

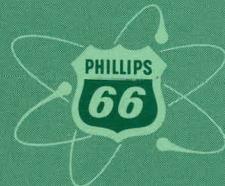
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PROPANE VIBRATIONAL ANALYSIS

G. D. Marshall



PHILLIPS
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ATOMIC ENERGY DIVISION

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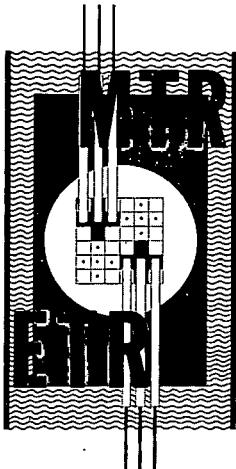
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PROPANE VIBRATIONAL ANALYSIS

By

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PHILLIPS
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Atomic Energy Division

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PROPANE VIBRATIONAL ANALYSIS*

by

G. D. Marshall

A B S T R A C T

Using the group vibration method of McMurry, the normal frequencies and coordinates of propane and three of its symmetrical deuterium substituted compounds have been obtained. The force constants used were taken from a variety of previous work on hydrocarbons. The results give reasonable agreements with the experimental frequency and mode assignments of McMurry and Thornton.

*Work performed under the auspices of the U. S. Atomic Energy Commission.

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PROPANE VIBRATIONAL ANALYSIS

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INTRODUCTION

This work analyzes the normal vibrations of $\text{CH}_2\text{CH}_2\text{CH}_3$, $\text{CH}_3\text{CD}_2\text{CH}_3$, $\text{CD}_3\text{CH}_2\text{CD}_3$, and $\text{CD}_3\text{CD}_2\text{CD}_3$ by the group vibration method of McMurry [1]. His method divides the symmetry coordinates into two parts called skeletal coordinates and intragroup coordinates. The skeletal coordinates consist of combinations of individual group rotations and translations while the intragroup coordinates are combinations of individual atom translations within the groups. The combinations are selected so that linear and angular momentum are conserved for each symmetry coordinate. The secular determinant used to determine the normal frequencies and coordinates is equation 31 from McMurry's work

$$|\lambda^2 E - BD'FDB'| = 0$$

where E is the identity matrix,

λ^2 is a frequency parameter,

B is the symmetry coordinate matrix,

D is the relation between valence coordinates and the σ , Ω , Q coordinates which are in-group translations, group rotations and group translations respectively,

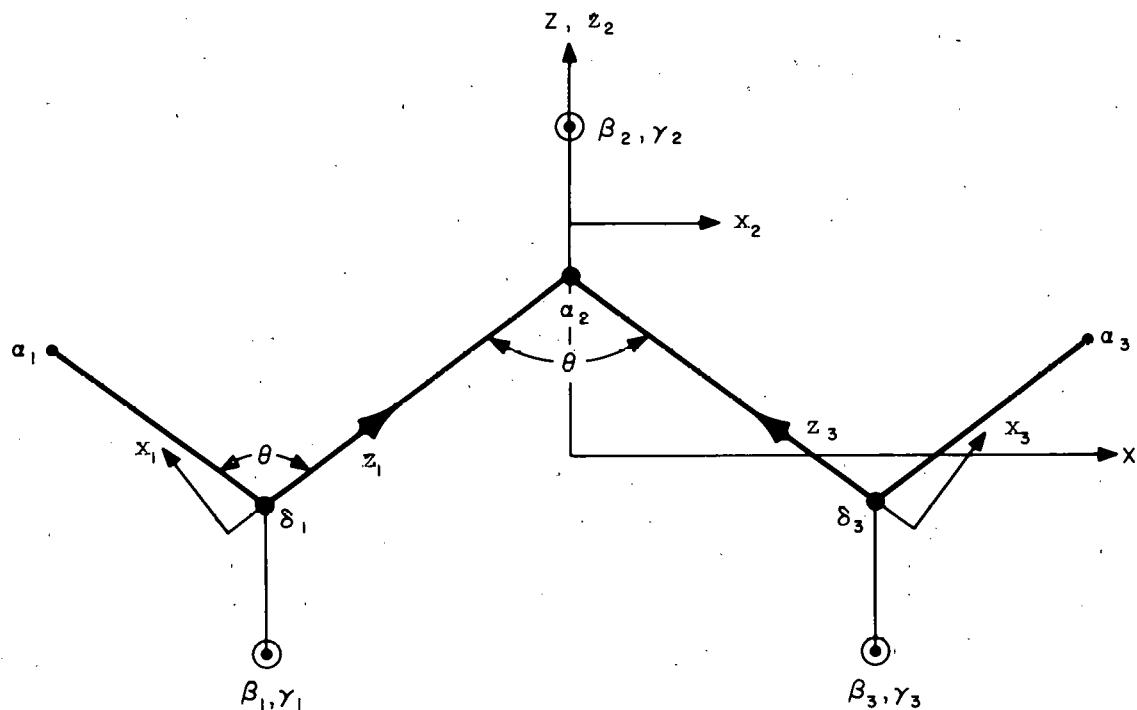
F is the symmetrical force constant matrix with respect to valence coordinates,

and ' (prime) denotes a transposed matrix.

SYMMETRY COORDINATES, B

The symmetry of propane is that of the point group C_{2v} [2]. It has 27 normal vibrations (all non-degenerate) distributed like $9A_1 + 5A_2 + 7B_1 + 6B_2$. The first three coordinates in each representation were made up of group translations, group rotations, or combinations of both, with the remaining being made up of intragroup coordinates.

The diagram below shows a propane molecule and the particular atom numbering and coordinate conventions that are used.



PROPANE MOLECULE

Greek letters with subscripts indicate a particular atom in group number 1, 2, or 3. The δ_1 , α_2 , and δ_3 are the carbon atoms and the convention was made that atoms β_1 , β_2 , and β_3 have positive components along their respective y group axes. The circles β and γ atoms denote that one atom is above and one is below the plane of the paper. The capital X , Y , and Z represent the molecular center of mass coordinates while the x_i , y_i and z_i refer to the i th group's center of mass coordinates. We have assumed that all C - H distances are 1.09 Å and the C - C distances are 1.54 Å while the angles labeled θ are the angles whose cosine is $-1/3$. From a microwave experiment [2] the C - C - C angle is actually 3° larger than the C - C - C angle used here, and the distances vary slightly from the numbers used here.

Since there are eleven atoms in propane the dimensions of each symmetry coordinate are 1×51 (33 σ , 9 Ω , and 9 Q components). Pages 22-27 in the appendix give the numerical values of the B matrix for $\text{CH}_3\text{CH}_2\text{CH}_3$, $\text{CH}_3\text{CD}_2\text{CH}_3$, $\text{CD}_3\text{CH}_2\text{CD}_3$, and $\text{CD}_3\text{CD}_2\text{CD}_3$. The B matrix satisfies the relation $\text{BB}' = \text{E}$. The significance of this matrix is amplified in the appendix where it is presented for the molecules considered here.

VALENCE TRANSFORMATION MATRIX D

The potential function is most easily expressed in terms of changes in bond distance and interbond angles. These are related in the σ, Ω, Q coordinates by the D matrix. This transformation is discussed in the appendix.

Part of the D matrix used here was obtained directly from McMurry's work on ethane [1]. The remainder of the D matrix was constructed in the same fashion as for ethane. Pages 28-31 of the appendix give the numerical values of the D' matrix in terms of $\frac{1}{m}$, the reciprocal mass of the hydrogen atom for $\text{CH}_3\text{CH}_2\text{CH}_3$ and $\text{CD}_3\text{CD}_2\text{CD}_3$. The D' matrices for the other two propanes are combinations of these two.

FORCE CONSTANT MATRIX, F

Sixteen valence interaction force constants, f_i 's, were used. The subscripts on the f 's in the following table have the interaction meaning:*

| | |
|----------------|--|
| r | C-H distance squared |
| φ | H-C-H angle squared |
| χ | C-H-H angle squared |
| R | C-C distance squared |
| r_x | C-H distance times C-H-H angle |
| rR | C-H distance times C-C distance |
| XR | C-H-H angle times C-C distance |
| RR | C-C distance times another C-C distance |
| $R\theta_c$ | C-C distance times C-C-C angle |
| θ_c | C-C-C angle squared |
| χ' | a trans C-H-H angle times C-H-H angle |
| $\chi\theta_c$ | a trans C-H-H angle times C-C-C angle |
| ψ | torsional angle squared of a CH_3 or CD_3 group about a C-C axis |
| $\chi\chi_2$ | HCC_1 angle times an HCC_3 angle |

The additional subscript 2 denotes values used for group number 2. The actual F matrix used is shown on page 28 of the appendix.

*Distances and angles actually refer to changes in the distances and angles from their equilibrium values.

TABLE I

F Matrix Values

| <u>Constant</u> | <u>Value</u> ($\times 10^5$ <u>dynes</u> <u>cm</u>) |
|-----------------|--|
| f_r | 4.86 |
| f_ϕ | .46 |
| $f_{\phi 2}$ | .46 |
| f_{r2} | 4.86 |
| f_x | .58 |
| f_{x2} | .58 |
| f_{rR} | .34 |
| f_{xR} | .31 |
| f_R | 4.40 |
| f_{RR} | .22 |
| $f_{R\theta_c}$ | .17 |
| f_{θ_c} | .84 |
| f_x' | .08 |
| f_ψ | .16 |
| $f_{x\theta_c}$ | .08 |
| f_{xx_2} | .1 |

All of the angle constants have been evaluated in terms of $r_o = 1.09\text{A}$ or r_o^2 as a multiplying factor. These constants were mainly taken from Simanouti [3] and Stitt [4]. The f_ψ constant was calculated using a potential barrier for rotation of a methyl group about the C-C axis of 3 kcal/mole. There is some experimental evidence that it should be greater than 3 [5]. The values of the trans angle interaction constants, f_x'

and $f_{X\theta_c}$, were taken from work of J. R. Scherer [6]. He has made a somewhat similar calculation on propane using a modified Urey-Bradley potential instead of a valence potential. The need for the inclusion of this trans interaction is also evident from work on ethane [1,4]. The value of the constant that was used in ethane is $.11 \times 10^5$ dynes/cm. A few adjustments were made before arriving at the set of f values quoted above but no least square fitting to the experimental data was done.

RESULTS

Since the secular determinant was symmetric the Jacobi method was used to solve for the eigenvalues and eigenvectors. The majority of the work was done on an IBM 650 computer. Pages 33-39 of the appendix show the eigenvectors and corresponding eigenvalues, while Table II shows the eigenvalues and their comparison to the experimental data of McMurry and Thornton [7]. This table also shows the results of some decoupling calculations to test the validity of assuming zero coupling between intragroup and skeletal motions. This calculation was made by first putting the intragroup symmetry coordinates equal to zero and then the skeletal coordinates equal to zero.

For work on slow neutron scattering the normal coordinates of $\text{CH}_3\text{CH}_2\text{CH}_3$ were needed referred not to the symmetry coordinates but to the molecular center of mass axes. The transformation matrix, γ , from the σ , Ω , Q coordinates to the molecular axes is listed in the appendix on page 40 and the resulting molecular normal coordinates for $\text{CH}_3\text{CH}_2\text{CH}_3$ in terms of the molecular axes on pages 41-44.

TABLE II
Propane Frequencies

| Symmetry | Description ^(a) | CH ₃ CH ₂ CH ₃ | | | | CH ₃ CD ₂ CH ₃ | | | | CD ₃ CH ₂ CD ₃ | | | | CD ₃ CD ₂ CD ₃ | | | |
|----------------|---|---|------|---------------------------|------|---|------|---------------------------|------|---|------|---------------------------|------|---|---|---------------------------|--|
| | | Experimental ^(b) | | Calculated ^(c) | | Experimental ^(b) | | Calculated ^(c) | | Experimental ^(b) | | Calculated ^(c) | | Experimental ^(b) | | Calculated ^(c) | |
| | | | I | II | | I | II | | I | II | | I | II | | I | II | |
| A ₁ | ν_1 CH ₂ (CD ₂) s.st. | 2940 | 2930 | 2929 | 2154 | 2122 | 2120 | 2905 | 2925 | 2924 | 2120 | 2127 | 2126 | | | | |
| | ν_2 CH ₃ (CD ₃) u.st. | 2940 | 3023 | 3022 | 2920 | 3023 | 3023 | 2210 | 2259 | 2257 | 2230 | 2260 | 2257 | | | | |
| | ν_3 CH ₃ (CD ₃) s.st. | 2940 | 2882 | 2880 | 2920 | 2888 | 2886 | 2090 | 2065 | 2065 | 2120 | 2059 | 2058 | | | | |
| | ν_4 CH ₂ (CD ₂) s.def. | 1460 | 1489 | 1477 | 1062 | 1069 | 1072 | 1463 | 1485 | 1471 | 1070 | 1081 | 1070 | | | | |
| | ν_5 CH ₃ (CD ₃) u.def. | 1460 | 1472 | 1455 | 1460 | 1474 | 1460 | 1070 | 1059 | 1057 | 1070 | 1056 | 1055 | | | | |
| | ν_6 CH ₃ (CD ₃) s.def. | 1380 | 1411 | 1411 | 1380 | 1413 | 1413 | 1070 | 1135 | 1088 | 1070 | 1135 | 1094 | | | | |
| | ν_7 CH ₃ (CD ₃) r., C ₃ s.st. | 1155 | 1181 | 1206 | 1130 | 1170 | 1181 | 940 | 1014 | 1082 | 958 | 992 | 1045 | | | | |
| | ν_8 CH ₃ (CD ₃) r., C ₃ s.st. | 870 | 879 | 904 | 850 | 877 | 892 | 720 | 734 | 752 | 720 | 734 | 749 | | | | |
| | ν_9 C ₃ s.def. | 372 ^(d) | 367 | 371 | --- | 363 | 367 | --- | 312 | 317 | --- | 310 | 314 | | | | |
| A ₂ | ν_{10} CH ₃ (CD ₃) u.st. | --- | 3021 | 3021 | --- | 3021 | 3021 | --- | 2254 | 2252 | --- | 2254 | 2252 | | | | |
| | ν_{11} CH ₃ (CD ₃) u.def. | --- | 1472 | 1458 | --- | 1472 | 1459 | --- | 1055 | 1054 | --- | 1058 | 1054 | | | | |
| | ν_{12} CH ₃ (CD ₃) r. | --- | 928 | 942 | --- | 1058 | 1075 | --- | 727 | 735 | --- | 670 | 676 | | | | |
| | ν_{13} CH ₂ t. | --- | 1195 | 1202 | --- | 751 | 755 | --- | 1147 | 1148 | --- | 888 | 891 | | | | |
| | ν_{14} CH ₃ t. | --- | 312 | 312 | --- | 312 | 312 | --- | 218 | 218 | --- | 218 | 218 | | | | |

TABLE II (Cont)

Propane Frequencies

| Symmetry | Description(a) | Frequency (cm^{-1}) | | | | | | | | | | | | | |
|----------------|--|-------------------------------------|------|---------------|--|-------------------------------------|------|---------------|--|-------------------------------------|------|---------------|------|-------------------------------------|------|
| | | $\text{CH}_3\text{CH}_2\text{CH}_3$ | | | | $\text{CH}_3\text{CD}_2\text{CH}_3$ | | | | $\text{CD}_3\text{CH}_2\text{CD}_3$ | | | | $\text{CD}_3\text{CD}_2\text{CD}_3$ | |
| | | Experimental(b) | | Calculated(c) | | Experimental(b) | | Calculated(c) | | Experimental(b) | | Calculated(c) | | Experimental(b) | |
| B ₁ | $\nu_{15} \text{CH}_3(\text{CD}_3)$ u.st. | 2940 | 3020 | 3020 | | 2920 | 3020 | 3020 | | 2210 | 2252 | 2250 | 2230 | 2251 | 2250 |
| | $\nu_{16} \text{CH}_3(\text{CD}_3)$ s.st. | 2940 | 2888 | 2885 | | 2920 | 2888 | 2885 | | 2050 | 2065 | 2064 | 2120 | 2065 | 2064 |
| | $\nu_{17} \text{CH}_3(\text{CD}_3)$ u.def. | 1460 | 1484 | 1459 | | 1460 | 1477 | 1459 | | 1140 | 1058 | 1053 | 1070 | 1060 | 1053 |
| | $\nu_{18} \text{CH}_3(\text{CD}_3)$ s.def. | 1380 | 1380 | 1410 | | 1380 | 1416 | 1416 | | 1070 | 1062 | 1083 | 1070 | 1049 | 1083 |
| | $\nu_{19} \text{CH}_2(\text{CD}_2)$ r., C ₃ u.st. | 1336 | 1445 | 1429 | | 1199 | 1312 | 1328 | | 1327 | 1418 | 1402 | 1200 | 1309 | 1286 |
| | $\nu_{20} \text{CH}_2(\text{CD}_2)$ r., C ₃ u.st. | 1053 | 973 | 992 | | 964 | 971 | 987 | | 940 | 905 | 910 | 860 | 769 | 774 |
| | $\nu_{21} \text{CH}_3(\text{CD}_3)$ r. | 923 | 927 | 937 | | 850 | 741 | 746 | | --- | 743 | 752 | --- | 703 | 708 |
| B ₂ | $\nu_{22} \text{CH}_2(\text{CD}_2)$ u.st. | 2940 | 3029 | 3026 | | 2160 | 2260 | 2254 | | 2905 | 3023 | 3022 | 2120 | 2273 | 2266 |
| | $\nu_{23} \text{CH}_3(\text{CD}_3)$ u.st. | 2940 | 3016 | 3016 | | 2920 | 3022 | 3021 | | 2210 | 2256 | 2253 | 2230 | 2241 | 2241 |
| | $\nu_{24} \text{CH}_3(\text{CD}_3)$ u.def. | 1478 | 1476 | 1459 | | 1460 | 1474 | 1459 | | 1070 | 1059 | 1055 | 1070 | 1059 | 1055 |
| | $\nu_{25} \text{CH}_2(\text{CD}_2)$ r. | 748 | 795 | 802 | | 720 | 662 | 666 | | --- | 668 | 675 | --- | 577 | 582 |
| | $\nu_{26} \text{CH}_3(\text{CD}_3)$ r. | 1188(e) | 1204 | 1224 | | --- | 1141 | 1171 | | --- | 1092 | 1101 | --- | 985 | 1001 |
| | $\nu_{27} \text{CH}_3(\text{CD}_3)$ t. | --- | 277 | 277 | | --- | 286 | 286 | | --- | 181 | 181 | --- | 189 | 189 |

(a) The abbreviations u.st., s.st., u.def., s.def., denote vibrations which are unsymmetrical stretching, symmetrical stretching, unsymmetrical deformation, and symmetrical deformation, respectively, within the groups indicated. The letters r and t denote rocking and twisting motions of the indicated groups. The descriptions are only qualitative.

(b) E. L. McMurry and V. Thornton, J. Chem. Phys., 19, 1617 (1951).

(c) Columns I and II show the calculated frequencies resulting from the skeletal and intragroup motions being coupled and decoupled respectively.

(d) J. R. Nielsen, from unpublished Raman data on propane gas.

(e) M. Randic, and D. M. Simpson, Trans. Faraday Soc. 56, 1 (1960).

CONCLUSION

The frequency results are generally within 5% of the experimental values. In some cases the normal coordinates are rather mixed and include appreciable percentages of both skeletal and intragroup coordinates. In $\text{CH}_3\text{CH}_2\text{CH}_3$ the resultant decoupled frequencies were not greatly changed from those previously calculated with a maximum change of about 30cm^{-1} . In the other propanes the maximum frequency change was about 60cm^{-1} . In particular the low frequencies near 300cm^{-1} and the high frequencies near 2940cm^{-1} remained nearly constant.

The normal coordinate results of $\text{CH}_3\text{CH}_2\text{CH}_3$ have been used to calculate slow neutron scattering cross sections from propane gas.

ACKNOWLEDGMENTS

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APPENDIX

1. The B Matrix

Each of the three groups in propane has its own axes x , y , z and, for example $\Delta x_{\alpha 1}$ means the displacement of atom α of group 1 of Fig. 1 along the x axis for this group. Rotations of a group around its axes are denoted by symbols like $\Delta\theta_{1x}$ (meaning a rotation of group 1 about its x axis). Displacements of the entire group along the axes X , Y , Z for the whole molecule are denoted by symbols like ΔX_1 (meaning a displacement of group 1 along the X axis for the whole molecule).

The B matrix relates the symmetry coordinates to mass adjusted displacements σ, Ω, Q in the following manner

$$[S] = \begin{bmatrix} S_{A_1} \\ S_{A_2} \\ S_{B_1} \\ S_{B_2} \end{bmatrix} = B \begin{bmatrix} \sigma \\ \Omega \\ Q \end{bmatrix} \quad (A-1)$$

In the equation $[S]$ is a column matrix containing the 27 symmetry coordinates which are divided into those belonging to the A_1 , A_2 , B_1 and B_2 irreducible representations of the C_{2v} point group which pertains to this molecule.

$$[\sigma] = \begin{bmatrix} \sigma_{\alpha 1} \\ \sigma_{\beta 1} \\ - \\ - \\ - \\ \sigma_{\gamma 3} \end{bmatrix} ; \quad [\sigma_{\alpha 1}] = \begin{bmatrix} \sigma_{\alpha 1x} \\ \sigma_{\alpha 1y} \\ \sigma_{\alpha 1z} \end{bmatrix} ; \quad \sigma_{\alpha 1x} = \sqrt{m_{\alpha}} \Delta x_{\alpha 1} \quad (A-2)$$

The meanings of $[\sigma_{\beta 1}]$ etc. can be inferred from $[\sigma_{\alpha 1}]$. The $[\Omega]$ matrix is of the form

$$[\Omega] = \begin{bmatrix} \Omega_1 \\ \Omega_2 \\ \Omega_3 \end{bmatrix} ; [\Omega_1] = \begin{bmatrix} \Omega_{1x} \\ \Omega_{1y} \\ \Omega_{1z} \end{bmatrix} ; \Omega_{1x} = \sqrt{L_{1x}} \Delta\theta_{1x} \quad (A-3)$$

Here L_{1x} is the moment of inertia of group 1 about its x axis. The meaning of the other quantities can be inferred from that for $[\Omega_1]$ and Ω_{1x} .

The $[Q]$ matrix is of the form

$$[Q] = \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \end{bmatrix} ; [Q_1] = \begin{bmatrix} Q_{1x} \\ Q_{1y} \\ Q_{1z} \end{bmatrix} ; Q_{1x} = \sqrt{M_1} \Delta x_1 \quad (A-4)$$

Here M_1 is the mass of group 1. The other meanings can be inferred from the definition of $[Q_1]$.

The matrix B in Eq. (A-1) has 27 rows and 51 columns. In the tabulations on pages 22 and 27 eight columns of figures are given of which the first two are used for identifying rows and columns of B_1 and the last six give numerical values for the identified matrix elements. Thus, the first two digits of each number in the first column denote which of the 27 rows in the B matrix is being dealt with. The succeeding numbers, taken 2 at a time, in the first and if necessary, the second, column denote which columns in the B matrix are being dealt with. The numerical values of the matrix elements appear in respective order in the next six columns. For example, the row of the B matrix for propane on page 22 which begins with the number 0901040507 has the following form and significance 09|01|04|05|07| 08|22|00|00|00

40824829|50+ 20412414|50- 35355339|50- 20412414|50- 35355339|50+

40824829|50+ . The number 09 denotes that the ninth symmetry coordinate is involved. The following two digit numbers 01,04,05,07,08,22, ... denote that the matrix elements which come in columns 1, 4, 5, 7, 8 and 22 of the ninth row of the B matrix are being presented. These occur in columns 3 to 8 on page 22 in the respective order (so that the number in column three is for the matrix element in column 1 of the B matrix, etc). They are in floating point arithmetic with 50 in the last place denoting the tenth base. Thus 4082482950+ in column 3 of the tabulation on page 22 means that the matrix element for the ninth row and first column of B has the value 0.40825 and is positive. The 2041241450- in column four means that the matrix element in row nine, column four of B has the value -0.20412.

By counting elements downward from the top of the column matrix in Eq. (A-1) it can be seen that the 1 corresponds to $\sigma_{\alpha lx}$, the 4 to $\sigma_{\beta lx}$, the 5 to $\sigma_{\beta ly}$, and the 6th, 6 to $\sigma_{\beta lz}$.

2. The D Matrix

The potential energy is expressed most easily in terms of changes in bond distances and interbond angles. These changes are related to the coordinates σ , Ω , Q appearing in Eq. (A-1) by the equation

$$[\mathbf{H}] = \mathbf{D} \begin{bmatrix} \sigma \\ \Omega \\ Q \end{bmatrix} \quad (A-5)$$

In Eq. (A-5) $[\mathbf{H}]$ is a column matrix which, in McMurry's notation(1), may be written for propane in the form

$$[\mathbf{H}] = \begin{bmatrix} \Sigma \\ \mathbf{x} \\ \tau \end{bmatrix} ; \quad [\Sigma] = \begin{bmatrix} \Sigma_1 \\ \Sigma_2 \\ \Sigma_3 \end{bmatrix} ; \quad [\Sigma_1] = \begin{bmatrix} \Delta r_{\alpha 1} \\ \Delta r_{\beta 1} \\ \Delta r_{\gamma 1} \\ r_o^{\Delta \phi_{\alpha \beta 1}} \\ r_o^{\Delta \phi_{\alpha \gamma 1}} \\ r_o^{\Delta \phi_{\beta \gamma 1}} \end{bmatrix} \quad (A-6)$$

The elements in $[\Sigma_2]$ and $[\Sigma_3]$ can be inferred from the form of $[\Sigma_1]$.

$$[\mathbf{x}] = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} ; \quad [x_1] = \begin{bmatrix} r_o^{\Delta x_{\alpha 1}} \\ r_o^{\Delta x_{\beta 1}} \\ r_o^{\Delta x_{\gamma 1}} \\ r_o^{\theta_{z1}} \end{bmatrix} ; \quad [x_z] = \begin{bmatrix} r_o^x_{\beta 1 \delta 1} \\ r_o^x_{\gamma \delta 1} \\ r_o^x_{\beta 2 \delta 2} \\ r_o^x_{\gamma 2 \delta 2} \\ r_o^{\theta_{z2}} \end{bmatrix} \quad (A-7)$$

The $[x_3]$ can be inferred from $[x_1]$. The $r_o^{\theta_z}$ coordinates are torsional rotations about the symmetry axes of the groups.

$$\text{The } [\tau] = \begin{bmatrix} \Delta R_{\delta 1, \alpha 2} \\ \Delta R_{\delta 2, \alpha 2} \\ r_o^{\Delta \theta_c} \end{bmatrix} \quad (A-8)$$

The D' or D transpose matrix for $\text{CH}_3\text{CH}_2\text{CH}_3$ and $\text{CD}_3\text{CD}_2\text{CD}_3$ is given on pages 28-31 in the same format as for the B matrix.

3. The γ Matrix

The γ matrix relates the displacements of the atoms along the molecular axes X, Y, Z to the σ , Ω , Q coordinates. Thus

$$\begin{bmatrix} \Delta X_{\alpha 1} \\ - \\ - \\ - \\ \Delta Z_{\gamma 3} \end{bmatrix} = \gamma \begin{bmatrix} \sigma \\ \Omega \\ Q \end{bmatrix} \quad (A-9)$$

The γ matrix has 33 rows and 51 columns. It is given on page 40 for propane. The elements are identified in essentially the same manner as for the B matrix.

4. The Normal Coordinate Transformation

The symmetry coordinates in Eq. (A-1) are used in a normal coordinate analysis to obtain true normal coordinates in terms of which both the kinetic and potential energies appear as sums of squared terms.

The orthogonal transformation derived in this way is

$$[Q] = N[S] = \begin{bmatrix} N_{A1} & 0 & 0 & 0 \\ 0 & N_{A2} & 0 & 0 \\ 0 & 0 & N_{B1} & 0 \\ 0 & 0 & 0 & N_{B2} \end{bmatrix} \begin{bmatrix} S_{A1} \\ S_{A2} \\ S_{B1} \\ S_{B2} \end{bmatrix} \quad (A-10)$$

The $[Q]$ is a column matrix with its elements being the $3N-6$ normal coordinates and N is a $3N-6$ by $3N-6$ square matrix. (The elements in $[Q]$ are not to be confused with those in Eq. (A-1) which are mass adjusted cartesian displacements.) For propane the coordinates Q can

be separated into those belonging to different irreducible representations of the point group C_{2v} of the molecule. This is brought out in the form of Eq. (A-10).

The elements in the N matrices for the various propanes are given on pages 33-39. The first column gives the frequency of the normal coordinate and serves to identify which one is involved. The fractions contributed to this normal mode by each of the symmetry coordinates of the same species are given in columns 2 through 7 and, if necessary, are continued on a second line.

5. The Cartesian Displacements in Terms of Normal Coordinates

Slow neutron scattering calculations require the transformation which gives the cartesian displacements of each atom relative to the molecular axes. ⁽⁸⁾ This can be written

$$\begin{bmatrix} \Delta x_{\alpha 1} \\ - \\ - \\ - \\ \Delta z_{\gamma 3} \end{bmatrix} = \gamma \begin{bmatrix} \sigma \\ \Omega \\ Q \end{bmatrix} = T'[\Omega] \quad (A-11)$$

$$T' = \gamma B' N' \quad (A-12)$$

The T' matrix for propane is given on pages 41-44. The first two digits in the first column identify the atom and the coordinate displacement Δx , Δy , or Δz . The order is $\alpha 1$, $\beta 1$, $\gamma 1$, $\delta 1$, $\alpha 2$, $\beta 2$, $\gamma 2$, $\alpha 3$, $\beta 3$, $\gamma 3$, and $\delta 3$. Thus, for example, the numbers 01, 02, 03 refer to $\Delta x_{\alpha 1}$, $\Delta y_{\alpha 1}$, $\Delta z_{\alpha 1}$, respectively and 16, 17, 18 refer to

$\Delta X_{\beta 2}$, $\Delta Y_{\beta 2}$, $\Delta Z_{\beta 2}$, respectively. The coefficients for the normal modes are read across the columns and are in the order appearing in the N matrix. For example, in the case of $\Delta X_{\gamma 1}$ (number 09 in the first column) the coefficient for mode 24 is -0.21823. This mode is shown on page 34 of the N matrix to be the 1204 cm^{-1} frequency belonging to the B_2 species.

B MATRIX -- SYMMETRY COORDINATES FOR CH₃CH₂CH₃

0145485100+ 0000000000+ 3988620250- 8257228250+ 3988620250- * * *
 0243490000+ 0000000000+ 7071067850- 7071067850+ * * * *
 0335410000+ 0000000000+ 7071067850+ 7071067850+ * * * *
 0403060912+ 2427000000+ 3651483750- 3651483750- 3651483750- 3162277750+ 3651483750- 3651483750-
 0430330000+ 0000000000+ 3651483750- 3162277750+ * * * *
 0501040507+ 0822000000+ 4082482950+ 2041241450- 3535533950+ 2041241450- 3535533950- 4082482950+
 0525262829+ 0000000000+ 2041241450- 3535533950+ 2041241450- 3535533950- * *
 0615182100+ 0000000000+ 3779644750- 6546536750+ 6546536750+ * * * *
 0717200000+ 0000000000+ 7071067850- 7071067850+ * * * *
 0801030406+ 0709000000+ 3333333350- 2357022650+ 3333333350- 1178511350- 3333333350- 1178511350-
 0810222425+ 2728000000+ 2886751350+ 3333333350- 2357022650+ 3333333350- 1178511350- 3333333350-
 0830310000+ 0000000000+ 1178511350- 2886751350+ * * * *
 0901040507+ 0822000000+ 4082482950+ 2041241450- 3535533950- 2041241450- 3535533950+ 4082482950+
 0925262829+ 0000000000+ 2041241450- 3535533950- 2041241450- 3535533950+ * *
 1034364042+ 0000000000+ 4767312950+ 5222329750- 4767312950+ 5222329750- * *
 1134363940+ 4200000000+ 2633200450+ 2403772150+ 8635755450- 2633200450+ 2403772150+ *
 1234363940+ 4244000000+ 4261825350+ 3890496450+ 4764865650+ 4261825350+ 3890496450+ 2312771250+
 1250000000+ 0000000000+ 2312771250- * * * * * *
 1302050608+ 0911000000+ 3333333350- 3333333350- 2041241450+ 3333333350- 2041241450- 2886751350+
 1323262729+ 3032000000+ 3333333350- 3333333350- 2041241450+ 3333333350- 2041241450- 2886751350+
 1402040507+ 0823000000+ 4082482950+ 3535533950+ 2041241450- 3535533950- 2041241450- 4082482950+
 1425262829+ 0000000000+ 3535533950+ 2041241450- 3535533950- 2041241450- * *
 1543454649+ 5100000000+ 3654371450+ 2833537150+ 7565267650- 3654371450+ 2833537150- *
 1635384100+ 0000000000+ 2752409450- 9211323750- 2752409450+ * * * *
 1735384143+ 4546000000+ 6289934950- 3758955150+ 6289934950+ 4150644449+ 1682379450- 8592650349-
 1749510000+ 0000000000+ 4150644449+ 1682379450+ * * * *
 1803060912+ 2427000000+ 3651483750- 3651483750- 3651483750- 3162277750+ 3651483750+ 3651483750+
 1830330000+ 0000000000+ 3651483750+ 3162277750- * * * *
 1901040507+ 0822000000+ 4082482950+ 2041241450- 3535533950+ 2041241450- 3535533950- 4082482950-
 1925262829+ 0000000000+ 2041241450+ 3535533950- 2041241450+ 3535533950+ * *
 2001030406+ 0709000000+ 3333333350- 2357022650+ 3333333350- 1178511350- 3333333350- 1178511350-
 2010222425+ 2728000000+ 2886751350+ 3333333350+ 2357022650- 3333333350+ 1178511350+ 3333333350+
 2030310000+ 0000000000+ 1178511350+ 2886751350- * * * *
 2101040507+ 0822000000+ 4082482950+ 2041241450- 3535533950- 2041241450- 3535533950+ 4082482950-

B MATRIX - SYMMETRY COORDINATES FOR CH₃CH₂CH₃

2125262829+ 0000000000+ 2041241450+ 3535533950+ 2041241450+ 3535533950- * *
 2234364042+ 0000000000+ 6201736750+ 3396831150+ 6201736750- 3396831150- * *
 2334363740+ 4200000000+ 1835008350+ 3350251450- 8415290950+ 1835008350- 3350251450+ * *
 2434363740+ 4244000000+ 2142945350+ 3912464950- 4049791850- 2142945350- 3912464950+ 2639732650+
 2447500000+ 0000000000+ 5464765850- 2639732650+ * * * *
 2502050608+ 0911000000+ 3333333350- 3333333350- 2041241450+ 3333333350- 2041241450- 2886751350+
 2523262729+ 3032000000+ 3333333350+ 3333333350+ 2041241450- 3333333350+ 2041241450+ 2886751350-
 2602040507+ 0823000000+ 4082482950+ 3535533950+ 2041241450- 3535533950- 2041241450- 4082482950-
 2625262829+ 0000000000+ 3535533950- 2041241450+ 3535533950+ 2041241450+ * *
 2714171820+ 2100000000+ 3162277750- 5477225650+ 3872983350+ 5477225650+ 3872983350- *

* * B MATRIX*- SYMMETRY COORDINATES FOR CH₃CD₂CH₃ * + *
 0145485100+ 0000000000+ 4170288350- 8075728550+ 4170288350- * * *
 0243490000+ 0000000000+ 7071067850- 7071067850+ * * * *
 0335410000+ 0000000000+ 7071067850+ 7071067850+ * * * *
 0403060912+ 2427000000+ 3651483750- 3651483750- 3651483750- 3162277750+ 3651483750- 3651483750-
 0430330000+ 0000000000+ 3651483750- 3162277750+ * * * *
 0501040507+ 0822000000+ 4082482950+ 2041241450- 3535533950+ 2041241450- 3535533950- 4082482950+
 0525262829+ 0000000000+ 2041241450- 3535533950+ 2041241450- 3535533950- * *
 0615182100+ 0000000000+ 5000000050- 6123724450+ 6123724450+ * * *
 0717200000+ 0000000000+ 7071067850- 7071067850+ * * * *
 0801030406+ 0709000000+ 3333333350- 2357022650+ 3333333350- 1178511350- 3333333350- 1178511350-
 0810222425+ 2728000000+ 2886751350+ 3333333350- 2357022650+ 3333333350- 1178511350- 3333333350-
 0830310000+ 0000000000+ 1178511350- 2886751350+ * * * *
 0901040507+ 0822000000+ 4082482950+ 2041241450- 3535533950- 2041241450- 3535533950+ 4082482950+
 0925262829+ 0000000000+ 2041241450- 3535533950- 2041241450- 3535533950+ * *
 1034364042+ 0000000000+ 4767312950+ 5222329750- 4767312950+ 5222329750- * *
 1134363940+ 4200000000+ 3325133250+ 3035417550+ 7710996050- 3325133250+ 3035417550+ *
 1234363940+ 4244000000+ 3754730250+ 3427584150+ 5936749850+ 3754730250+ 3427584150+ 2555615250+
 1250000000+ 0000000000+ 2555615250- * * * *
 1302050608+ 0911000000+ 3333333350- 3333333350- 2041241450+ 3333333350- 2041241450- 2886751350+
 1323262729+ 3032000000+ 3333333350- 3333333350- 2041241450+ 3333333350- 2041241450- 2886751350+

B MATRIX - SYMMETRY COORDINATES FOR CH3CD2CH3

1402040507+ 0823000000+ 4082482950+ 3535533950+ 2041241450- 3535533950- 2041241450- 4082482950+
 1425262829+ 0000000000+ 3535533950+ 2041241450- 3535533950- 2041241450- * *
 1543454649+ 5100000000+ 3748579350+ 3098538450+ 7259092650- 3748579350+ 3098538450- *
 1635384100+ 0000000000+ 3450327850- 8728715650- 3450327850+ * * *
 1735384143+ 4546000000+ 5945984050- 4700713150+ 5945984050+ 4901381549+ 1704771550- 9491484449-
 1749510000+ 0000000000+ 4901381549+ 1704771550+ * * * *
 1803060912+ 2427000000+ 3651483750- 3651483750- 3651483750- 3162277750+ 3651483750+ 3651483750+
 1830330000+ 0000000000+ 3651483750+ 3162277750- * * * *
 1901040507+ 0822000000+ 4082482950+ 2041241450- 3535533950+ 2041241450- 3535533950- 4082482950-
 1925262829+ 0000000000+ 2041241450+ 3535533950- 2041241450+ 3535533950+ * *
 2001030406+ 0709000000+ 3333333350- 2357022650+ 3333333350- 1178511350- 3333333350- 1178511350-
 2010222425+ 2728000000+ 2886751350+ 3333333350+ 2357022650- 3333333350+ 1178511350+ 3333333350+
 2030310000+ 0000000000+ 1178511350+ 2886751350- * * * *
 2101040507+ 0822000000+ 4082482950+ 2041241450- 3535533950- 2041241450- 3535533950+ 4082482950-
 2125262829+ 0000000000+ 2041241450+ 3535533950+ 2041241450+ 3535533950- * *
 2234364042+ 0000000000+ 6201736750+ 3396831150+ 6201736750- 3396831150- * *
 2334363740+ 4200000000+ 2259235550+ 4124780950- 7467534750+ 2259235550- 4124780950+ *
 2434363740+ 4244000000+ 1892409050+ 3455050450- 4961938350- 1892409050- 3455050450+ 2776986150+
 2447500000+ 0000000000+ 5377610550- 2776986150+ * * * *
 2502053608+ 0911000000+ 3333333350- 3333333350- 2041241450+ 3333333350- 2041241450- 2886751350+
 2523262729+ 3032000000+ 3333333350+ 3333333350+ 2041241450- 3333333350+ 2041241450+ 2886751350-
 2602040507+ 0823000000+ 4082482950+ 3535533950+ 2041241450- 3535533950- 2041241450- 4082482950-
 2625262829+ 0000000000+ 3535533950- 2041241450+ 3535533950+ 2041241450+ * *
 2714171820+ 2100000000+ 4264014350- 5222329750+ 3692744750+ 5222329750+ 3692744750- *

* * B MATRIX*- SYMMETRY COORDINATES FOR CD3CH2CD3 * + *
 0145485100+ 0000000000+ 3741657450- 8485281450+ 3741657450- * * *
 0243490000+ 0000000000+ 7071067850- 7071067850+ * * * *
 0335410000+ 0000000000+ 7071067850+ 7071067850+ * * * *
 0403060912+ 2427000000+ 3333333350- 3333333350- 3333333350- 4082482950+ 3333333350- 3333333350-
 0430330000+ 0000000000+ 3333333350- 4082482950+ * * * *
 0501040507+ 0822000000+ 4082482950+ 2041241450- 3535533950+ 2041241450- 3535533950- 4082482950+

B MATRIX - SYMMETRY COORDINATES FOR CD3CH2CD3

0525262829+ 0000000000+ 2041241450- 3535533950+ 2041241450- 3535533950- * *
 0615182100+ 0000000000+ 3779644750- 6546536750+ 6546536750+ * * * *
 0717200000+ 0000000000+ 7071067850- 7071067850+ * * * * *
 0801030406+ 0709000000+ 3086067050- 2182178950+ 3086067050- 1091089450- 3086067050- 1091089450-
 0810222425+ 2728000000+ 3779644750+ 3086067050- 2182178950+ 3086067050- 1091089450- 3086067050-
 0830310000+ 0000000000+ 1091089450- 3779644750+ * * * * *
 0901040507+ 0822000000+ 4082482950+ 2041241450- 3535533950- 2041241450- 3535533950+ 4082482950+
 0925262829+ 0000000000+ 2041241450- 3535533950- 2041241450- 3535533950+ * *
 1034364042+ 0000000000+ 4803844650+ 5188745250- 4803844650+ 5188745250- * *
 1134363940+ 4200000000+ 1993052250+ 1845207850+ 9232870750- 1993052250+ 1845207850+ *
 1234363940+ 4244000000+ 4443971450+ 4114318050+ 3563103950+ 4443971450+ 4114318050+ 2641145850+
 1250000000+ 0000000000+ 2641145850- * * * * *
 1302050608+ 0911000000+ 3086067050- 3086067050- 1889822450+ 3086067050- 1889822450- 3779644750+
 1323262729+ 3032000000+ 3086067050- 3086067050- 1889822450+ 3086067050- 1889822450- 3779644750+
 1402040507+ 0823000000+ 4082482950+ 3535533950+ 2041241450- 3535533950- 2041241450- 4082482950+
 1425262829+ 0000000000+ 3535533950+ 2041241450- 3535533950- 2041241450- * *
 1543454649+ 5100000000+ 3462898150+ 2678176750+ 7853114850- 3462898150+ 2678176750- *
 1635384100+ 0000000000+ 2050757850- 9570203050- 2050757850+ * * *
 1735384143+ 4546000000+ 6439364750- 2759727750+ 6439364750+ 4357171149+ 2012088550- 9881135349-
 1749510000+ 0000000000+ 4357171149+ 2012088550+ * * * * *
 1803060912+ 2427000000+ 3333333350- 3333333350- 3333333350- 4082482950+ 3333333350+ 3333333350+
 1830330000+ 0000000000+ 3333333350+ 4082482950- * * * * *
 1901040507+ 0822000000+ 4082482950+ 2041241450- 3535533950+ 2041241450- 3535533950- 4082482950-
 1925262829+ 0000000000+ 2041241450+ 3535533950- 2041241450+ 3535533950+ * *
 2001030406+ 0709000000+ 3086067050- 2182178950+ 3086067050- 1091089450- 3086067050- 1091089450-
 2010222425+ 2728000000+ 3779644750+ 3086067050+ 2182178950- 3086067050+ 1091089450+ 3086067050+
 2030310000+ 0000000000+ 1091089450+ 3779644750- * * * * *
 2101040507+ 0822000000+ 4082482950+ 2041241450- 3535533950- 2041241450- 3535533950+ 4082482950-
 2125262829+ 0000000000+ 2041241450+ 3535533950+ 2041241450+ 3535533950- * *
 2234364042+ 0000000000+ 6221710250+ 3360107550+ 6221710250- 3360107550- * *
 2334363740+ 4200000000+ 1392543650+ 2578489650- 9100792750+ 1392543550- 2578489650+ *
 2434363740+ 4244000000+ 2067324250+ 3827941050- 2801770050- 2067324250- 3827941050+ 2757075550+
 2447500000+ 0000000000+ 6252459650- 2757075550+ * * * * *
 2502050608+ 0911000000+ 3086067050- 3086067050- 1889822450+ 3086067050- 1889822450- 3779644750+

B MATRIX - SYMMETRY COORDINATES FOR CD3CH2CD3

2523262729+ 3032000000+ 3086067050+ 3086067050+ 1889822450- 3086067050+ 1889822450+ 3779644750-
 2602040507+ 0823000000+ 4082482950+ 3535533950+ 2041241450- 3535533950- 2041241450- 4082482950-
 2625262829+ 0000000000+ 3535533950- 2041241450+ 3535533950+ 2041241450+ * *
 2714171820+ 21000000C0+ 3162277750- 5477225650+ 3872983350+ 5477225650+ 3872983350- *

B MATRIX - SYMMETRY COORDINATES FOR CD3CD2CD3

0145485100+ 00000000C0+ 3922322750- 8320502950+ 3922322750- * * *
 0243490000+ 0000000000+ 7071067850- 7071067850+ * * *
 0335410000+ 0000000000+ 7071067850+ 7071067850+ * * *
 0403060912+ 2427000000+ 3333333350- 3333333350- 3333333350- 4082482950+ 3333333350- 3333333350-
 0430330000+ 0000000000+ 3333333350- 4082482950+ * * *
 0501040507+ 0822000000+ 4082482950+ 2041241450- 3535533950+ 2041241450- 3535533950- 4082482950+
 0525262829+ 0000000000+ 2041241450- 3535533950+ 2041241450- 3535533950- * *
 0615182100+ 0000000000+ 5000000050- 6123724450+ 6123724450+ * * *
 0717200000+ 0000000000+ 7071067850- 7071067850+ * * *
 0801030406+ 0709000000+ 3086067050- 2182178950+ 3086067050- 1091089450- 3086067050- 1091089450-
 0810222425+ 2728000000+ 3779644750+ 3086067050- 2182178950+ 3086067050- 1091089450- 3086067050-
 0830310000+ 0000000000+ 1091089450- 3779644750+ * * *
 0901040507+ 0822000000+ 4082482950+ 2041241450- 3535533950- 2041241450- 3535533950+ 4082482950+
 0925262829+ 0000000000+ 2041241450- 3535533950- 2041241450- 3535533950+ * *
 1034364042+ 0000000000+ 4803844650+ 5188745250- 4803844650+ 5188745250- * *
 1134363940+ 4200000000+ 2631174050+ 2435993850+ 8618916150- 2631174050+ 2435993850+ *
 1234363940+ 4244000000+ 4106414650+ 3801801250+ 4656236550+ 106414650+ 3801801250+ 2800606750+
 1250000000+ 0000000000+ 2800606750- * * * *
 1302050608+ 0911000000+ 3086067050- 3086067050- 1889822450+ 3086067050- 1889822450- 3779644750+
 1323262729+ 3032000000+ 3086067050- 3086067050- 1889822450+ 3086067050- 1889822450- 3779644750+
 1402040507+ 0823000000+ 4082482950+ 3535533950+ 2041241450- 3535533950- 2041241450- 4082482950+
 1425262829+ 0000000000+ 3535533950+ 2041241450- 3535533950- 2041241450- * *
 1543454649+ 5100000000+ 3568015850+ 2936853150+ 7568904550- 3568015850+ 2936853150- *
 1635384100+ 0000000000+ 2631174050- 9281909650- 2631174050+ * * *
 1735384143+ 4546000000+ 6237421250- 3536285450+ 6237421250+ 5069490749+ 2001668950- 1075401450-
 1749510000+ 0000000000+ 5069490749+ 2001668950+ * * * *

B MATRIX - SYMMETRY COORDINATES FOR CD3CD2CD3

1803050912+ 2427000000+ 3333333350- 3333333350- 3333333350- 4082482950+ 3333333350+ 3333333350+
1830330000+ 0000000000+ 3333333350+ 4082482950- * * * *
1901040507+ 0822000000+ 4082482950+ 2041241450- 3535533950+ 2041241450- 3535533950- 4082482950-
1925262829+ 0000000000+ 2041241450+ 3535533950- 2041241450+ 3535533950+ * *
2001030406+ 0709000000+ 3086067050- 2182178950+ 3086067050- 1091089450- 3086067050- 1091089450-
2010222425+ 2728000000+ 3779644750+ 3086067050+ 2182178950- 3086067050+ 1091089450+ 3086067050+
2030310000+ 0000000000+ 1091089450+ 3779644750- * * * *
2101040507+ 0822000000+ 4082482950+ 2041241450- 3535533950- 2041241450- 3535533950+ 4082482950-
2125262829+ 0000000000+ 2041241450+ 3535533950+ 2041241450+ 3535533950- * *
2234364042+ 0000000000+ 6221710250+ 3360107550+ 6221710250- 3360107550- * *
2334363740+ 4200000000+ 1794758650+ 3323247150- 8453977850+ 1794758650- 3323247150+ *
2434363740+ 4244000000+ 1957392450+ 3624386450- 3680581850- 1957392450- 3624386450+ 2842485250+
2447500000+ 0000000000+ 6029821750- 2842485250+ * * * *
2502050608+ 0911000000+ 3086067050- 3086067050- 1889822450+ 3086067050- 1889822450- 3779644750+
2523262729+ 3032000000+ 3086067050+ 3086067050+ 1889822450- 3086067050+ 1889822450+ 3779644750-
2602040507+ 0823000000+ 4082482950+ 3535533950+ 2041241450- 3535533950- 2041241450- 4082482950-
2625262829+ 0000000000+ 3535533950- 2041241450+ 3535533950+ 2041241450+ * *
2714171820+ 2100000000+ 4264014350- 5222329750+ 3692744750+ 5222329750+ 3692744750- *

D PRIME MATRIX FOR CH₃CH₂CH₃

| | | | | | | | |
|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 0101040516+ | 0000000000+ | 9428090450+ | 1666666750+ | 1666666750+ | 333333350- | * | * |
| 0204050000+ | 0000000000+ | 8660254150- | 8660254150+ | * | * | * | * |
| 0301040516+ | 0000000000+ | 3333333350- | 4714045250+ | 4714045250+ | 9428090450- | * | * |
| 0402040617+ | 0000000000+ | 4714045250- | 8333333350- | 6666666750+ | 1666666750+ | * | * |
| 0502040617+ | 0000000000+ | 8164965850+ | 2886751450- | 5773502750+ | 2886751450- | * | * |
| 0602040617+ | 0000000000+ | 3333333350- | 4714045250+ | 4714045250+ | 9428090450- | * | * |
| 0703050618+ | 0000000000+ | 4714045250- | 8333333350- | 6666666750+ | 1666666750+ | * | * |
| 0803050618+ | 0000000000+ | 8164965850- | 2886751450+ | 5773502750- | 2886751450+ | * | * |
| 0903050618+ | 0000000000+ | 3333333350- | 4714045250+ | 4714045250+ | 9428090450- | * | * |
| 1001020304+ | 0506000000+ | 2721655350- | 1360827650+ | 1360827650+ | 1924500950+ | 1924500950+ | 3849001850- |
| 1016171820+ | 2131000000+ | 3005470550+ | 1502735350- | 1502735350- | 1021610150- | 1021610150- | 2043220150+ |
| 1102030405+ | 1718000000+ | 2357022650- | 2357022650+ | 3333333350+ | 3333333350- | 2602813850+ | 2602813850- |
| 1120210000+ | 0000000000+ | 1769480550+ | 1769480550- | * | * | * | * |
| 1201020304+ | 0506000000+ | 9622504549+ | 9622504549+ | 9622504549+ | 2721655350- | 2721655350- | 2721655350- |
| 1216171829+ | 0000000000+ | 2721655350+ | 2721655350+ | 2721655350+ | 2886751450- | * | * |
| 1316171820+ | 2122000000+ | 1179653750+ | 5898268449- | 5898268449- | 3089826850- | 3089826850- | 3089826850+ |
| 1323252627+ | 2930000000+ | 3089826850+ | 1179653750- | 5898268449+ | 5898268449+ | 2357022650+ | 2357022650- |
| 1407081718+ | 2021000000+ | 2357022650- | 2357022650+ | 1769480550+ | 1769480550- | 2602813950+ | 2602813950- |
| 1422232627+ | 0000000000+ | 2602813950+ | 2602813950- | 1769480550- | 1769480550+ | * | * |
| 1507080916+ | 1718000000+ | 1666666750- | 1666666750- | 4714045250+ | 1668282250- | 8341411249+ | 8341411249+ |
| 1520212223+ | 2526000000+ | 3443701849- | 3443701849- | 3443701849- | 3443701849- | 1668282250- | 8341411249+ |
| 1527293031+ | 0000000000+ | 8341411249+ | 1666666750+ | 1666666750+ | 3336564550- | * | * |
| 1620220000+ | 0000000000+ | 8660254150+ | 8660254150- | * | * | * | * |
| 1707092022+ | 0000000000+ | 8164965850+ | 5773502750+ | 2886751450- | 2886751450- | * | * |
| 1807092022+ | 0000000000+ | 5773502750+ | 8164965850- | 4082482950+ | 4082482950+ | * | * |
| 1921230000+ | 0000000000+ | 8660254150+ | 8660254150- | * | * | * | * |
| 2008092123+ | 0000000000+ | 8164965850- | 5773502750- | 2886751450+ | 2886751450+ | * | * |
| 2108092123+ | 0000000000+ | 5773502750+ | 8164965850- | 4082482950+ | 4082482950+ | * | * |
| 2210131425+ | 0000000000+ | 9428090450+ | 1666666750+ | 1666666750+ | 3333333350- | * | * |
| 2313140000+ | 0000000000+ | 8660254150- | 8660254150+ | * | * | * | * |
| 2410131425+ | 0000000000+ | 3333333350- | 4714045250+ | 4714045250+ | 9428090450- | * | * |
| 2511131526+ | 0000000000+ | 4714045250- | 8333333350- | 6666666750+ | 1666666750+ | * | * |
| 2611131526+ | 0000000000+ | 8164965850+ | 2886751450- | 5773502750+ | 2886751450- | * | * |
| 2711131526+ | 0000000000+ | 3333333350- | 4714045250+ | 4714045250+ | 9428090450- | * | * |
| 2812141527+ | 0000000000+ | 4714045250- | 8333333350- | 6666666750+ | 1666666750+ | * | * |

D PRIME MATRIX FOR CH₃CH₂CH₃

2912141527+ 0000000000+ 8164965850- 2886751450+ 5773502750- 2886751450+ * *
 3012141527+ 0000000000+ 3333333350- 4714045250+ 4714045250+ 9428090450- * *
 3110111213+ 1415000000+ 2721655350- 1360827650+ 1360827650+ 1924500950+ 1924500950+ 3849001850-
 3122232526+ 2731000000+ 1021610150- 1021610150- 3005470550+ 1502735350- 1502735350- 2043220150+
 3211121314+ 2223000000+ 2357022650- 2357022650+ 3333333350+ 3333333350- 1769480550- 1769480550+
 3226270000+ 0000000000+ 2602813850+ 2602813850- * * * * *
 3310111213+ 1415000000+ 9622504549+ 9622504549+ 9622504549+ 2721655350- 2721655350- 2721655350-
 3325262730+ 0000000000+ 2721655350+ 2721655350+ 2721655350+ 2886751350- * *
 3417182021+ 0000000000+ 7169593450- 7169593450+ 3230614649- 3230614649+ * *
 3516171820+ 2131000000+ 8278733450+ 4139366750- 4139366750- 1865196249- 1865196249- 3730392549+
 3619000000+ 0000000000+ 6123724550+ * * * * *
 3717182021+ 222300000+ 3663172749+ 3663172749- 3989161550+ 3989161550- 3989161550+ 3989161550-
 3726270000+ 0000000000+ 3663172749- 3663172749+ * * * * *
 3816171820+ 2122000000+ 4458671849- 2229335949+ 2229335949+ 6837311950+ 6837311950+ 6837311950-
 3823252627+ 2930000000+ 6837311950- 4458671849+ 2229335949- 2229335949- 8908707949- 8908707949+
 3920212223+ 2400000000+ 6123724550- 6123724550+ 6123724550+ 6123724550- 8660254350+ *
 4022232627+ 0000000000+ 3230614649+ 3230614649- 7169593450- 7169593450+ * *
 4122232526+ 2731000000+ 1865196249- 1865196249- 8278733450+ 4139366750- 4139366750- 3730392549+
 4228000000+ 0000000000+ 6123724450+ * * * * *
 4316171820+ 2129000000+ 1055114350- 5275571749+ 5275571649+ 5275571649+ 5275571649+ 2108185150-
 4331000000+ 0000000000+ 1055114350- * * * * *
 4417182021+ 0000000000+ 1582671550- 1582671550+ 1582671550- 1582671550+ * *
 4516171820+ 2129000000+ 1492157050+ 7460784949- 7460784949- 7460784949- 7460784949- 1490712050-
 4531000000+ 0000000000+ 1492157050+ * * * * *
 4616171820+ 2122000000+ 1092147150+ 5460735449- 5460735449- 5460735449- 5460735449- 5460735449+
 4623252627+ 2930000000+ 5460735449+ 1092147150- 5460735449+ 5460735449+ 2182178950+ 2182178950-
 4717182021+ 2223000000+ 1638220750+ 1638220750- 1638220650+ 1638220650- 1638220650+ 1638220650-
 4726270000+ 0000000000+ 1638220750- 1638220750+ * * * * *
 4816171820+ 2122000000+ 1544529250- 7722646449+ 7722646449+ 7722646149+ 7722646149+ 7722646149+
 4823252627+ 2930000000+ 7722646149+ 1544529250- 7722646449+ 7722646449+ 1543033550+ 1543033550+
 4831000000+ 0000000000+ 3089058450- * * * * *
 4922232526+ 2730000000+ 5275571649- 5275571649- 1055114350+ 5275571749- 5275571749- 2108185150+
 4931000000+ 0000000000+ 1055114350+ * * * * *
 5022232627+ 0000000000+ 1582671550- 1582671550+ 1582671550- 1582671550- * *
 5122232526+ 2730000000+ 7460785349- 7460785349- 1492157050+ 7460784949- 7460784949- 1490712050-
 5131000000+ 0000000000+ 1492157050+ * * * * *

D PRIME MATRIX FOR CD3CD2CD3

| | | | | | | | |
|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 0101040516+ | 0000000000+ | 6666666750+ | 1178511350+ | 1178511350+ | 2357022650- | * | * |
| 0204050000+ | 0000000000+ | 6123724450- | 6123724450+ | * | * | * | * |
| 0301040516+ | 0000000000+ | 2357022650- | 3333333350+ | 3333333350+ | 6666666750- | * | * |
| 0402040617+ | 0000000000+ | 3333333350- | 5892556550- | 4714045250+ | 1178511350+ | * | * |
| 0502040617+ | 0000000000+ | 5773502750+ | 2041241450- | 4082482950+ | 2041241450- | * | * |
| 0602040617+ | 0000000000+ | 2357022650- | 3333333350+ | 3333333350+ | 6666666750- | * | * |
| 0703050618+ | 0000000000+ | 3333333350- | 5892556550- | 4714045250+ | 1178511350+ | * | * |
| 0803050618+ | 0000000000+ | 5773502750- | 2041241450+ | 4082482950- | 2041241450+ | * | * |
| 0903050618+ | 0000000000+ | 2357022650- | 3333333350+ | 3333333350+ | 6666666750- | * | * |
| 1001020304+ | 0506000000+ | 2721655350- | 1360827650+ | 1360827650+ | 1924500950+ | 1924500950+ | 3849001850- |
| 1016171820+ | 2131000000+ | 3005470550+ | 1502735350- | 1502735350- | 1021610150- | 1021610150- | 2043220150+ |
| 1102030405+ | 1718000000+ | 2357022650- | 2357022650+ | 3333333350+ | 3333333350- | 2602813850+ | 2602813850- |
| 1120210000+ | 0000000000+ | 1769480550+ | 1769480550- | * | * | * | * |
| 1201020304+ | 0506000000+ | 9622504549+ | 9622504549+ | 9622504549+ | 2721655350- | 2721655350- | 2721655350- |
| 1216171829+ | 0000000000+ | 2721655350+ | 2721655350+ | 2721655350+ | 2886751450- | * | * |
| 1316171820+ | 2122000000+ | 1179653750+ | 5898268449- | 5898268449- | 3089826850- | 3089826850- | 3089826850+ |
| 1323252627+ | 2930000000+ | 3089826850+ | 1179653750- | 5898268449+ | 5898268449+ | 2357022650+ | 2357022650- |
| 1407081718+ | 2021000000+ | 2357022650- | 2357022650+ | 1769480550+ | 1769480550- | 2602813950 | 2602813950- |
| 1422232627+ | 0000000000+ | 2602813950+ | 2602813950- | 1769480550- | 1769480550+ | * | * |
| 1507080916+ | 1718000000+ | 1666666750- | 1666666750- | 4714045250+ | 1668282250- | 8341411249+ | 8341411249+ |
| 1520212223+ | 2526000000+ | 3443701849- | 3443701849- | 3443701849- | 3443701849- | 1668282250- | 8341411249+ |
| 1527293031+ | 0000000000+ | 8341411249+ | 1666666750+ | 1666666750+ | 3336564550- | * | * |
| 1620220000+ | 0000000000+ | 6123724450+ | 6123724450- | * | * | * | * |
| 1707092022+ | 0000000000+ | 5773502750+ | 4082482950+ | 2041241450- | 2041241450- | * | * |
| 1807092022+ | 0000000000+ | 4082482950+ | 5773502750- | 2886751450+ | 2886751450+ | * | * |
| 1921230000+ | 0000000000+ | 6123724450+ | 6123724450- | * | * | * | * |
| 2008092123+ | 0000000000+ | 5773502750- | 4082482950- | 2041241450+ | 2041244250+ | * | * |
| 2108092123+ | 0000000000+ | 4082482950+ | 5773502750- | 2886751450+ | 2886751450+ | * | * |
| 2210131425+ | 0000000000+ | 6666666750+ | 1178511350+ | 1178511350+ | 2357022650- | * | * |
| 2313140000+ | 0000000000+ | 6123724450- | 6123724450+ | * | * | * | * |
| 2410131425+ | 0000000000+ | 2357022650- | 3333333350+ | 3333333350+ | 6666666750- | * | * |
| 2511131526+ | 0000000000+ | 3333333350- | 5892556550- | 4714045250+ | 1178511350+ | * | * |
| 2611131526+ | 0000000000+ | 5773502750+ | 2041241450- | 4082482950+ | 2041241450- | * | * |
| 2711131526+ | 0000000000+ | 2357022650- | 3333333350+ | 3333333350+ | 6666666750- | * | * |
| 2812141527+ | 0000000000+ | 3333333350- | 5892556550- | 4714045250+ | 1178511350+ | * | * |

D PRIME MATRIX FOR CD3CD2CD3

2912141527+ 0000000000+ 5773502750- 2041241450+ 4082482950- 2041241450+ * *
 3012141527+ 0000000000+ 2357022650- 3333333350+ 3333333350+ 6666666750- * *
 3110111213+ 1415000000+ 2721655350- 1360827650+ 1360827650+ 1924500950+ 1924500950+ 3849001850-
 3122232526+ 2731000000+ 1021610150- 1021610150- 3005470550+ 1502735350- 1502735350- 2043220150+
 3211121314+ 2223000000+ 2357022650- 2357022650+ 3333333350+ 3333333350- 1769480550- 1769480550+
 3226270000+ 0000000000+ 2602813850+ 2602813850- * * * *
 3310111213+ 1415000000+ 9622504549+ 9622504549+ 9622504549+ 2721655350- 2721655350- 2721655350-
 3325262730+ 0000000000+ 2721655350+ 2721655350+ 2721655350+ 2886751350- * *
 3417182021+ 0000000000+ 5296034850- 5296034850+ 3861323049- 3861323049+ * *
 3516171820+ 2131000000+ 6115334350+ 3057667150- 3057667150- 2229335949- 2229335949- 4458671849+
 3619000000+ 0000000000+ 4330127050+ * * * *
 3717182021+ 2223000000+ 4620405349+ 4620405349- 3073205450+ 3073205450- 3073205450+ 3073205450-
 3726270000+ 0000000000+ 4620405349- 4620405349+ * * * *
 3816171820+ 2122000000+ 5898268449- 2949134249+ 2949134249+ 5294913450+ 5294913450+ 5294913450-
 3823252627+ 2930000000+ 5294913450- 5898268449+ 2949134249- 2949134249- 1178511350- 1178511350+
 3920212223+ 2400000000+ 4330127050- 4330127050+ 4330127050+ 4330127050- 6123724450+ *
 4022232627+ 0000000000+ 3861323049+ 3861323049- 5296034850- 5296034850+ * *
 4122232526+ 2731000000+ 2229335949- 2229335949- 6115334350+ 3057667150- 3057667150- 4458671849+
 4228000000+ 0000000000+ 4330127050+ * * * *
 4316171820+ 2129000000+ 9631832049- 4815916049+ 4815916049+ 4815916049+ 4815916049+ 1924500950-
 4331000000+ 0000000000+ 9631832049- * * * *
 4417182021+ 0000000000+ 1444774850- 1444774850+ 1444774850- 1444774850+ * *
 4516171820+ 2129000000+ 1362146750+ 6810733749- 6810733749- 6810733749- 6810733749- 1360827650-
 4531000000+ 0000000000+ 1362146750+ * * * *
 4616171820+ 2122000000+ 1021610150+ 5108050349- 5108050349- 5108050349- 5108050349- 5108050349+
 4623252627+ 2930000000+ 5108050349+ 1021610150- 5108050349+ 5108050349+ 2041241450+ 2041241450-
 4717182021+ 2223000000+ 1532415150+ 1532415150- 1532415150+ 1532415150- 1532415150+ 1532415150-
 4726270000+ 0000000000+ 1532415150- 1532415150+ * * * *
 4816171820+ 2122000000+ 1444774850- 7223874049+ 7223874049+ 7223874049+ 7223874049+ 7223874049+
 4823252627+ 2930000000+ 7223874049+ 1444774850- 7223874049+ 7223874049+ 1443375750+ 1443375750+
 4831000000+ 0000000000+ 2889549650- * * * *
 4922232526+ 2730000000+ 4815916049- 4815916049- 9631832049+ 4815916049- 4815916049- 1924500950+
 4931000000+ 0000000000+ 9631832049+ * * * *
 5022232627+ 0000000000+ 1444774850- 1444774850+ 1444774850+ 1444774850- * *
 5122232526+ 2730000000+ 6810733749- 6810733749- 1362146750+ 6810733749- 6810733749- 1360827650-
 5131000000+ 0000000000+ 1362146750+ * * * *

F MATRIX -*FORCE CONSTANTS

| | | | | | | | | |
|-------------|---------------|-------------|-------------|-------------|-------------|-------------|-------------|---|
| 0101162900+ | 0000000000+ | 4860000051+ | 0000000000+ | 3400000050+ | * | + * | + * | + |
| 0202172900+ | 0000000000+ | 4860000051+ | 0000000000+ | 3400000050+ | * | + * | + * | + |
| 0303182900+ | 0000000000C0+ | 4860000051+ | 0000000000+ | 3400000050+ | * | + * | + * | + |
| 0404000000+ | 0000000000C0+ | 4600000050+ | * | + * | + * | + * | + * | + |
| 0505000000+ | 0000000000C0+ | 4600000050+ | * | + * | + * | + * | + * | + |
| 0606000000+ | 00000000000+ | 4600000050+ | * | + * | + * | + * | + * | + |
| 0707202229+ | 3000000000+ | 4860000051+ | 0000000000+ | 0000000000+ | 3400000050+ | 3400000050+ | * | + |
| 0808212329+ | 3000000000C0+ | 4860000051+ | 0000000000+ | 0000000000+ | 3400000050+ | 3400000050+ | * | + |
| 0909000000+ | 00000000000+ | 4600000050+ | * | + * | + * | + * | + * | + |
| 1010253000+ | 00000000000+ | 4860000051+ | 0000000000+ | 3400000050+ | * | + * | + * | + |
| 1111263000+ | 00000000000+ | 4860000051+ | 0000000000+ | 3400000050+ | * | + * | + * | + |
| 1212273000+ | 00000000000+ | 4860000051+ | 0000000000+ | 3400000050+ | * | + * | + * | + |
| 1313000000+ | 00000000000+ | 4600000050+ | * | + * | + * | + * | + * | + |
| 1414000000+ | 00000000000+ | 4600000050+ | * | + * | + * | + * | + * | + |
| 1515000000+ | 00000000000+ | 4600000050+ | * | + * | + * | + * | + * | + |
| 1601162931+ | 00000000000+ | 0000000000+ | 5800000050+ | 3100000050+ | 8000000049+ | * | + * | + |
| 1702172029+ | 00000000000+ | 0000000000+ | 5800000050+ | 8000000049+ | 3100000050+ | * | + * | + |
| 1803182129+ | 00000000000+ | 0000000000+ | 5800000050+ | 8000000049+ | 3100000050+ | * | + * | + |
| 1919000000+ | 00000000000+ | 1600000050+ | * | + * | + * | + * | + * | + |
| 2007172022+ | 29300000000+ | 0000000000+ | 8000000049+ | 5800000050+ | 1000000050+ | 3100000050+ | 3100000050+ | + |
| 2108182123+ | 29300000000+ | 0000000000+ | 8000000049+ | 5800000050+ | 1000000050+ | 3100000050+ | 3100000050+ | + |
| 2207202227+ | 29300000000+ | 0000000000+ | 1000000050+ | 5800000050+ | 8000000049+ | 3100000050+ | 3100000050+ | + |
| 2308212326+ | 29300000000+ | 0000000000+ | 1000000050+ | 5800000050+ | 8000000049+ | 3100000050+ | 3100000050+ | + |
| 2424000000+ | 0000000000+ | 0000000000+ | * | + * | + * | + * | + * | + |
| 2510253031+ | 0000000000+ | 0000000000+ | 5800000050+ | 3100000050+ | 8000000049+ | * | + * | + |
| 2611232630+ | 0000000000+ | 0000000000+ | 8000000049+ | 5800000050+ | 3100000050+ | * | + * | + |
| 2712222730+ | 0000000000+ | 0000000000+ | 8000000049+ | 5800000050+ | 3100000050+ | * | + * | + |
| 2828000000+ | 0000000000+ | 1600000050+ | * | + * | + * | + * | + * | + |
| 2901020307+ | 0816000000+ | 3400000050+ | 3400000050+ | 3400000050+ | 3400000050+ | 3400000050+ | 3100000050+ | + |
| 2917182021+ | 2223000000+ | 3100000050+ | 3100000050+ | 3100000050+ | 3100000050+ | 3100000050+ | 3100000050+ | + |
| 2929303100+ | 0000000000+ | 4400000051+ | 2200000050+ | 1700000050+ | * | + * | + * | + |
| 3007081011+ | 1220000000+ | 3400000050+ | 3400000050+ | 3400000050+ | 3400000050+ | 3400000050+ | 3100000050+ | + |
| 3021222325+ | 2627000000+ | 3100000050+ | 3100000050+ | 3100000050+ | 3100000050+ | 3100000050+ | 3100000050+ | + |
| 3029303100+ | 0000000000+ | 2200000050+ | 4400000051+ | 1700000050+ | * | + * | + * | + |
| 3116252930+ | 3100000000+ | 8000000049+ | 8000000049+ | 1700000050+ | 1700000050+ | 8400000050+ | * | + |

A1 NORMAL FREQUENCIES AND COORDINATES FOR CH3CH2CH3

3793252953+ 0523103311+ 0593046916+ 0592222317+ 0023212152- 0019117343- 0118710877- 0900940101+
3793252953+ 0051684133- 0044294336+ 0065583372+ 0000000000+ 0000000000+ 0000000000+ 0900940102+
3666812253+ 0465596381- 0797795761+ 0381386227- 0016767147- 0001917780+ 0011024332+ 0900940201+
3666812253+ 0018230089+ 0016856826- 0016236188- 0000000000+ 0000000000+ 0000000000+ 0900940202+
1180871654+ 0680889447- 0070689592- 0679912652+ 0008724570- 0026348543+ 0132458750+ 0900940301+
1180871654+ 0092584056+ 0108078586+ 0174765038+ 0000000000+ 0000000000+ 0000000000+ 0900940302+
1411461054+ 0018810125+ 0032410993+ 0011070389+ 0916363592+ 0363698051- 0139667593+ 0900940401+
1411461054+ 0083295659+ 0004113754- 0003535029- 0000000000+ 0000000000+ 0000000000+ 0900940402+
2881667154+ 0030298010+ 0027521691+ 0002609908+ 0341297883+ 0876424703+ 0195864425+ 0900940501+
2881667154+ 0274384740- 0006371871- 0004772681+ 0000000000+ 0000000000+ 0000000000+ 0900940502+
1488982054+ 0150467342+ 0067951209+ 0032667924+ 0143266510- 0065511346+ 0720331769+ 0900940601+
1488982054+ 0569033809+ 0194841083- 0257327739- 0000000000+ 0000000000+ 0000000000+ 0900940602+
2929922254+ 0010461031- 0017101424- 0009530178- 0143668372+ 0306537593+ 0579411411- 0900940701+
2929922254+ 0740266140+ 0028085979+ 0020024665- 0000000000+ 0000000000+ 0000000000+ 0900940702+
3023321754+ 0014628670- 0004763704+ 0018216232+ 0000777601- 0003868520- 0019631026+ 0900940801+
3023321754+ 0029258716- 0789105092- 0612770417- 0000000000+ 0000000000+ 0000000000+ 0900940802+
1472247954+ 0147434090+ 0008933117+ 0199791913- 0041604533- 0016371924+ 0235351018+ 0900940901+
1472247954+ 0183166343+ 0569716249- 0723015173+ 0000000000+ 0000000000+ 0000000000+ 0900940902+

A2 NORMAL FREQUENCIES AND COORDINATES FOR CH3CH2CH3

3118574153+ 0752316399+ 0346280838- 0560454817- 0000000063- 0000000080+ 0000000000+ 0500270101+
9276101553+ 0547150564+ 0786408582+ 0248569786+ 0082795763- 0116386036+ 0000000000+ 0500270201+
1194927654+ 0344820705+ 0509305580- 0777541805+ 0063499670- 0114468451+ 0000000000+ 0500270301+
3021215954+ 0010731690- 0005301658+ 0017681162- 0789172773+ 0613799985+ 0000000000+ 0500270401+
1471811954+ 0125019160- 0047231636- 0138634638- 0605242909- 0772399396+ 0000000000+ 0500270501+

B1 NORMAL FREQUENCIES AND COORDINATES FOR CH3CH2CH3

9268168253+ 0844481570+ 0495337021+ 0170144372- 0108747777+ 0013229055- 0015909217- 0700520101+
9268168253+ 0016994135- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700520102+
1445398954+ 0219107563- 0450631804+ 0264573333- 0637171651- 0234882132+ 0280287517+ 0700520201+

B1 NORMAL FREQUENCIES AND COORDINATES FOR CH₃CH₂CH₃

1445398954+ 0373102330+ 0000000C00+ 0000000000+ 0000000000+ C000000000+ 0000000000+ 0700520202+
9734934753+ 0181914800- 0568837388+ 0784438598+ 0012009082+ C015158264- 0092745313- 0700520301+
9734934753+ 0137880761- 0000000C00+ 0000000000+ 0000000000+ C000000000+ 0000000000+ 0700520302+
1380489554+ 0396282259- 0414408859+ 0359596353- 0641027683+ 0281857093- 0132442841+ 0700520401+
1380489554+ 0184431768+ 0000000C00+ 0000000000+ 0000000000+ C000000000+ 0000000000+ 0700520402+
2887790654+ 0042402912- 0013487150+ 0007345247- 0369172996+ 0928263191+ 0001903743- 0700520501+
2887790654+ 0001114506+ 0000000C00+ 0000000000+ 0000000000+ C000000000+ 0000000C00+ 0700520502+
3020230354+ 0003378296- 0003889088+ 0018205982- 0000240383- 0002096170+ 0789025669+ 0700520601+
3020230354+ 0614065169- 0000000C00+ 0000000000+ 0000000000+ 0000000000+ 0000000C00+ 0700520602+
1484182054+ 0216565666+ 0236779384- 0394984758+ 0186645963+ 0057488347- 0521994114+ 0700520701+
1484182054+ 0656050586+ 0000000C00+ 0000000000+ 0000000000+ 0000000000+ 0700520702+

B2 NORMAL FREQUENCIES AND COORDINATES FOR CH₃CH₂CH'3

2771916253+ 0550531870+ 0542982346- 0634101573- 0000000262+ 0000000174- 0000000C29+ 0600420101+
7946889953+ 0560196444+ 0799290796+ 0198067354- 0055193077- 0070654017+ 0006723708+ 0600420201+
1203669154+ 0589176845+ 0256675744- 0731319689+ 0119972235- 0191725231+ 0031745949- 0600420301+
3016234454+ 0000387044+ 0004444918- 00041423.75+ 0590361612+ 0456671816+ 0665497512+ 0600420401+
1475769354+ 0188350810- 0014375242- 0151218533- 0599725119- 0762684564+ 0009607171+ 0600420501+
3028565754+ 0022114520+ 0013983303- 0031173860+ 0523797014- 0409893323- 0745632443+ 0600420601+

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A1 NORMAL FREQUENCIES AND COORDINATES FOR CH₃CD₂CH₃

8766867753+ 0521524879+ 0601408911+ 0576850444+ 0022283515- 0019550970- 0144714291- 0900920101+
8766867753+ 0076351312- 0043126104+ 0063657221+ 0000000000+ 0000000000+ 0000000C00+ 0900920102+
3633394253+ 0483763373- 0788692905+ 0377564841- 0016776156- 0001986277+ 0007746936+ 0900920201+
3633394253+ 0022319874+ 0016728858- 0016057253- 0000000000+ 0000000000+ 0000000000+ 0900920202+
1169774854+ 0644581858- 0065727359- 0691400782+ 0012689732- 0026675390+ 0170707524+ 0900920301+
1169774854+ 0178416304+ 0105553287+ 0170796730+ 0000000000+ 0000000000+ 0000000C00+ 0900920302+
1413418954+ 0023625413- 001833005+ 0023927703+ 0927463144+ 0369075356- 0008719213+ 0900920401+
1413418954+ 0042977871- 0010541155- 0009723279- 0000000000+ 0000000000+ 0000000C00+ 0900920402+
2887534054+ 0023824404+ 0019502590+ 0001304033- 0370280231+ 0927981591+ 0026075543- 0900920501+

A1 NORMAL FREQUENCIES AND COORDINATES FOR CH3CD2CH3

2887534054+ 0010553098+ 0001239062+ 0000454388- 0000000C00+ 0000000000+ 0000000000+ 0900920502+
1069494154+ 0266359352+ 0100623618+ 0080809826- 0026346348+ 0006248114- 0725736935+ 0900920601+
1069494154+ 0620446458+ 0003644123+ 0001721700- 0000000000+ 0000000000+ 0000000000+ 0900920602+
2121608454+ 0002543455+ 0029494564- 0035375505- 0027956667+ 0037530044- 0649629889- 0900920701+
2121608454+ 0757334717+ 0010283701+ 0001204852+ 0000000000+ 0000000000+ 0000000000+ 0900920702+
3023202554+ 0014331496- 0004153278+ 0017921032+ 0000898983+ 0001214968- 0005039012+ 0900920801+
3023202554+ 0004470543- 0789609712+ 0613127239- 0000000000+ 0000000000+ 0000000000+ 0900920802+
1473736054+ 0078829353+ 0014902190- 0194874889- 0017002837+ 0009313774- 0019032253- 0900920901+
1473736054+ 0036766318- 0602497783+ 0768436201+ 0000000000+ 0000000000+ 0000000000+ 0900920902+

A2 NORMAL FREQUENCIES AND COORDINATES FOR CH3CD2CH3

0005788165+ 0751941584+ 0437055643- 0493524271- 0000000123- 0000000056+ 0000000000+ 0500250101+
7511877353+ 0271438939+ 0886053925+ 0371103603- 0038036657- 0045438537+ 0000000000+ 0500250201+
1058141254+ 0588023297+ 0133696171+ 0777523101+ 0094437566- 0151305275+ 0000000000+ 0500250301+
0542664571+ 0010606125- 0000816514- 0015436697- 0789201440+ 0613848212+ 0000000000+ 0500250401+
0128773619+ 0/557V=597- 00XX-5=794- 0/1-U4=797- 07Y-6T777U- 0773-7-956+ 0000000000+ 0500250701+

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B1 NORMAL FREQUENCIES AND COORDINATES FOR CH3CD2CH3

1312368454+ 0609663510+ 0437028382- 0602467690+ 0133262380- 0094155694+ 0124411734- 0700570101+
1312368454+ 0179573981- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700570102+
7409054053+ 0695257191+ 0686628125+ 0196838470- 0074185516+ 0013056149- 0017824237- 0700570201+
7409054053+ 0020547343- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700570202+
9709547853+ 0362154735- 0568744389+ 0721833218+ 0013194506- 0012056637- 0085840952- 0700570301+
9709547853+ 0129005474- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700570302+
1415813054+ 0040986048+ 0117480416- 0111858185+ 0916364079+ 0359371117- 0032002691- 0700570401+
1415813054+ 0045949130- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700570402+
2887788654+ 0040718612- 0015899496+ 0010732185- 0369194662+ 0928258993+ 0001844888- 0700570501+
2887788654+ 0001067250+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700570502+
3020184554+ 0002906193- 0000109679+ 0017429292- 0000174810- 0002012888+ 0789040627+ 0700570601+
3020184554+ 0614083503- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700570602+
1476712454+ 0102105134+ 0004832073+ 0253599807+ 0023144643+ 0001565062- 0594325367+ 0700570701+
1476712454+ 0755961341+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700570702+

B2 NORMAL FREQUENCIES AND COORDINATES FOR CH3CD2CH3

1141398654+ 0682554268+ 0018922937- 0693644258+ 0115652790- 0182689424+ 0076604379- 0600380101+
6624720753+ 0464145854+ 0759998730+ 0450990701- 0036092781- 0042869330+ 0020915457+ 0600380201+
2858657853+ 0533829408- 0648228696+ 0542978542+ 0000000033+ 0000000026- 0000000053+ 0600380301+
3021714654+ 0014646868- 0002103373+ 0016911176- 0789149575+ 0613671455+ 0012055380- 0600380401+
1474462504+ 0176793962- 0039663483- 0126463128- 0601870269- 0766938086+ 0027127715+ 0600380501+
2260253554+ 0047368813+ 0016302685- 0066033339+ 0017800337+ 0000310170- 0996400046+ 0600380601+

A1 NORMAL FREQUENCIES AND COORDINATES FOR CD3CH2CD3

1013584454+ 0646650512+ 0098686498+ 0417873606- 0552680742+ 0271038902- 0063605441- 0900910101+
1013584454+ 0051284502- 0028019239- 0105388692- 0000000000+ 0000000000+ 0000000000+ 0900910102+
3124837253+ 0430573521- 0756113042+ 0490912084- 0007037168- 0001021622- 0010491357+ 0900910201+
3124837253+ 0015281102+ 0026533230- 0028401460- 0000000000+ 0000000000+ 0000000000+ 0900910202+
7341266653+ 0268198972+ 0624487842+ 0718106522+ 0092214986+ 0061222463- 0066227365- 0900910301+
7341266653+ 0022420141- 0022295430+ 0069062542+ 0000000000+ 0000000000+ 0000000000+ 0900910302+
1135186854+ 0536124349- 0152960920- 0228552529+ 0713734235+ 0303874366- 0159216079+ 0900910401+
1135186854+ 0086486699+ 0004021830- 0048324513+ 0000000000+ 0000000000+ 0000000000+ 0900910402+
2065136154+ 0019808237+ 0016959016+ 0000695317- 0413887105+ 0908930324+ 0015755337- 0900910501+
2065136154+ 0040028938- 0002218689- 0002678675+ 0000000000+ 0000000000+ 0000000000+ 0900910502+
1485037254+ 0177565660+ 0065475749+ 0017135106- 0062656440- 0063410982+ 0768776480+ 0900910601+
1485037254+ 0603328631+ 0000509831- 0030330946- 0000000000+ 0000000000+ 0000000000+ 0900910602+
2924813654+ 0018668356- 0022944431- 0007786691- 0029078220+ 0011724715+ 0612014684- 0900910701+
2924813654+ 0789594342+ 0006602464- 0004073196+ 0000000000+ 0000000000+ 0000000000+ 0900910702+
2259413954+ 0040350868- 0007801624+ 0035053123+ 0006142611+ 0001429971+ 0011836558- 0900910801+
2259413954+ 0000004195- 0824686725+ 0562844668- 0000000000+ 0000000000+ 0000000000+ 0900910802+
1059360954+ 0056487896+ 0003147451+ 0122025636- 0021508850+ 0011585260- 0011867783+ 0900910901+
1059360954+ 0009315320+ 0563773590+ 0814397811+ 0000000000+ 0000000000+ 0000000000+ 0900910902+

A2 NORMAL FREQUENCIES AND COORDINATES FOR CD3CH2CD3

2183723953+ 0754807995+ 0268422519- 0598510005- 0000000127- 0000000084- 0000000000+ 0500290101+
1147447754+ 0166615769- 0786816026+ 0563001536- 0067898220+ 0177704257- 0000000000+ 0500290201+
7266061553+ 0623577428+ 0549973826+ 0539766852+ 0057962132- 0118203636+ 0000000000+ 0500290301+
2254333954+ 0020669090- 0025462722+ 0037486618- 0823278821+ 0565447754+ 0000000000+ 0500290401+
1055388054+ 0115013217- 0075830804+ 0179057310- 0560573095- 0796691859+ 0000000000+ 0500290501+

B1 NORMAL FREQUENCIES AND COORDINATES FOR CD3CH2CD3

9047263053+ 0873078739+ 0451380280+ 0120297449- 0083616165- 0071355141+ 0053028869- 0700550101+
9047263053+ 0067989520- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700550102+
1417598454+ 0468958608- 0748546426+ 0398100296- 0235140976- 0066124267+ 0025871564- 0700550201+
1417598454+ 0030645761+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700550202+
7428284653+ 0104194682- 0426660282+ 0887233393+ 0046907003+ 0026599069- 0054001603- 0700550301+
7428284653+ 0118732486- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700550302+
1062212554+ 0040271206- 0165459404+ 0191665473- 0811548670+ 0372663917- 0216842218- 0700550401+
1062212554+ 0299592303- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700550402+
2065066354+ 0044657644- 0016431985+ 0007511148- 0410638217+ 0910519556+ 0002676055- 0700550501+
2065066354+ 0001576367+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700550502+
2251704054+ 0011795636- 0023027447+ 0038029233- 0002281002- 0003119733+ 0822566188+ 0700550601+
2251704054+ 0566792992- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700550602+
1057983854+ 0056564731+ 0160368264+ 0040289764+ 0329054067+ 0147967924- 0519576339+ 0700550701+
1057983854+ 0754538603+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700550702+

B2 NORMAL FREQUENCIES AND COORDINATES FOR CD3CH2CD3

5675088453+ 0682646395+ 0711030277+ 0120267455+ 0060864106- 0101291895+ 0001039839+ 0600350101+
1813533953+ 0588568247- 0451658244+ 0670516394+ 0000000001- 0000000039+ 0000000052+ 0600350201+
1092025954+ 0417655512+ 0536032570- 0727681395+ 0006426755+ 0088163948+ 0029975787- 0600350301+
2255669854+ 0028309960- 0024130998+ 0041104640- 0823278915+ 0564756007+ 0013752122+ 0600350401+
1059168554+ 0110409981- 0047287130- 0065063615- 0564236472- 0814232696+ 0001610637+ 0600350501+
3022965054+ 0012383650+ 0017072385- 0022370006+ 0010162665- 0006544143- 0999454176+ 0600350601+

*A1 NORMAL FREQUENCIES AND COORDINATES FOR CD3CD2CD3

9917801453+ 0680958201+ 0129728002+ 0425336552- 0490456557+ 0235568698- 0165825070+ 0900910101+
9917801453+ 0111591724+ 0009569715+ 0049727799- 0000000000+ 0000C00000+ 0000000000+ 0900910102+
3099287853+ 0448225043- 0748741841+ 0486287870- 0007630436- 0000759900- 0009183896+ 0900910201+
3099287853+ 0019235625+ 0026415325- 0028162192- 0000000000+ 0000C00000+ 0000000000+ 0900910202+
7336915853+ 0266913652+ 0628626732+ 0712429158+ 0093757999+ 0061953423- 0084362897- 0900910301+
7336915853+ 0032949140- 0022249644+ 0068582884+ 0000000000+ 0000000000+ 0000000000+ 0900910302+
1134743854+ 0494344472- 0162185788- 0186935185+ 0758212838+ 0332674869- 0023009649- 0900910401+
1134743854+ 0051761115- 0016778824+ 0072972947+ 0000000000+ 0000000000+ 0000000000+ 0900910402+
2058624654+ 0018989329+ 0024219088+ 0006182441+ 0385164072+ 0868739195+ 0184723002+ 0900910501+
2058624654+ 024807890- 0013404635- 0010488658+ 0000000000+ 0000000000+ 0000000000+ 0900910502+
1080752954+ 0131786859- 0004871665+ 0193648821+ 0023547101- 0035901667+ 0682780467+ 0900910601+
1080752954+ 0592146359+ 0211709194- 0285688515- 0000000000+ 0000000000+ 0000000000+ 0900910602+
2127060754+ 0003841325+ 0019038576- 0019936030- 0154315774+ 0269904548+ 0621544646- 0900910701+
2127060754+ 0715103719+ 0057174241+ 0040043731- 0000000000+ 0000000000+ 0000000000+ 0900910702+
2259914554+ 003712980- 0009962522+ 0036245670+ 0000333802+ 0005463051- 0048030507+ 0900910801+
2259914554+ 0052009988- 0822710866+ 0561527606- 0000000000+ 0000000000+ 0000000000+ 0900910802+
1055775854+ 0025477117- 0002906752+ 0029385910- 0054749808- 0033480563+ 0275380986+ 0900910901+
1055775854+ 0239068109+ 0522792036+ 0766851125+ 0000000000+ 0000000000+ 0000000000+ 0900910902+
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A2 NORMAL FREQUENCIES AND COORDINATES FOR CD3CD2CD3

2185002153+ 0754365523+ 0354157041- 0552725462- 0000000028+ 0000000240- 0000000000+ 0500260101+
6699899953+ 0497970536+ 0849435482+ 0135362356+ 0056273928- 0094841828+ 0000000000+ 0500260201+
8875447953+ 0421645721+ 0382520851- 0820565488+ 0013303695+ 0048866755+ 0000000000+ 0500260301+
2253672754+ 0020108226- 0008382365+ 0032815096- 0823494536+ 0565955209+ 0000000000+ 0500260401+
1057975354+ 0069054590- 0081484177- 0042036085- 0564369553- 0817503366+ 0000000000+ 0500260501+

B1 NORMAL FREQUENCIES AND COORDINATES FOR CD3CD2CD3

1309370754+ 0593579014+ 0583640021- 0436080670+ 0324973311+ 0101636136- 0028138232+ 0700590101+
1309370754+ 0011514243- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700590102+
7027645653+ 0466421824+ 0787304181+ 0388582861+ 0039265799+ 0007868748- 0048845632- 0700590201+

B1 NORMAL FREQUENCIES AND COORDINATES FOR CD3CD2CD3

7027645653+ 0087272705- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700590202+
7687541053+ 0621963279- 0026744176- 0777322057+ 0033437937+ 0034829958- 0023053683- 0700590301+
7687541053+ 0073171945- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700590302+
1048882154+ 0178176336- 0194862307+ 0136777283- 0740907217+ 0348054927- 0273283000+ 0700590401+
1048882154+ 0408417044+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700590402+
2065062754+ 0042636463- 0018948892+ 0010272410- 0410723582+ 0910502779+ 0002508402- 0700590501+
2065062754+ 0001440077+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700590502+
2251400354+ 0009935720- 0012110477+ 0036304472- 0001819752- 0002857438+ 0822729857+ 0700590601+
2251400354+ 0567045583- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700590602+
1060134954+ 0098045340+ 0018003772- 0185676697+ 0417243033- 0195523212+ 0494688330+ 0700590701+
1060134954+ 0706080374+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0700590702+

B2 NORMAL FREQUENCIES AND COORDINATES FOR CD3CD2CD3

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1891939553+ 0564182808+ 0557993655- 0608556338- 0000000058+ 0000000093+ 0000000097+ 0600440101+
5769945353+ 0609040500+ 0774793084+ 0145786726- 0047964369- 0071529801+ 0009719413+ 0600440201+
9848258353+ 0541083540+ 0294396567- 0771566125+ 0037105103- 0138691425+ 0068065094- 0600440301+
2241200854+ 0000826268+ 0008347643- 0008420324+ 0615726007+ 0423114108+ 0664616164+ 0600440401+
1058956054+ 0127356015- 0027210286- 0093120155- 0563989872- 0810076271+ 0007780013+ 0600440501+
2272926954+ 0042139910+ 0029314101- 0065945747+ 0546918204- 0374698603- 0743974113+ 0600440601+

GAMMA MATRIX FOR CH3CH2CH3

0101033543+ 0000000000+ 5773500050- 8164970050+ 4868650050- 2581990050+ * *
 0202343644+ 0000000000+ 1000000051- 2108180050- 5773500050- 2581990050+ * *
 0301033545+ 0000C00000+ 8164970050+ 5773500050+ 6024640050- 2581990050+ * *
 0404063435+ 3643000000+ 5773500050- 8164970050+ 5270460050+ 4260060050+ 2886750050+ 2581990050+
 0505343644+ 0000000000+ 1000000051- 2108180050- 2886750050+ 2581990050+ * *
 0604063435+ 3645000000+ 8164970050+ 5773500050+ 3726780050+ 4303310049+ 4082480050- 2581990050+
 0707093435+ 3643C00000+ 5773500050- 8164970050+ 5270460050- 4260060050+ 2886750050- 2581990050+
 0808343644+ 0000000000+ 1000000051- 2108180050- 2886750050+ 2581990050+ * *
 0907093435+ 3645000000+ 8164970050+ 5773500050+ 3726780050- 4303310049+ 4082480050+ 2581990050+
 1010123543+ 0000C00000+ 1666666750- 2357022650+ 3042900049- 2581990050+ * *
 1111344400+ 0000C00000+ 2886751750- 5270460049+ 2581990050+ * *
 1210123545+ 0000000000+ 2357022650+ 1666666750+ 4303310049+ 2581990050+ * *
 1313384600+ 0000000000+ 2886751750+ 1091090050- 2672610050+ * *
 1414374700+ 0000000000+ 2886751750+ 5976140049+ 2672610050+ * *
 1515480000+ 0000000000+ 2886751750+ 2672610050+ * *
 1616383946+ 0000000000+ 1000000051+ 6546540050+ 8164970050- 2672610050+ * *
 1717374700+ 0000C00000+ 1000000051+ 3585690050- 2672610050+ * *
 1818374800+ 0000000000+ 1000000051+ 6831300050+ 2672610050+ * *
 1919383946+ 0000C00000+ 1000000051+ 6546540050+ 8164970050+ 2672610050+ * *
 2020374700+ 0000000000+ 1000000051+ 3585690050- 2672610050+ * *
 2121374800+ 0000000000+ 1000000051+ 6831300050- 2672610050+ * *
 2222244149+ 0000000000+ 5773500050+ 8164970050- 4868650050+ 2581990050+ * *
 2323404250+ 0000000000+ 1000000051+ 2108180050+ 5773500050+ 2581990050+ * *
 2422244151+ 0000C00000+ 8164970050+ 5773500050+ 6024640050- 2581990050+ * *
 2525274041+ 42490000C0+ 5773500050+ 8164970050- 5270460050- 4260060050- 2886750050- 2581990050+
 2626404250+ 00000000C0+ 1000000051+ 2108180050+ 2886750050- 2581990050+ * *
 2725274041+ 42510000C0+ 8164970050+ 5773500050+ 3726780050+ 4303310049+ 4082480050- 2581990050+
 2828304041+ 4249C00000+ 5773500050+ 8164970050- 5270460050+ 4260060050- 2886750050+ 2581990050+
 2929404250+ 0000C00000+ 1000000051+ 2108180050+ 2886750050- 2581990050+ * *
 3028304041+ 42510000C0+ 8164970050+ 5773500050+ 3726780050- 4303310049+ 4082480050+ 2581990050+
 3131334149+ 0000C00000+ 1666666750+ 2357022650- 3042900049+ 2581990050+ * *
 3232405000+ 0000C00000+ 2886751750+ 5270460049- 2581990050+ * *
 3331334151+ 0000C00000+ 2357022650+ 1666666750+ 4303310049+ 2581990050+ * *

NORMAL COORDINATES FOR CH₃CH₂CH₃ (MOLECULAR C.M. AXES)

0100000007+ 2991395650- 1247315049- 2243666750- 1979612950- 3178313250- 1072157149- 9315187749-
 0100070007+ 4421607450+ 1245633650+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 0100140007+ 6070951249+ 1104034450+ 3044876450+ 2130101850- 3343836550- 4424421950+ 1180817650+
 0100210006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 0200270007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 0200340007+ 0000000000+ 0000000000+ 3612674650+ 1812492750- 9770947049- 1379182849+ 4977142650-
 0200410007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 0200480006+ 4217752150- 1559566950- 1685577850- 1056828749+ 4895664250- 8894762048- 0000000000+
 0300540007+ 2918081650- 2114787250+ 1653556550- 3216908450- 2184157550+ 3663380249- 6653165249+
 0300610007+ 3190199850- 2476338550+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 0300680007+ 5600171449+ 2687752850+ 3032746450+ 2665601350- 2288848650+ 3170225350- 1982390150+
 0300750006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 0400810007+ 8677987049+ 2588530950- 2544198350+ 3194642950- 2757055348- 1206014048- 6113740148-
 0400880007+ 8109406348+ 9254791349+ 1852974350- 2648927450+ 1566578150+ 3053499347+ 3276461150-
 0400950007+ 2785366349+ 2831360550+ 3161925950- 1833357650- 4408234548- 7782884848+ 1171537249+
 0401020006+ 2339310350+ 2144165750+ 1912207850+ 5340414048+ 3356701550- 5766401248+ 0000000000+
 0501080007+ 2994622449+ 6418396948- 5247315549+ 1273368650+ 3081755250- 1141408550- 1154571950-
 0501150007+ 2152793050- 2498361150+ 2398882350- 1099771350- 2761199749- 3896660050+ 2471820349-
 0501220007+ 1331157248- 4886822049+ 4338541949- 1648580150+ 3277965650- 2178459350- 2522741150+
 0501290006+ 1125700150+ 1126901950- 5115055049- 2902214650+ 2251925449- 2599021050- 0000000000+
 0601350007+ 5377150549- 4800063949+ 2236224549+ 1321815650- 2196912750- 1139569850+ 8680781949-
 0601420007+ 1634610950- 3295447850- 2940562050+ 2377038350+ 1603400850+ 2659990650+ 1027781150+
 0601490007+ 5543651849+ 6507271049- 2082565649- 1725081350- 2348207050- 1653960950- 3258950150-
 0601560006+ 2124249850- 1822096450+ 2182330950+ 2015209450+ 9289744049+ 1734115450- 0000000000+
 0701620007+ 8677987049+ 2588530950- 2544198350+ 3194642950- 2757055348- 1206014048- 6113740148-
 0701690007+ 8109406348+ 9254791349+ 1852974350+ 2648927450- 1566578150- 3053499347- 3276461150+
 0701760007+ 2785366349+ 2831360550+ 3161925950- 1833357650- 4408234548- 7782884848+ 1171537249+
 0701830006+ 2339310350- 2144165750- 1912207850- 5340414048- 3356701550+ 5766401248- 0000000000+
 0801890007+ 2994622449- 6418396948+ 5247315549- 1273368650- 3081755250+ 1141408550+ 1154571950+
 0801960007+ 2152793050+ 2498361150- 2398882350- 1099771350- 2761199749- 3896660050+ 2471820349-
 0802030007+ 1331157248+ 4886822049- 4338541949+ 1648580150- 3277965650+ 2178459350+ 2522741150-
 0802100006+ 1125700150+ 1126901950- 5115055049- 2902214650+ 2251925449- 2599021050- 0000000000+
 0902160007+ 5377150549- 4800063949+ 2236224549+ 1321815650- 2196912750- 1139569850+ 8680781949-
 0902230007+ 1634610950- 3295447850- 2940562050- 2377038350- 1603400850- 2659990650- 1027781150-

NORMAL COORDINATES FOR -CH₃CH₂CH₃ (MOLECULAR C.M. AXES)

0902300007+ 5543651849+ 6507271049- 2082565649- 1725081350- 2348207050- 1653960950- 3258950150-
 0902370006+ 2124249850+ 1822096450- 2182330950- 2015209450- 9289744049- 1734115450+ 0000000000+
 1002430007+ 1248789450- 1378895850- 7573501048- 6234402249+ 2066450249+ 1441320249- 1268445849+
 1002500007+ 3928547649- 2784362949- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1002570007+ 8762117149+ 8577638749- 1637748249+ 3249702048- 2350041249+ 3880969049- 1904126649+
 1002640006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1102700007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1102770007+ 0000000000+ 0000000000+ 3195906249- 5198802849+ 7078363549+ 6741346149- 3524758449+
 1102840007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1102910006+ 3763730049- 1490338549+ 8487789349+ 4889802349- 3166703149+ 4671417849+ 0000000000+
 1202970007+ 3406100849- 3431393549+ 9770497849+ 4641638349+ 1451358149+ 3531000849- 1027034149+
 1203040007+ 5571166349+ 1530844849+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1203110007+ 7256195249+ 1722439649- 8103229549- 3424945149+ 1558405749+ 5466414049+ 3615417749+
 1203180006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1303240007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1303310007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1303380007+ 1100769850- 1065185850+ 4376459049+ 1447804250+ 1039387149+ 2238715648+ 9285515549-
 1303450006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1403510007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1403580007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1403650007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1403720006+ 8065122449+ 7330507049+ 1345205750- 6168013549- 2414560449+ 7407733449- 0000000000+
 1503780007+ 1283926950+ 1039522950- 1647135150- 1108790149- 1468429349- 4538898949- 6091039949+
 1503850007+ 5370227143- 6857366048+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1503920007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1503990006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1604050007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1604120007+ 0000000000+ 0000000000+ 2608486649- 4577960350+ 6516173750- 1061708849+ 2063243649+
 1604190007+ 5074074750- 2864706950- 1312193050- 2500056750- 1168308548- 5724210248- 1871236750+
 1604260006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1704320007+ 3654620149+ 1289062049- 6546681449- 5889892549- 1940193150+ 4023676750- 5234472150-
 1704390007+ 2068903649+ 1295181650- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1704460007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1704530006+ 1643748550+ 2373341150- 5944947049+ 3658457650+ 9726596048+ 4125929750+ 0000000000+

NORMAL COORDINATES FOR CH₃CH₂CH₃ (MOLECULAR C.M. AXES)

1804590007+ 3772576049+ 9553232049- 5354646049- 9558498449+ 1349096450+ 5047735050+ 3816223950-
 1804660007+ 9623217048+ 1866096850+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1804730007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1804800006+ 1367199350- 5168914050+ 3621734050- 2540448050+ 3729201649+ 2721192150+ 0000000000+
 1904860007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 1904930007+ 0000000000+ 0000000000+ 2608486649+ 4577960350- 6616173750+ 1061708849- 2063243649-
 1905000007+ 5074074750- 2864706950- 1312193050- 2500056750- 1168308548- 5724210248- 1871236750+
 1905070006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 2005130007+ 3654620149- 1289062049+ 6546681449+ 5889892549+ 1940193150- 4023676750+ 5234472150+
 2005200007+ 2068903649- 1295181650+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 2005270007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 2005340006+ 1543748550+ 2373341150- 5944947049+ 3658457650+ 9726596048+ 4125929750+ 0000000000+
 2105400007+ 3772576049+ 9553232049- 6354646049- 9558498449+ 1349096450+ 5047735050+ 3816223950-
 2105470007+ 9623217048+ 1866096850+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 2105540007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 2105610006+ 1367199350+ 5168914050- 3621734050+ 2540448050- 3729201649- 2721192150- 0000000000+
 2205670007+ 2991395650+ 1247315049+ 2243666750+ 1979612950+ 3178313250+ 1072157149+ 9315187749+
 2205740007+ 4421607450- 1245633650- 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 2205810007+ 6070951249+ 1104034450+ 3044876450+ 2130101850- 3343836550- 4424421950+ 1180817650+
 2205880006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 2305940007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 2306010007+ 0000000000+ 0000000000+ 3612674650- 1812492750+ 9770947049+ 1379182849- 4977142650+
 2306080007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 2306150006+ 4217752150- 1559566950- 1685577850- 1056828749+ 4895664250- 8894762048- 0000000000+
 2406210007+ 2918081650- 2114787250+ 1653556550- 3216908450- 2184157550+ 3663380249- 6653165249+
 2406280007+ 3190199850- 2476338550+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 2406350007+ 5600171449- 2687752850- 3032746450- 2665601350+ 2288848650- 3170225350+ 1982390150-
 2406420006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 2506480007+ 8677987049- 2588530950+ 2544198350- 3194642950+ 2757055348+ 1206014048+ 6113740148+
 2506550007+ 8109406348- 9254791349- 1852974350+ 2648927450- 1566578150- 3053499347- 3276461150+
 2506620007+ 2785366349+ 2831360550+ 3161925950- 1833357650- 4408234548- 7782884848+ 1171537249+
 2506690006+ 2339310350+ 2144165750+ 1912207850+ 5340414048+ 3356701550- 5766401248+ 0000000000+
 2606750007+ 2994622449- 6418396948+ 5247315549- 1273368650- 3081755250+ 1141408550+ 1154571950+
 2606820007+ 2152793050+ 2498361150- 2398882350+ 1099771350+ 2761199749+ 3896660050- 2471820349+

NORMAL COORDINATES FOR CH3CH2CH3 (MOLECULAR C.M. AXES)

2606890007+ 1331157248- 4886822049+ 4338541949- 1648580150+ 3277965650- 2178459350- 2522741150+
 2606960006+ 1125700150+ 1126901950- 5115055049- 2902214650+ 2251925449- 2599021050- 0000000000+
 2707020007+ 5377150549- 4800063949+ 2236224549+ 1321815650- 2196912750- 1139569850+ 8680781949-
 2707090007+ 1634610950- 3295447850- 2940562050+ 2377038350+ 1603400850+ 2659990650+ 1027781150+
 2707160007+ 5543651849- 6507271049+ 2082565649+ 1725081350+ 2348207050+ 1653960950+ 3258950150+
 2707230006+ 2124249850+ 1822096450- 2182330950- 2015209450- 9289744049- 1734115450+ 0000000000+
 2807290007+ 8677987049- 2588530950+ 2544198350- 3194642950+ 2757055348+ 1206014048+ 6113740148+
 2807360007+ 8109406348- 9254791349- 1852974350- 2648927450+ 1566578150+ 3053499347+ 3276461150-
 2807430007+ 2785366349+ 2831360550+ 3161925950- 1833357650- 4408234548- 7782884848+ 1171537249+
 2807500006+ 2339310350- 2144165750- 1912207850- 5340414048- 3356701550+ 5766401248- 0000000000+
 2907560007+ 2994622449+ 6418396948- 5247315549+ 1273368650+ 3081755250- 1141408550- 1154571950-
 2907630007+ 2152793050- 2498361150+ 2398882350+ 1099771350+ 2761199749+ 3896660050- 2471820349+
 2907700007+ 1331157248+ 4886822049- 4338541949+ 1648580150- 3277965650+ 2178459350+ 2522741150-
 2907770006+ 1125700150+ 1126901950- 5115055049- 2902214650+ 2251925449- 2599021050- 0000000000+
 3007830007+ 5377150549- 4800063949+ 2236224549+ 1321815650- 2196912750- 1139569850+ 8680781949-
 3007900007+ 1634610950- 3295447850- 2940562050- 2377038350- 1603400850- 2659990650- 1027781150-
 3007970007+ 5543651849- 6507271049+ 2082565649+ 1725081350+ 2348207050+ 1653960950+ 3258950150+
 3008040006+ 2124249850- 1822096450+ 2182330950+ 2015209450+ 9289744049+ 1734115450- 0000000000+
 3108100007+ 1248789450+ 1378895850+ 7573501048+ 6234402249- 2066450249- 1441320249+ 1268445849-
 3108170007+ 3928547649+ 2784362949+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 3108240007+ 8762117149+ 8577638749- 1537748249+ 3249702048- 2350041249+ 3880969049- 1904126649+
 3108310006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 3208370007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 3208440007+ 0000000000+ 0000000000+ 3195906249+ 5198802849- 7078363549- 6741346149+ 3524758449-
 3208510007+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 3208580006+ 3763730049- 1490338549+ 8487789349+ 4889802349- 3166703149+ 4671417849+ 0000000000+
 3308640007+ 3406100849- 3431393549+ 9770497849+ 4641638349+ 1451358149+ 3531000849- 1027034149+
 3308710007+ 5571166349+ 1530844849+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+
 3308780007+ 7256195249- 1722439649+ 8103229549+ 3424945149- 1658405749- 5466414049- 3615417749-
 3308850006+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+ 0000000000+