	-0.183872	-0.308131
ROW 9	0.0	0.0	0.0	0.841749	0.0	0.0
	-1.221092	0.0	-0.000000	0.252895	0.0	0.704370
	0.063224	-0.109507	-0.352185	0.063224	0.109507	-0.352185
ROW 10	0.0	0.0	0.0	0.0	0.841750	0.0
	0.0	-1.221092	0.0	0.0	0.0	0.0
	-0.109507	0.189671	0.610002	0.109507	0.189671	-0.610002
ROW 11	0.862813	0.0	-0.000001	-1.550098	0.0	0.000001
	0.687285	0.0	-0.000001	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0
ROW 12	0.0	0.862813	0.0	0.0	-1.550098	0.0
	0.0	0.687285	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0

SYMMETRIZED G MATRIX

		S 1	S 2	S 3	S 4	S 5	S 6
S 1	ME S STR	1.020782					
S 2	ME BEND	-0.103595	2.060365				
S 3	CC STR	-0.048774	0.176998	0.166667			
S 4	CN STR	0.0	0.000000	-0.083333	0.154746		
S 5	ME STR A	0.000000	0.000000	-0.000000	0.0	1.102962	
S 6	ME STR B	-0.000000	0.0	0.0	0.0	0.000000	1.102962
S 7	ME BND A	0.000000	0.000001	0.000000	0.0	0.142788	-0.000000
S 8	ME BND B	-0.000000	0.000000	0.0	0.0	0.000000	0.142788
S 9	ME RCK A	0.0	-0.000001	-0.000000	-0.000000	-0.117296	0.0
S 10	ME RCK B	0.0	0.000000	0.0	0.0	0.0	-0.117296
S 11	CCN A	0.000000	-0.000000	-0.000000	0.000000	0.066019	0.0
S 12	CCN B	0.0	0.0	0.0	0.0	0.0	0.066019

		S 7	S 8	S 9	S 10	S 11	S 12
S 7	ME BND A	2.259574					
S 8	ME BND B	-0.000000	2.259574				
S 9	ME RCK A	0.269825	0.000000	1.016916			
S 10	ME RCK B	0.0	0.269825	0.000000	1.016916		
S 11	CCN A	0.085136	0.0	-0.178669	0.0	0.292760	
S 12	CCN B	0.0	0.085136	0.0	-0.178669	0.0	0.292760

FORCE CONSTANTS

1	F(1,1)	5.3310	2	F(1,2)	-0.0510
3	F(1,3)	0.2130	4	F(1,4)	-0.0720
5	F(2,2)	0.6090	6	F(2,3)	-0.3740
7	F(2,4)	-0.0490	8	F(3,3)	5.1560
9	F(3,4)	0.1680	10	F(4,4)	18.3300
11	F(5,5)	5.3320	12	F(5,7)	-0.1440
13	F(5,9)	0.1000	14	F(5,11)	-0.2570
15	F(7,7)	0.5370	16	F(7,9)	0.0280
17	F(7,11)	0.0030	18	F(9,9)	0.6800
19	F(9,11)	-0.0890	20	F(11,11)	0.3570

SYMMETRIZED F MATRIX

		S 1	S 2	S 3	S 4	S 5	S 6
S 1	ME S STR	5.33100					
S 2	ME BEND	-0.05100	0.60900				
S 3	CC STR	0.21300	-0.37400	5.15600			
S 4	CN STR	-0.07200	-0.04900	0.16800	18.33000		
S 5	ME STR A	0.0	0.0	0.0	0.0	5.33200	
S 6	ME STR B	0.0	0.0	0.0	0.0	0.0	5.33200
S 7	ME BND A	0.0	0.0	0.0	0.0	-0.14400	0.0
S 8	ME BND B	0.0	0.0	0.0	0.0	0.0	-0.14400
S 9	ME RCK A	0.0	0.0	0.0	0.0	0.10000	0.0
S 10	ME RCK B	0.0	0.0	0.0	0.0	0.0	0.10000
S 11	CCN A	0.0	0.0	0.0	0.0	-0.25700	0.0
S 12	CCN B	0.0	0.0	0.0	0.0	0.0	-0.25700

		S 7	S 8	S 9	S 10	S 11	S 12
S 7	ME BND A	0.53700					
S 8	ME BND B	0.0	0.53700				
S 9	ME RCK A	0.02800	0.0	0.68000			
S 10	ME RCK B	0.0	0.02800	0.0	0.68000		
S 11	CCN A	0.00300	0.0	-0.08900	0.0	0.35700	
S 12	CCN B	0.0	0.00300	0.0	-0.08900	0.0	0.35700

EIGENVALUES, EIGENVECTORS AND FREQUENCIES

	EIGENVALUE	5.451035	3.083927	1.189502	0.497265	5.809691
	FREQUENCY	3041.776	2287.914	1420.922	918.716	3140.250
	ASSIGNMENT	ME S STR	CN STR	ME BEND	CC STR	ME STR A
	PED	100	90	104	87	101
	ASSIGNMENT		CC STR		CN STR	
	PED		11		10	
S 1	ME S STR	1.009740	0.011837	0.032599	-0.000383	0.0
S 2	ME BEND	-0.148280	-0.033239	1.426596	-0.045633	0.0
S 3	CC STR	-0.049148	-0.255322	0.122288	0.290011	0.0
S 4	CN STR	-0.004881	0.389919	0.010203	0.050805	0.0
S 5	ME STR A	0.0	0.0	0.0	0.0	1.049490
S 6	ME STR B	0.0	0.0	0.0	0.0	0.0
S 7	ME BND A	0.0	0.0	0.0	0.0	0.094474
S 8	ME BND B	0.0	0.0	0.0	0.0	0.0
S 9	ME RCK A	0.0	0.0	0.0	0.0	-0.103842
S10	ME RCK B	0.0	0.0	0.0	0.0	0.0
S11	CCN A	0.0	0.0	0.0	0.0	0.048418
S12	CCN B	0.0	0.0	0.0	0.0	0.0

	EIGENVALUE	5.809691	1.287027	1.287026	0.664491	0.664490
	FREQUENCY	3140.250	1478.024	1478.024	1062.019	1062.018
	ASSIGNMENT	ME STR B	ME BND B	ME BND A	ME RCK B	ME RCK A
	PED	101	87	87	81	81
	ASSIGNMENT		ME RCK B	ME RCK A	ME BND B	ME BND A
	PED		11	11	14	14
S 1	ME S STR	0.0	0.0	0.0	0.0	0.0
S 2	ME BEND	0.0	0.0	0.0	0.0	0.0
S 3	CC STR	0.0	0.0	0.0	0.0	0.0
S 4	CN STR	0.0	0.0	0.0	0.0	0.0
S 5	ME STR A	0.0	0.0	0.023748	0.0	-0.023950
S 6	ME STR B	1.049490	0.023748	0.0	-0.023950	0.0
S 7	ME BND A	0.0	0.0	1.442422	0.0	-0.411674
S 8	ME BND B	0.094474	1.442422	0.0	-0.411673	0.0
S 9	ME RCK A	0.0	0.0	0.449551	0.0	0.888965
S10	ME RCK B	-0.103843	0.449551	0.0	0.888965	0.0
S11	CCN A	0.0	0.0	-0.008579	0.0	-0.253742
S12	CCN B	0.048418	-0.008579	0.0	-0.253742	0.0

	EIGENVALUE	0.078045	0.078045
	FREQUENCY	363.965	363.965
	ASSIGNMENT	CCN A	CCN B
	PED	103	103
	ASSIGNMENT	ME RCK A	ME RCK B
	PED	12	12
S 1	ME S STR	0.0	0.0
S 2	ME BEND	0.0	0.0
S 3	CC STR	0.0	0.0
S 4	CN STR	0.0	0.0
S 5	ME STR A	0.019630	0.0
S 6	ME STR B	0.0	0.019630
S 7	ME BND A	-0.024241	0.0
S 8	ME BND B	0.0	-0.024241
S 9	ME RCK A	0.117355	0.0
S10	ME RCK B	0.0	0.117355
S11	CCN A	0.475349	0.0
S12	CCN B	0.0	0.475349

POTENTIAL ENERGY DISTRIBUTION

	FREQUENCY	3041.776	2287.914	1420.922	918.716	3140.250
S 1	ME S STR	99.71	0.02	0.48	0.00	0.0
S 2	ME BEND	0.25	0.02	104.20	0.26	0.0
S 3	CC STR	0.23	10.90	6.48	87.21	0.0
S 4	CN STR	0.01	90.37	0.16	9.51	0.0
S 5	ME STR A	0.0	0.0	0.0	0.0	101.09
S 6	ME STR B	0.0	0.0	0.0	0.0	0.0
S 7	ME BND A	0.0	0.0	0.0	0.0	0.08
S 8	ME BND B	0.0	0.0	0.0	0.0	0.0

S 9	ME RCK A	0.0	0.0	0.0	0.0	0.13
S10	ME RCK B	0.0	0.0	0.0	0.0	0.0
S11	CCN A	0.0	0.0	0.0	0.0	0.01
S12	CCN B	0.0	0.0	0.0	0.0	0.0
	FREQUENCY	3140.250	1478.024	1478.024	1062.019	1062.018
S 1	ME S STR	0.0	0.0	0.0	0.0	0.0
S 2	ME BEND	0.0	0.0	0.0	0.0	0.0
S 3	CC STR	0.0	0.0	0.0	0.0	0.0
S 4	CN STR	0.0	0.0	0.0	0.0	0.0
S 5	ME STR A	0.0	0.0	0.23	0.0	0.46
S 6	ME STR B	101.09	0.23	0.0	0.46	0.0
S 7	ME BND A	0.0	0.0	86.81	0.0	13.70
S 8	ME BND B	0.08	86.81	0.0	13.70	0.0
S 9	ME RCK A	0.0	0.0	10.68	0.0	80.87
S10	ME RCK B	0.13	10.68	0.0	80.87	0.0
S11	CCN A	0.0	0.0	0.00	0.0	3.46
S12	CCN B	0.01	0.00	0.0	3.46	0.0

	FREQUENCY	363.965	363.965
S 1	ME S STR	0.0	0.0
S 2	ME BEND	0.0	0.0
S 3	CC STR	0.0	0.0
S 4	CN STR	0.0	0.0
S 5	ME STR A	2.63	0.0
S 6	ME STR B	0.0	2.63
S 7	ME BND A	0.40	0.0
S 8	ME BND B	0.0	0.40
S 9	ME RCK A	12.00	0.0
S10	ME RCK B	0.0	12.00
S11	CCN A	103.36	0.0
S12	CCN B	0.0	103.36

TRANSPOSED LX MATRIX

3041.78	1	-0.000000	0.0	0.002138
	2	0.000000	0.0	-0.002744
	3	0.000000	0.0	-0.051892
	4	-0.526480	0.0	0.206947
	5	0.263240	-0.455945	0.206947
	6	0.263240	0.455945	0.206947
2287.91	1	0.000000	0.0	-0.164529
	2	-0.000000	0.0	0.225391
	3	0.000000	0.0	-0.029932
	4	-0.001455	0.0	-0.013760
	5	0.000727	-0.001260	-0.013760
	6	0.000727	0.001260	-0.013760
1420.92	1	0.000000	0.0	-0.008123
	2	-0.000000	0.0	0.002079
	3	0.000000	0.0	0.124369
	4	-0.231332	0.0	-0.464245
	5	0.115665	-0.200339	-0.464245
	6	0.115665	0.200339	-0.464245
918.72	1	0.000000	0.0	-0.141061
	2	0.000000	0.0	-0.090256
	3	-0.000000	0.0	0.199757
	4	0.007041	0.0	0.218714
	5	-0.003520	0.006098	0.218714
	6	-0.003520	-0.006098	0.218714
3140.25	1	-0.002576	0.0	0.000000
	2	0.005795	0.0	-0.000000
	3	0.086754	0.0	-0.000000
	4	-0.730496	0.0	0.259636
	5	-0.167842	0.324849	-0.129818
	6	-0.167842	-0.324849	-0.129818

3140.25	1	0.0	-0.002576	0.0
	2	0.0	0.005795	0.0
	3	0.0	0.086754	0.0
	4	0.0	0.019710	0.0
	5	0.324849	-0.542945	0.224851
	6	-0.324849	-0.542945	-0.224851
1478.02	1	0.0	-0.002147	0.0
	2	0.0	0.023535	0.0
	3	0.0	0.043292	0.0
	4	0.0	-0.675947	0.0
	5	-0.364302	-0.044957	0.344159
	6	0.364302	-0.044957	-0.344159
1478.02	1	-0.002147	0.0	0.000000
	2	0.023535	0.0	-0.000000
	3	0.043292	0.0	0.000000
	4	0.165372	0.0	0.397401
	5	-0.465618	-0.364302	-0.198701
	6	-0.465618	0.364302	-0.198701
1062.02	1	0.0	-0.015280	0.0
	2	0.0	0.096760	0.0
	3	0.0	-0.131782	0.0
	4	0.0	0.323227	0.0
	5	0.098258	0.153039	0.500055
	6	-0.098258	0.153039	-0.500055
1062.02	1	-0.015280	0.0	0.000000
	2	0.096760	0.0	-0.000000
	3	-0.131782	0.0	-0.000000
	4	0.096310	0.0	0.577415
	5	0.266498	0.098258	-0.288707
	6	0.266498	-0.098258	-0.288707
363.97	1	0.121690	0.0	-0.000000
	2	-0.220263	0.0	0.000000
	3	0.042087	0.0	-0.000000
	4	0.128803	0.0	0.288952
	5	0.150950	0.012787	-0.144476
	6	0.150950	-0.012787	-0.144476
363.97	1	0.0	0.121690	0.0
	2	0.0	-0.220263	0.0
	3	0.0	0.042087	0.0
	4	0.0	0.158333	0.0
	5	0.012787	0.136186	0.250240
	6	-0.012787	0.136186	-0.250240

JACOBIAN MATRIX(FREQUENCY)

	FREQUENCY	3041.776	2287.914	1420.922	918.716	3140.250
	ASSIGNMENT	ME S STR	CN STR	ME BEND	CC STR	ME STR A
	PED	100	90	104	87	101
	ASSIGNMENT		CC STR		CN STR	
	PED		11		10	
1	F(1,1)	5.3310	284.471	0.052	0.635	0.000	0.0
2	F(1,2)	-0.0510	-83.549	-0.292	55.554	0.032	0.0
3	F(1,3)	0.2130	-27.693	-2.242	4.762	-0.205	0.0
4	F(1,4)	-0.0720	-2.750	3.424	0.397	-0.036	0.0
5	F(2,2)	0.6090	6.135	0.410	1215.565	1.924	0.0
6	F(2,3)	-0.3740	4.067	6.296	208.398	-24.451	0.0
7	F(2,4)	-0.0490	0.404	-9.615	17.387	-4.283	0.0
8	F(3,3)	5.1560	0.674	24.182	8.932	77.695	0.0
9	F(3,4)	0.1680	0.134	-73.858	1.490	27.222	0.0
10	F(4,4)	18.3300	0.007	56.397	0.062	2.384	0.0
11	F(5,5)	5.3320	0.0	0.0	0.0	0.0	297.673
12	F(5,7)	-0.1440	0.0	0.0	0.0	0.0	53.592
13	F(5,9)	0.1000	0.0	0.0	0.0	0.0	-58.907
14	F(5,11)	-0.2570	0.0	0.0	0.0	0.0	27.466

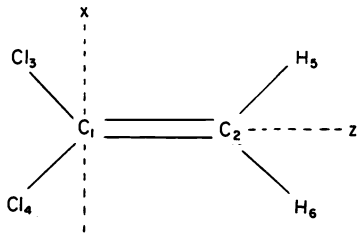
15	F(7,7)	0.5370	0.0	0.0	0.0	0.0	2.412
16	F(7,9)	0.0280	0.0	0.0	0.0	0.0	-5.303
17	F(7,11)	0.0030	0.0	0.0	0.0	0.0	2.472
18	F(9,9)	0.6800	0.0	0.0	0.0	0.0	2.914
19	F(9,11)	-0.0890	0.0	0.0	0.0	0.0	-2.718
20	F(11,11)	0.3570	0.0	0.0	0.0	0.0	0.634

	FREQUENCY	3140.250	1478.024	1478.024	1062.019	1062.018
	ASSIGNMENT	ME STR B	ME BND B	ME BND A	ME RCK B	ME RCK A
	PED	101	87	87	81	81
	ASSIGNMENT		ME RCK B	ME RCK A	ME BND B	ME BND A
	PED		11	11	14	14
1	F(1,1)	5.3310	0.0	0.0	0.0	0.0	0.0
2	F(1,2)	-0.0510	0.0	0.0	0.0	0.0	0.0
3	F(1,3)	0.2130	0.0	0.0	0.0	0.0	0.0
4	F(1,4)	-0.0720	0.0	0.0	0.0	0.0	0.0
5	F(2,2)	0.6090	0.0	0.0	0.0	0.0	0.0
6	F(2,3)	-0.3740	0.0	0.0	0.0	0.0	0.0
7	F(2,4)	-0.0490	0.0	0.0	0.0	0.0	0.0
8	F(3,3)	5.1560	0.0	0.0	0.0	0.0	0.0
9	F(3,4)	0.1680	0.0	0.0	0.0	0.0	0.0
10	F(4,4)	18.3300	0.0	0.0	0.0	0.0	0.0
11	F(5,5)	5.3320	297.673	0.324	0.324	0.458	0.458
12	F(5,7)	-0.1440	53.592	39.338	39.338	15.758	15.758
13	F(5,9)	0.1000	-58.907	12.260	12.260	-34.027	-34.027
14	F(5,11)	-0.2570	27.466	-0.234	-0.234	9.713	9.713
15	F(7,7)	0.5370	2.412	1194.676	1194.676	135.432	135.432
16	F(7,9)	0.0280	-5.303	744.675	744.675	-584.900	-584.901
17	F(7,11)	0.0030	2.472	-14.211	-14.211	166.951	166.952
18	F(9,9)	0.6800	2.914	116.044	116.044	631.515	631.516
19	F(9,11)	-0.0890	-2.718	-4.429	-4.429	-360.514	-360.514
20	F(11,11)	0.3570	0.634	0.042	0.042	51.452	51.452

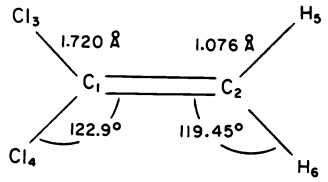
	FREQUENCY	363.965	363.965
	ASSIGNMENT	CCN A	CCN B
	PED	103	103
	ASSIGNMENT	ME RCK A	ME RCK B
	PED	12	12
1	F(1,1)	5.3310	0.0	0.0
2	F(1,2)	-0.0510	0.0	0.0
3	F(1,3)	0.2130	0.0	0.0
4	F(1,4)	-0.0720	0.0	0.0
5	F(2,2)	0.6090	0.0	0.0
6	F(2,3)	-0.3740	0.0	0.0
7	F(2,4)	-0.0490	0.0	0.0
8	F(3,3)	5.1560	0.0	0.0
9	F(3,4)	0.1680	0.0	0.0
10	F(4,4)	18.3300	0.0	0.0
11	F(5,5)	5.3320	0.899	0.899
12	F(5,7)	-0.1440	-2.219	-2.219
13	F(5,9)	0.1000	10.743	10.743
14	F(5,11)	-0.2570	43.516	43.516
15	F(7,7)	0.5370	1.370	1.370
16	F(7,9)	0.0280	-13.267	-13.267
17	F(7,11)	0.0030	-53.738	-53.738
18	F(9,9)	0.6800	32.114	32.114
19	F(9,11)	-0.0890	260.155	260.155
20	F(11,11)	0.3570	526.880	526.880

IV. Cl_2CCH_2 (1,1-Dichloroethylene)

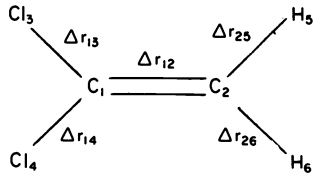
1. Numbering of atoms and the cartesian axes.

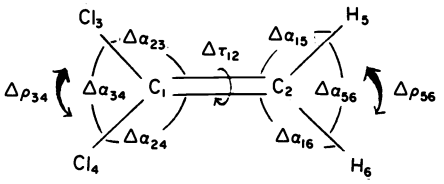


2. Structural parameters.



3. Internal coordinates.





$R_1 = \Delta r_{12}$ $R_4 = \Delta r_{25}$ $R_6 = \Delta\alpha_{23}$ $R_9 = \Delta\alpha_{15}$ $R_{12} = \Delta\rho_{34}$

$R_2 = \Delta r_{13}$ $R_5 = \Delta r_{26}$ $R_7 = \Delta\alpha_{24}$ $R_{10} = \Delta\alpha_{16}$ $R_{13} = \Delta\rho_{56}$

$R_3 = \Delta r_{14}$ $R_8 = \Delta\alpha_{34}$ $R_{11} = \Delta\alpha_{56}$ $R_{14} = \Delta\tau_{12}$

4. Symmetry coordinates.

a_1: S_1 (C=C) $= R_1$

S_2 S(C-CL) $= (R_2 + R_3)/\sqrt{2}$

S_3 S(C-H) $= (R_4 + R_5)/\sqrt{2}$

S_4 S(CLC=C) $= (-R_6 - R_7 + 2R_8)/\sqrt{6}$

S_5 S(HC=C) $= (-R_9 - R_{10} + 2R_{11})/\sqrt{6}$

a_2: S_6 TORSION $= R_{14}$

b_1: S_7 A(C-CL) $= (R_2 - R_3)/\sqrt{2}$

S_8 A(C-H) $= (R_4 - R_5)/\sqrt{2}$

S_9 A(CLC=C) $= (R_6 - R_7)/\sqrt{2}$

S_{10} A(HC=C) $= (R_9 - R_{10})/\sqrt{2}$

b_2: S_{11} OP(CL) $= R_{12}$

S_{12} OP(H) $= R_{13}$

5. Force constants.

Symmetrized valence force field. See the output data.

6. Reference.
Y. Yamaoka and K. Machida, J. Mol. Spectrosc., 83,21(1980).

7. Output data.

```
PROGRAM  NCTB     PROBLEM NO.   4

    **CL2C=CH2**CALCULATION OF FREQUENCY
    REPORTED BY M. NAKATA AND M. TASUMI (THE UNIVERSITY OF TOKYO)


INTRAMOLECULAR PARAMETER

       LENGTH                                   ANGLE

            NO.  1       1.326000                NO.  4     122.900000
            NO.  2       1.720000                NO.  5     119.450000
            NO.  3       1.076000                NO.  6       0.0
                                                 NO.  7     180.000000


CARTESIAN COORDINATE

                        X-            Y-            Z-

ATOM NO.    1            0.0           0.0           0.0
ATOM NO.    2            0.0           0.0           1.326000
ATOM NO.    3            1.444150      0.0          -0.934260
ATOM NO.    4           -1.444146     -0.000000     -0.934260
ATOM NO.    5            0.936965      0.0           1.855030
ATOM NO.    6           -0.936965     -0.000000      1.855030


ATOM DISTANCE CHECK

                    ATOM  1    ATOM  2    ATOM  3    ATOM  4    ATOM  5    ATOM  6
       ATOM  1     0.0
       ATOM  2     1.325999   0.0
       ATOM  3     1.720003   2.682226   0.0
       ATOM  4     1.719999   2.682224   2.888296   0.0
       ATOM  5     2.078230   1.076000   2.835026   3.667399   0.0
       ATOM  6     2.078230   1.076000   3.667402   2.835025   1.873929   0.0


MASSES OF ATOMS

ATOM  1       12.000000
ATOM  2       12.000000
ATOM  3       34.968857
ATOM  4       34.968857
ATOM  5        1.007825
ATOM  6        1.007825


SYMMETRIZED B MATRIX

ROW  1   0.0          0.0         -1.000000    0.0          0.0          1.000000
         0.0          0.0          0.0         0.0          0.0          0.0
         0.0          0.0          0.0         0.0          0.0          0.0
ROW  2  -0.000000     0.000000     0.768164    0.0          0.0          0.0
         0.593701     0.0         -0.384082   -0.593701    -0.000000    -0.384082
         0.0          0.0          0.0         0.0          0.0          0.0
ROW  3   0.0          0.0          0.0         0.0          0.000000    -0.695318
         0.0          0.0          0.0         0.0          0.0          0.0
         0.615738     0.0          0.347659   -0.615738    -0.000000     0.347659
ROW  4   0.000002    -0.000000    -1.195721   -0.000000    -0.000000     0.0
         0.386772     0.000000     0.597860   -0.386773     0.000000     0.597861
         0.0          0.0          0.0         0.0          0.0          0.0
ROW  5   0.0         -0.000000     0.0         0.0         -0.000000     1.982320
         0.0          0.0          0.0         0.0          0.0          0.0
         0.559631     0.000000    -0.991161   -0.559631     0.000000    -0.991161
```

```
ROW  6   0.000000  -0.000002   0.0        -0.000000   0.000001   0.0
         0.0       -0.346224   0.0        -0.000000   0.346226   0.0
         0.0        0.533638   0.0         0.000000  -0.533638   0.0
ROW  7  -1.187403  -0.000000  -0.000001    0.0         0.0        0.0
         0.593701   0.0       -0.384082    0.593701    0.000000   0.384082
         0.0        0.0        0.0         0.0         0.0        0.0
ROW  8   0.0        0.0        0.0        -1.231476   -0.000000   0.0
         0.0        0.0        0.0         0.0         0.0        0.0
         0.615738   0.0        0.347659    0.615738    0.000000  -0.347659
ROW  9   1.513134   0.000000  -0.000000   -1.066527   -0.000000   0.0
        -0.223303   0.0       -0.345175   -0.223304   -0.000000   0.345175
         0.0        0.0        0.0         0.0         0.0        0.0
ROW 10  -1.066527  -0.000000   0.0         1.712733    0.000000   0.0
         0.0        0.0        0.0         0.0         0.0        0.0
        -0.323103   0.0        0.572247   -0.323103   -0.000000  -0.572247
ROW 11   0.000000  -1.664175   0.000000   -0.000000    0.687873  -0.000000
        -0.000000   0.488150   0.0         0.0         0.488152   0.0
         0.0        0.0        0.0         0.0         0.0        0.0
ROW 12   0.000000  -0.645752  -0.000000   -0.000000    2.264311   0.000000
         0.0        0.0        0.0         0.0         0.0        0.0
         0.000000  -0.809279   0.0         0.0        -0.809279   0.0
```

SYMMETRIZED G MATRIX

```
                      S  1        S  2        S  3        S  4        S  5        S  6
S  1  (C=C)          0.166667
S  2  S(C-CL)       -0.064014   0.077770
S  3  S(C-H)        -0.057943   0.0         1.032524
S  4  S(CLC=C)       0.099643  -0.076542   -0.000000   0.148144
S  5  S(HC=C)        0.165193  -0.000000   -0.114862   0.000000   2.898519
S  6  TORSION        0.0       -0.000000   -0.000000   0.000000  -0.000000   0.571972
S  7  A(C-CL)       0.000000  -0.000000    0.0       -0.000000   0.000000  -0.000000
S  8  A(C-H)        0.0        0.0         0.0        0.000000   0.0        0.000000
S  9  A(CLC=C)      0.000000  -0.000000   -0.000000   0.000000   0.000000   0.000000
S 10  A(HC=C)       0.0        0.000000    0.0       -0.000000   0.0       -0.000000
S 11  OP(CL)       -0.000000  -0.000000    0.000000  -0.000000  -0.000000   0.000000
S 12  OP(H)         0.000000  -0.000000    0.000000   0.000000  -0.000000   0.000000

                      S  7        S  8        S  9        S 10        S 11        S 12
S  7  A(C-CL)       0.146090
S  8  A(C-H)        0.0         1.118613
S  9  A(CLC=C)     -0.149725   0.109450    0.295254
S 10  A(HC=C)       0.105533  -0.175766   -0.286706   1.196262
S 11  OP(CL)        0.000000  -0.000000   -0.000000   0.000000   0.283849
S 12  OP(H)         0.000000   0.0         0.0        0.000000   0.219350   1.761703
```

FORCE CONSTANTS

```
    1  F(1,1)      8.4300      2  F(2,2)      4.3500
    3  F(3,3)      5.5800      4  F(4,4)      1.0700
    5  F(5,5)      0.4260      6  F(1,3)      0.1700
    7  F(1,4)     -0.0900      8  F(1,5)     -0.2050
    9  F(2,4)      0.0270     10  F(3,5)      0.0930
   11  F(6,6)      0.4790     12  F(7,7)      3.6900
   13  F(8,8)      5.5500     14  F(9,9)      0.7920
   15  F(10,10)    0.5280     16  F(7,9)      0.6330
   17  F(8,10)     0.1610     18  F(11,11)    0.4880
   19  F(12,12)    0.2430
```

SYMMETRIZED F MATRIX

```
                      S  1        S  2        S  3        S  4        S  5        S  6
S  1  (C=C)          8.43000
S  2  S(C-CL)        0.0        4.35000
S  3  S(C-H)         0.17000    0.0         5.58000
S  4  S(CLC=C)      -0.09000    0.02700     0.0         1.07000
S  5  S(HC=C)       -0.20500    0.0         0.09300     0.0         0.42600
S  6  TORSION        0.0        0.0         0.0         0.0         0.0         0.47900
S  7  A(C-CL)       0.0        0.0         0.0         0.0         0.0         0.0
```

S 8	A(C-H)	0.0	0.0	0.0	0.0	0.0	0.0
S 9	A(CLC=C)	0.0	0.0	0.0	0.0	0.0	0.0
S 10	A(HC=C)	0.0	0.0	0.0	0.0	0.0	0.0
S 11	OP(CL)	0.0	0.0	0.0	0.0	0.0	0.0
S 12	OP(H)	0.0	0.0	0.0	0.0	0.0	0.0

		S 7	S 8	S 9	S 10	S 11	S 12
S 7	A(C-CL)	3.69000					
S 8	A(C-H)	0.0	5.55000				
S 9	A(CLC=C)	0.63300	0.0	0.79200			
S 10	A(HC=C)	0.0	0.16100	0.0	0.52800		
S 11	OP(CL)	0.0	0.0	0.0	0.0	0.48800	
S 12	OP(H)	0.0	0.0	0.0	0.0	0.0	0.24300

EIGENVALUES, EIGENVECTORS AND FREQUENCIES

	EIGENVALUE	5.754456	1.581854	1.153808	0.221493	0.055540
	FREQUENCY	3125.287	1638.593	1399.441	613.151	307.038
	ASSIGNMENT	S(C-H)	(C=C)	S(HC=C)	S(C-CL)	S(CLC=C)
	PED	100	81	86	73	83
	ASSIGNMENT		S(HC=C)		(C=C)	S(C-CL)
	PED		15		14	16
	ASSIGNMENT		S(C-CL)		S(CLC=C)	
	PED		8		11	
S 1	(C=C)	-0.065531	0.389071	-0.084723	-0.061580	-0.005132
S 2	S(C-CL)	0.004280	-0.173716	0.091879	-0.192723	0.044612
S 3	S(C-H)	1.015689	0.016119	-0.024802	-0.003914	-0.000514
S 4	S(CLC=C)	-0.006525	0.253581	-0.131005	0.153956	0.207207
S 5	S(HC=C)	-0.087553	0.749999	1.525048	0.050486	0.006082
S 6	TORSION	0.0	0.0	0.0	0.0	0.0
S 7	A(C-CL)	0.0	0.0	0.0	0.0	0.0
S 8	A(C-H)	0.0	0.0	0.0	0.0	0.0
S 9	A(CLC=C)	0.0	0.0	0.0	0.0	0.0
S10	A(HC=C)	0.0	0.0	0.0	0.0	0.0
S11	OP(CL)	0.0	0.0	0.0	0.0	0.0
S12	OP(H)	0.0	0.0	0.0	0.0	0.0

	EIGENVALUE	0.273974	6.175879	0.724194	0.385175	0.081414
	FREQUENCY	681.935	3237.704	1108.703	808.569	371.739
	ASSIGNMENT	TORSION	A(C-H)	A(HC=C)	A(C-CL)	A(CLC=C)
	PED	100	101	72	88	91
	ASSIGNMENT			A(C-CL)	A(HC=C)	
	PED			28	24	
	ASSIGNMENT			A(CLC=C)	A(CLC=C)	
	PED			16	9	
S 1	(C=C)	0.0	0.0	0.0	0.0	0.0
S 2	S(C-CL)	0.0	0.0	0.0	0.0	0.0
S 3	S(C-H)	0.0	0.0	0.0	0.0	0.0
S 4	S(CLC=C)	0.0	0.0	0.0	0.0	0.0
S 5	S(HC=C)	0.0	0.0	0.0	0.0	0.0
S 6	TORSION	0.756288	0.0	0.0	0.0	0.0
S 7	A(C-CL)	0.0	0.001200	0.233264	-0.302626	0.009717
S 8	A(C-H)	0.0	1.057534	-0.012759	-0.005822	-0.005614
S 9	A(CLC=C)	0.0	0.101609	-0.385442	0.207856	0.305220
S10	A(HC=C)	0.0	-0.151449	0.995024	0.420256	0.081434
S11	OP(CL)	0.0	0.0	0.0	0.0	0.0
S12	OP(H)	0.0	0.0	0.0	0.0	0.0

	EIGENVALUE	0.446613	0.119999
	FREQUENCY	870.669	451.312
	ASSIGNMENT	OP(H)	OP(CL)
	PED	94	94
S 1	(C=C)	0.0	0.0
S 2	S(C-CL)	0.0	0.0
S 3	S(C-H)	0.0	0.0
S 4	S(CLC=C)	0.0	0.0
S 5	S(HC=C)	0.0	0.0
S 6	TORSION	0.0	0.0
S 7	A(C-CL)	0.0	0.0
S 8	A(C-H)	0.0	0.0
S 9	A(CLC=C)	0.0	0.0

S10	A(HC=C)	0.0	0.0
S11	OP(CL)	0.227797	0.481620
S12	OP(H)	1.316701	-0.167332

POTENTIAL ENERGY DISTRIBUTION

	FREQUENCY	3125.287	1638.593	1399.441	613.151	307.038
S 1	(C=C)	0.63	80.67	5.24	14.43	0.40
S 2	S(C-CL)	0.00	8.30	3.18	72.95	15.59
S 3	S(C-H)	100.03	0.09	0.30	0.04	0.00
S 4	S(CLC=C)	0.00	4.35	1.59	11.45	82.71
S 5	S(HC=C)	0.06	15.15	85.87	0.49	0.03
S 6	TORSION	0.0	0.0	0.0	0.0	0.0
S 7	A(C-CL)	0.0	0.0	0.0	0.0	0.0
S 8	A(C-H)	0.0	0.0	0.0	0.0	0.0
S 9	A(CLC=C)	0.0	0.0	0.0	0.0	0.0
S10	A(HC=C)	0.0	0.0	0.0	0.0	0.0
S11	OP(CL)	0.0	0.0	0.0	0.0	0.0
S12	OP(H)	0.0	0.0	0.0	0.0	0.0

	FREQUENCY	681.935	3237.704	1108.703	808.569	371.739
S 1	(C=C)	0.0	0.0	0.0	0.0	0.0
S 2	S(C-CL)	0.0	0.0	0.0	0.0	0.0
S 3	S(C-H)	0.0	0.0	0.0	0.0	0.0
S 4	S(CLC=C)	0.0	0.0	0.0	0.0	0.0
S 5	S(HC=C)	0.0	0.0	0.0	0.0	0.0
S 6	TORSION	100.00	0.0	0.0	0.0	0.0
S 7	A(C-CL)	0.0	0.00	27.72	87.74	0.43
S 8	A(C-H)	0.0	100.50	0.12	0.05	0.21
S 9	A(CLC=C)	0.0	0.13	16.25	8.88	90.63
S10	A(HC=C)	0.0	0.20	72.18	24.21	4.30
S11	OP(CL)	0.0	0.0	0.0	0.0	0.0
S12	OP(H)	0.0	0.0	0.0	0.0	0.0

	FREQUENCY	870.669	451.312
S 1	(C=C)	0.0	0.0
S 2	S(C-CL)	0.0	0.0
S 3	S(C-H)	0.0	0.0
S 4	S(CLC=C)	0.0	0.0
S 5	S(HC=C)	0.0	0.0
S 6	TORSION	0.0	0.0
S 7	A(C-CL)	0.0	0.0
S 8	A(C-H)	0.0	0.0
S 9	A(CLC=C)	0.0	0.0
S10	A(HC=C)	0.0	0.0
S11	OP(CL)	5.67	94.33
S12	OP(H)	94.33	5.67

TRANSPOSED LX MATRIX

3125.29	1	-0.000000	-0.000000	0.005453
	2	0.000000	0.000000	-0.060078
	3	0.000053	-0.000000	-0.000038
	4	-0.000053	-0.000000	-0.000038
	5	0.606495	0.000000	0.326529
	6	-0.606495	-0.000000	0.326529
1638.59	1	0.000000	-0.000000	-0.208522
	2	-0.000000	-0.000000	0.180549
	3	-0.006418	0.000000	0.007703
	4	0.006418	0.000000	0.007703
	5	0.171908	0.000000	-0.100733
	6	-0.171908	-0.000000	-0.100733
1399.44	1	-0.000000	0.000000	0.106828
	2	0.000000	-0.000000	0.022105
	3	0.004582	-0.000000	-0.005698
	4	-0.004582	-0.000000	-0.005698
	5	0.314103	0.000000	-0.569874
	6	-0.314103	0.000000	-0.569874

613.15	1	0.000000	-0.000000	-0.110681
	2	-0.000000	-0.000000	-0.172261
	3	-0.055700	0.000000	0.054108
	4	0.055700	0.000000	0.054108
	5	0.008493	0.000000	-0.192934
	6	-0.008493	0.000000	-0.192934
307.04	1	0.000000	0.000000	-0.075748
	2	-0.000000	-0.000000	-0.080882
	3	0.105517	0.000000	0.029278
	4	-0.105517	-0.000000	0.029278
	5	0.000996	0.000000	-0.083387
	6	-0.000996	0.000000	-0.083387
681.93	1	0.000000	-0.000000	0.0
	2	-0.000000	0.000000	0.0
	3	0.0	-0.013091	0.0
	4	-0.000000	0.013092	0.0
	5	0.0	0.700122	0.0
	6	0.000000	-0.700122	0.0
3237.70	1	-0.000742	-0.000000	-0.000000
	2	-0.096206	-0.000000	0.0
	3	0.000105	0.0	-0.000252
	4	0.000105	0.000000	0.000252
	5	0.573530	0.0	0.334776
	6	0.573530	0.000000	-0.334776
1108.70	1	-0.175939	-0.000000	-0.000000
	2	0.109815	0.000000	0.0
	3	0.015849	0.0	-0.007206
	4	0.015849	0.000000	0.007206
	5	-0.156258	0.0	0.452886
	6	-0.156258	-0.000000	-0.452886
808.57	1	0.193268	0.000000	0.000000
	2	0.078675	0.000000	0.0
	3	-0.042976	0.0	0.028782
	4	-0.042976	-0.000000	-0.028782
	5	-0.127840	0.0	0.357383
	6	-0.127840	-0.000000	-0.357383
371.74	1	0.059575	0.000000	-0.000000
	2	-0.174063	-0.000000	0.0
	3	0.028325	0.0	-0.060957
	4	0.028325	0.000000	0.060957
	5	-0.301199	0.0	0.217093
	6	-0.301199	-0.000000	-0.217093
870.67	1	0.000000	-0.073071	-0.000000
	2	-0.000000	0.149449	0.000000
	3	-0.000000	0.003475	0.0
	4	0.0	0.003475	0.0
	5	0.000000	-0.575275	0.0
	6	0.0	-0.575275	0.0
451.31	1	0.000000	-0.253386	0.000000
	2	-0.000000	0.048334	-0.000000
	3	-0.000000	0.027341	0.0
	4	0.0	0.027341	0.0
	5	-0.000000	0.272094	0.0
	6	0.0	0.272094	0.0

JACOBIAN MATRIX(FREQUENCY)

	FREQUENCY	3125.287	1638.593	1399.441	613.151	307.038
	ASSIGNMENT	S(C-H)	(C=C)	S(HC=C)	S(C-CL)	S(CLC=C)
	PED	100	81	86	73	83
	ASSIGNMENT		S(HC=C)		(C=C)	S(C-CL)
	PED		15		14	16
1 F(1,1)	8.4300	1.166	78.403	4.353	5.249	0.073

2	F(2,2)	4.3500	0.005	15.630	5.120	51.410	5.501
3	F(3,3)	5.5800	280.142	0.135	0.373	0.021	0.001
4	F(4,4)	1.0700	0.012	33.305	10.408	32.807	118.676
5	F(5,5)	0.4260	2.082	291.338	1410.455	3.528	0.102
6	F(1,3)	0.1700	-36.149	6.496	2.549	0.667	0.015
7	F(1,4)	-0.0900	0.232	102.200	13.462	-26.245	-5.878
8	F(1,5)	-0.2050	3.116	302.271	-156.715	-8.606	-0.173
9	F(2,4)	0.0270	-0.015	-45.631	-14.599	-82.137	51.102
10	F(3,5)	0.0930	-48.297	12.523	-45.877	-0.547	-0.017
11	F(6,6)	0.4790	0.0	0.0	0.0	0.0	0.0
12	F(7,7)	3.6900	0.0	0.0	0.0	0.0	0.0
13	F(8,8)	5.5500	0.0	0.0	0.0	0.0	0.0
14	F(9,9)	0.7920	0.0	0.0	0.0	0.0	0.0
15	F(10,10)	0.5280	0.0	0.0	0.0	0.0	0.0
16	F(7,9)	0.6330	0.0	0.0	0.0	0.0	0.0
17	F(8,10)	0.1610	0.0	0.0	0.0	0.0	0.0
18	F(11,11)	0.4880	0.0	0.0	0.0	0.0	0.0
19	F(12,12)	0.2430	0.0	0.0	0.0	0.0	0.0

	FREQUENCY		681.935	3237.704	1108.703	808.569	371.739
	ASSIGNMENT		TORSION	A(C-H)	A(HC=C)	A(C-CL)	A(CLC=C)
		PED	100	101	72	88	91
	ASSIGNMENT				A(C-CL)	A(HC=C)	
		PED			28	24	
1	F(1,1)	8.4300	0.0	0.0	0.0	0.0	0.0
2	F(2,2)	4.3500	0.0	0.0	0.0	0.0	0.0
3	F(3,3)	5.5800	0.0	0.0	0.0	0.0	0.0
4	F(4,4)	1.0700	0.0	0.0	0.0	0.0	0.0
5	F(5,5)	0.4260	0.0	0.0	0.0	0.0	0.0
6	F(1,3)	0.1700	0.0	0.0	0.0	0.0	0.0
7	F(1,4)	-0.0900	0.0	0.0	0.0	0.0	0.0
8	F(1,5)	-0.2050	0.0	0.0	0.0	0.0	0.0
9	F(2,4)	0.0270	0.0	0.0	0.0	0.0	0.0
10	F(3,5)	0.0930	0.0	0.0	0.0	0.0	0.0
11	F(6,6)	0.4790	711.834	0.0	0.0	0.0	0.0
12	F(7,7)	3.6900	0.0	0.000	41.651	96.126	0.216
13	F(8,8)	5.5500	0.0	293.156	0.125	0.036	0.072
14	F(9,9)	0.7920	0.0	2.706	113.723	45.348	212.684
15	F(10,10)	0.5280	0.0	6.012	757.877	185.378	15.140
16	F(7,9)	0.6330	0.0	0.064	-137.647	-132.047	13.542
17	F(8,10)	0.1610	0.0	-83.966	-19.436	-5.136	-2.088
18	F(11,11)	0.4880	0.0	0.0	0.0	0.0	0.0
19	F(12,12)	0.2430	0.0	0.0	0.0	0.0	0.0

	FREQUENCY		870.669	451.312
	ASSIGNMENT		OP(H)	OP(CL)
		PED	94	94
1	F(1,1)	8.4300	0.0	0.0
2	F(2,2)	4.3500	0.0	0.0
3	F(3,3)	5.5800	0.0	0.0
4	F(4,4)	1.0700	0.0	0.0
5	F(5,5)	0.4260	0.0	0.0
6	F(1,3)	0.1700	0.0	0.0
7	F(1,4)	-0.0900	0.0	0.0
8	F(1,5)	-0.2050	0.0	0.0
9	F(2,4)	0.0270	0.0	0.0
10	F(3,5)	0.0930	0.0	0.0
11	F(6,6)	0.4790	0.0	0.0
12	F(7,7)	3.6900	0.0	0.0
13	F(8,8)	5.5500	0.0	0.0
14	F(9,9)	0.7920	0.0	0.0
15	F(10,10)	0.5280	0.0	0.0
16	F(7,9)	0.6330	0.0	0.0
17	F(8,10)	0.1610	0.0	0.0
18	F(11,11)	0.4880	50.581	436.193
19	F(12,12)	0.2430	1689.927	52.653