IN-1076
May 1967

MASTER

D MATRIX
A COMPUTER PROGRAM FOR CALCULATING
VALENCE FORCE COORDINATES IN TERMS OF
ATOM DISPLACEMENTS OF A MOLECULE OR CRYSTAL

J. K. Boyter and H. L. McMurry

IDAHO NUCLEAR CORPORATION
NATIONAL REACTOR TESTING STATION
IDAHO FALLS, IDAHO

U. S. ATOMIC ENERGY COMMISSION

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Per

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Printed in the United States of America
Available from
Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U. S. Department of Commerce
Springfield, Virginia 22151
Price: Printed Copy \$3.00; Microfiche \$0.65

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, express or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

IN-1076
Issued: May 1967
Mathematics and Computers
TID-4500

~~SECRET~~ RECES

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

HQ \$3.00; MN 65

D MATRIX

A COMPUTER PROGRAM FOR CALCULATING VALENCE FORCE COORDINATES

IN TERMS OF ATOM DISPLACEMENTS OF A MOLECULE OR CRYSTAL

by

J. K. Boyter and H. L. McMurry

IDAHO NUCLEAR CORPORATION

A JOINTLY OWNED SUBSIDIARY OF
AEROJET ALLIED
GENERAL CHEMICAL
CORPORATION CORPORATION

U. S. Atomic Energy Commission Research and Development Report
Issued Under Contract AT(10-1)-1230
Idaho Operations Office

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the help given by Dr. A. W. Solbrig for his help in clarifying the problem to be programmed. Also the assistance of R. S. Marsden in checking out the program.

D MATRIX

by

J. K. Boyter and H. L. McMurry

ABSTRACT

This report describes a Fortran program written for the IBM 7040 which calculates the valence force coordinates of the valence force potential function in terms of the atom displacements, and mass adjusted displacements in a molecule or crystal.

The input data is explained with illustrative applications given for propane and diamond in the Appendix. Two other test examples are also given.

CONTENTS

ACKNOWLEDGEMENTS	ii
ABSTRACT	iii
I. INTRODUCTION	1
II. THEORY	2
A. Introduction	2
B. The Valence Force Potential Function	2
C. The Relation Between Valence Force Coordinates and Cartesian Displacement of Atoms	3
D. Equation for the Coordinates Associated with Molecular Rotation	3
E. Equation to Group Rotation	4
III. CALCULATIONS	5
A. Molecules	5
B. Coordinates for Crystal	5
C. Indexing Types of Valence Coordinates	6
D. Valence Coordinates	7
E. Computation of $\mathbf{D}$	9
IV. GENERAL INPUT-OUTPUT INFORMATION	11
A. Input	11
B. Output	11
C. Card Formats	12
V. REFERENCES	17
APPENDIX A	19
APPENDIX B	27
APPENDIX C	35
APPENDIX D	39

D MATRIX

I. INTRODUCTION

This report describes an IBM 7040 program for calculating the changes in bond distances and interbond angles in terms of the rectangular Cartesian displacements, or mass adjusted Cartesian displacements of the atoms in a molecule or crystal. This transformation is needed to calculate the vibrational frequencies and normal modes when a valence force potential is suitable. The program saves much handwork and eliminates a major possibility of error in computation.

The computing program* which calculates molecular vibration frequencies and normal modes requires as input a set of three coordinates associated with the rotation of the molecule. As a byproduct, the program described here calculates these coordinates so they can be inserted directly into the program for calculating the molecular vibrations.

In some cases it is convenient to think of a molecule as divided into groups of atoms and to describe some of the vibrations in terms of translational and rotational displacements of the groups as rigid units. A convenient recipe has been given for defining coordinates associated with the group rotations⁽¹⁾ and the computer program gives these as part of the output.

*The program is described in Phillips Petroleum Company program description PPCo 40-0206 (available from Phillips Computing Center, P. O. Box 2067, Idaho Falls, Idaho).

II. THEORY

A. Introduction

Much of the work is based on Reference 1 which gives the theory and notation for molecules. A report describing the theory for the case of crystals is in preparation; however, it draws on that for a molecule, and also employs properties of crystals in which the primitive cell is an important concept. This report assumes the reader is familiar with the way primitive cells are used to describe the properties of crystals.

B. The Valence Force Potential Function

The valence force potential energy, V , for a molecule has the form

$$V = \underline{H}' \underline{F} \underline{H} = \sum_{ij} H_i F_{ij} H_j \quad (1)$$

$\underline{H}$ is a column matrix containing elements H_i which are the changes in bond distances and interbond angles. $\underline{F}$, a square and symmetric matrix, is the force constant matrix.

In the case of molecules the elements in $\underline{H}$ are easy to set down since they include all changes in bond distances and interbond angles, together with appropriate torsional motions (such as the torsional rotations of the CH_3 groups in C_2H_6) and possible changes between a bond and a plane defined by two other bonds.

In crystals the valence bond coordinates must be chosen so that each primitive cell has the same set of coordinates, and no valence coordinate is identified with more than one cell. This will be discussed in a forthcoming publication.

C. The Relation Between Valence Force Coordinates and Cartesian Displacements of Atoms

To use Eq. (1) $\tilde{H}$ must be expressed in terms of the mass adjusted Cartesian coordinates of the atoms which give the internal kinetic energy. For molecules, Wilson⁽²⁾ has given convenient formulas for expressing the components in $\tilde{H}$ in terms of these mass adjusted Cartesian displacements. The same relations are valid for crystals. They lead to the relation

$$\tilde{H} = \tilde{D} \tilde{q} \quad (2)$$

Here $\tilde{q}$ is a column vector containing the mass adjusted Cartesian displacements ($\sqrt{m_v} \Delta X_v$, etc.) of the atoms in a primitive unit cell in a crystal, or in a molecule.

Any element H_i of $\tilde{H}$ is given by*

$$H_i = \tilde{D}_{i\tilde{q}} = [\tilde{D}_{i1} \tilde{D}_{i2} \dots \tilde{D}_{ij} \dots] \tilde{q} \quad (3)$$

$$\tilde{D}_{ij} = [\tilde{D}_{ij1} \tilde{D}_{ij2} \dots \tilde{D}_{ijv} \dots \tilde{D}_{ijm}]$$

$$\tilde{D}_{ijv} = \frac{1}{\sqrt{m_v}} [S_{x_{ijv}} \ S_{y_{ijv}} \ S_{z_{ijv}}],$$

where m is the number of atoms/unit cell in a crystal or atoms/molecule, and m_v is the mass of atom v . In Eq. (4) the $S_{x_{ijv}}$, $S_{y_{ijv}}$, $S_{z_{ijv}}$ are the components of Wilson's $\tilde{S}_{ijv}$ vector along the indicated axes and are computed from his equations⁽²⁾.

D. Equation for the Coordinates Associated with Molecular Rotation

For molecules, the theory defines a three rowed matrix $\mathfrak{B}$, each row of which is associated with molecular rotation about one of the axes. The $\mathfrak{B}$ has the form

*In crystals the subscript j denotes the cell involved. See Sec. III B.

There is no need for a j subscript in molecules.

$$\underline{\underline{B}} = [\underline{\underline{B}}_1 \underline{\underline{B}}_2 \dots \underline{\underline{B}}_v \dots \underline{\underline{B}}_n] \quad (5)$$

where

$$\underline{\underline{B}}_v = \sqrt{m_v} \begin{bmatrix} 0 & -Z_v & Y_v \\ Z_v & 0 & X_v \\ Y_v & X_v & 0 \end{bmatrix}$$

Here m_v is the mass of atom v and x_v , y_v , z_v are the coordinates relative to Cartesian axes at the molecular center of mass.

E. Equation to Group Rotation

When a molecule is considered as made up of groups of atoms rigid rotations of any groups are conveniently expressed by a three row matrix $\underline{\underline{B}}_J$ in the form

$$\underline{\underline{B}}_J = [\underline{\underline{B}}_{1J} \underline{\underline{B}}_{2J} \dots \underline{\underline{B}}_{vJ} \dots \underline{\underline{B}}_{mJ}]$$

$$\underline{\underline{B}}_{vJ} = \sqrt{m_v} \begin{bmatrix} 0 & -Z_{vJ} & Y_{vJ} \\ Z_{vJ} & 0 & -X_{vJ} \\ Y_{vJ} & X_{vJ} & 0 \end{bmatrix}$$

Here m_v is the mass of atom v , and X_{vJ} , Y_{vJ} , Z_{vJ} are the position of atom v relative to axes fixed at the cm. of the group and parallel to the molecular axis. The subscript m is the number of atoms in the molecule.

III. CALCULATIONS

A. Molecules

The atoms are numbered from 1 to m. In what follows an atom is identified by its assigned number in this sequence.

Initially, the positions of the atoms are given in rectangular Cartesian coordinates relative to a conveniently chosen origin. Then the center of mass is calculated (only for the origin cell in the case of a crystal) and the coordinates of each atom are corrected to put the origin at the center of mass. All calculations of the $\underline{D}$ matrix and $\underline{B}$ matrix are made with these coordinates. The $\underline{B}_J$ matrix is calculated for molecules where the coordinates of each atom are relative to an origin at the center of mass of the group J to which that atom belongs.

B. Coordinates for Crystals

The primitive cells adjacent to the origin cell are indexed. The program is set up so a molecule is a special case of a crystal with but one primitive cell. "Adjacent cells" are all the cells which contain atoms whose motions alter one of the bond distances, interbond angles, etc. associated with the origin cell. These adjacent cells are reached by displacing the origin cell by

$$\underline{t} = l_{1j} \underline{\alpha}_1 + l_{2j} \underline{\alpha}_2 + l_{3j} \underline{\alpha}_3 \quad (7)$$

where $l_{ij} = 0, \pm 1, \dots$. The $\underline{\alpha}_1, \underline{\alpha}_2, \underline{\alpha}_3$ are the primitive translation vectors characteristic of the crystal involved. The cells involved in a calculation are called by the set of ordered triplets l_{1j}, l_{2j}, l_{3j} . Each ordered triplet is called by the index j.

The indices j of the ordered triplets are 1, 2, 3, . . . j , . . . , n where n is the maximum number of cells involved. The indices j of the cells are assigned so that the $\underline{D}$ matrix is grouped for direct insertion into a program for calculating the crystal or molecular vibrations*. To use this program the indices are assigned to the cells as follows:

<u>j</u>	<u>l_{1j}</u>	<u>l_{2j}</u>	<u>l_{3j}</u>
1	1	0	0
2	0	1	0
3	0	0	1
.			
.			
.			
.			
m	0	0	0 (the origin cell is assigned the median index m)
m + 1	-1	0	0
m + 2	0	-1	0
m + 3	0	0	-1
.	.	.	.
.	.	.	.
.	.	.	.
.	.	.	.
n			

C. Indexing Types of Valence Coordinates

To each element H_i in $\underline{H}$ there corresponds a valence coordinate.

These valence coordinates are indexed as follows:

1. bond stretching
2. angle bending

*The program referred to is under further development. It has not been described in a report.

3. torsional rotation about a bond
4. dihedral torsion
5. angle bending between a bond and a plane defined by two bonds

Except for the torsional rotation coordinates the recipes given by Wilson (see Ref. 2, Section 4.1) are used to compute the elements in $\underline{D}$.

A set of vectors is used to compute each valence coordinate. Each of these vectors, $\underline{S}_{ijv}$, is obtained in terms of a unit vector, $\underline{e}_{vv'}$, connecting atom v and other atoms v' whose motion effects H_i .

The vector position of atom v in the cell with indices l_{1j} , l_{2j} , l_{3j} ($=[0, 0, 0]$ for a molecule) is given by

$$\underline{R}_{jv} = X_{vj} \underline{i} + Y_{vj} \underline{j} + Z_{vj} \underline{k} + l_{1j} \underline{\alpha}_1 + l_{2j} \underline{\alpha}_2 + l_{3j} \underline{\alpha}_3 \quad (8)$$

The unit vector directed from atom v to atom v' is

$$\underline{e}_{vv'} = \frac{\underline{R}_{j'v'} - \underline{R}_{jv}}{r_{vv'}} \quad (9)$$

$$r_{vv'} = |\underline{R}_{j'v'} - \underline{R}_{jv}| \quad (10)$$

D. Valence Coordinates

1. Bond stretching ($= \Delta r_{vv'}$) from atom v' and to atom v .

$$\underline{S}_{ijv} = \underline{e}_{v'v} \quad (11)$$

$$\underline{S}_{ij'v'} = -\underline{e}_{v'v} = -\underline{S}_{ijv} \quad (12)$$

2. Interbond angle ($= r_o \Delta \theta$) between $\underline{e}_{v'v}$ and $\underline{e}_{v'v''}$

$$\theta = (\underline{e}_{vv'}, \underline{e}_{vv''}) \quad (13)$$

$$\cdot \tilde{S}_{ijv} = \frac{r_o}{r_{v'v}} \cdot \frac{\cos \emptyset \tilde{e}_{v'v} - \tilde{e}_{v'v'}}{\sin \emptyset} \quad (14)$$

$$\tilde{S}_{ij''v''} = \frac{r_o}{r_{v'v''}} \cdot \frac{\cos \emptyset \tilde{e}_{v'v''} - \tilde{e}_{v'v}}{\sin \emptyset}$$

$$\tilde{S}_{ij'v'} = - (\tilde{S}_{ijv} + \tilde{S}_{ij''v''}) \quad (16)$$

r_o , a constant chosen to give dimensions of length to $\Delta \emptyset$.

3. Torsional rotation of group J about an axis along w passing through, R_J , the center of mass of group J*.

$$\tilde{e}_{Jv} = \frac{R_{Jv} - R_J}{r_{Jv}} \quad (17)$$

$$\tilde{w}_J = w_x \tilde{i} + w_y \tilde{j} + w_z \tilde{k}, \quad (18)$$

A unit vector specified by the user

$$\tilde{S}_{iJv} = \frac{\tilde{w}_J \times \tilde{e}_{Jv}}{\sin (\tilde{w}_J, \tilde{e}_{Jv})} \quad (19)$$

4. Torsion involving a dihedral angle ($r_o \Delta \tau$)

$$\tilde{S}_{ij_1 v_1} = \frac{r_o}{r_{12}} \cdot \frac{\tilde{e}_{12} \times \tilde{e}_{23}}{\sin^2 \emptyset_2} \quad (20)$$

$$\tilde{S}_{ij_2 v_2} = r_o \cdot \frac{r_{23} - r_{12} \cos \emptyset_2}{r_{23} r_{12} \sin \emptyset_2} \frac{\tilde{e}_{12} \times \tilde{e}_{23}}{\sin \emptyset_2} + r_o \cdot \frac{\cos \emptyset_3}{r_{23} \sin \emptyset_3} \frac{\tilde{e}_{43} \times \tilde{e}_{32}}{\sin \emptyset_3}$$

*Note that this as observed from a laboratory fixed coordinate system can change. It must be used with care in crystals -- usually in combination with an opposite rotation of a like group.

$$= r_o \cdot \frac{r_{23} - r_{12} \cos \theta_2}{r_{23} r_{12} \sin \theta_2} \frac{\underline{e}_{12} \times \underline{e}_{23}}{\sin \theta_2} - r_o \cdot \frac{\cos \theta_3}{r_{23} \sin \theta_3} \frac{\underline{e}_{23} \times \underline{e}_{34}}{\sin \theta_3} \quad (21)$$

$$\begin{aligned} \underline{s}_{ij_3 v_3} &= r_o \cdot \frac{r_{32} - r_{43} \cos \theta_3}{r_{32} r_{43} \sin \theta_3} \frac{\underline{e}_{43} \times \underline{e}_{32}}{\sin \theta_3} + r_o \cdot \frac{\cos \theta_2}{r_{32} \sin \theta_2} \frac{\underline{e}_{12} \times \underline{e}_{23}}{\sin \theta_2} \\ &= - r_o \cdot \frac{r_{23} - r_{34} \cos \theta_3}{r_{23} r_{34} \sin \theta_3} \frac{\underline{e}_{23} \times \underline{e}_{34}}{\sin \theta_3} + r_o \cdot \frac{\cos \theta_2}{r_{23} \sin \theta_2} \frac{\underline{e}_{12} \times \underline{e}_{23}}{\sin \theta_2} \end{aligned} \quad (22)$$

$$\underline{s}_{ij_4 v_4} = - r_o \cdot \frac{\underline{e}_{43} \times \underline{e}_{32}}{r_{43} \sin^2 \theta_3} = - r_o \cdot \frac{\underline{e}_{23} \times \underline{e}_{34}}{r_{34} \sin^2 \theta_3} \quad (23)$$

5. Angle ($= r_{41} \Delta \theta$) between the bond connecting atoms 1,4 and the plane defined by bonds 4, 3 and 4, 2

$$\sin \theta = \frac{\underline{e}_{42} \times \underline{e}_{43}}{\sin \theta_1} \cdot \underline{e}_{41} \quad (24)$$

$$\underline{s}_{ij_1 v_1} = \frac{\underline{e}_{42} \times \underline{e}_{43}}{\cos \theta \sin \theta_1} - \tan \theta \underline{e}_{41} \quad (25)$$

$$\underline{s}_{ij_2 v_2} = \frac{r_{41}}{r_{42}} \left[\frac{\underline{e}_{43} \times \underline{e}_{41}}{\cos \theta \sin \theta_1} - \frac{\tan \theta}{\sin^2 \theta_1} (\underline{e}_{43} - \cos \theta_1 \underline{e}_{43}) \right] \quad (26)$$

$$\underline{s}_{ij_3 v_3} = \frac{r_{41}}{r_{42}} \left[\frac{\underline{e}_{41} \times \underline{e}_{42}}{\cos \theta \sin \theta_1} - \frac{\tan \theta}{\sin^2 \theta_1} (\underline{e}_{43} - \cos \theta_1 \underline{e}_{42}) \right] \quad (27)$$

$$\underline{s}_{ij_4 v_4} = - (\underline{s}_{ij_1 v_1} + \underline{s}_{ij_2 v_2} + \underline{s}_{ij_3 v_3}) \quad (28)$$

E. Computation of $\underline{D}$

The construction of the $\underline{S}$ matrix is

$$S = \begin{bmatrix} S_{111} & S_{112} & \dots & S_{11m} & \dots & S_{1j1} & S_{1j2} & \dots & S_{1jm} \\ S_{211} & S_{212} & \dots & S_{21m} & \dots & S_{2j1} & S_{2j2} & \dots & S_{2jm} \\ \cdot & \cdot & & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & & \cdot & \cdot & & \cdot \\ S_{m_i 11} & S_{m_i 12} & \dots & S_{m_i 1m} & \dots & S_{m_i j1} & S_{m_i j2} & \dots & S_{m_i nm} \end{bmatrix}$$

where

m = number atoms/cell or atoms/molecule

n = number of cells (= 1 for a molecule)

m_i = number of H_i 's

$$D = S \begin{bmatrix} \left(\frac{1}{\sqrt{m_1}} \right) & 0 & 0 \dots 0 \\ 0 & \left(\frac{1}{\sqrt{m_2}} \right) & 0 \dots 0 \\ 0 & 0 & \left(\frac{1}{\sqrt{m_3}} \right) \dots 0 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \left(\frac{1}{\sqrt{m_n}} \right) \end{bmatrix}$$

$\frac{1}{\sqrt{m_v}}$ denotes a 3 element diagonal matrix with $\frac{1}{\sqrt{m_v}}$ for each element.

IV. GENERAL INPUT-OUTPUT INFORMATION

A. Input

The various card types are:

<u>Card Type</u>	<u>Maximum Value</u>	<u>Usage</u>
1	1 card	Comments.
2	1 card	Program constants and control information.
3	as many as needed	Number of atoms in each group. Omit if crystal.
4	3 cards	Primitive vectors of cell. Omit if molecule.
5	maximum of 8	Cell multipliers. Maximum of 40 ordered triplets. Omit if molecule.
6	maximum of 8	Coordinates and mass of atoms. Maximum of 30 atoms.
7	maximum of 6	Index of atoms of each group. Omit for crystal or if only one group.
8	one card for each element in $\underline{H}$	Information for calculation of row i of $\underline{H}$ matrix.
9	See C-9	Additional information for calculation of torsional rotation if needed.

B. Output

The input, $\underline{B}$ and $\underline{B}$ matrixes and $\underline{D}$ or $\underline{S}$ matrix are listed. The $\underline{D}$ ($\underline{S}$) matrix is punched, and an option exists to generate the $\underline{D}$ ($\underline{S}$) matrix on tape (SSU .05). Sample outputs are given in Appendix A for a diamond crystal and also for a propane molecule.

C. Card Formats

<u>Type</u>	<u>Columns</u>	<u>Mnemonic Name</u>	<u>Format</u>	<u>Meaning</u>
1	1-80		A	Comments.
2*	1-5	MI	I	Number of elements in H.
	6-10	J	I	Number of cells, if molecule a 1 punch in column 10.
	11-15	M	I	Number of atoms/cell or atoms/molecule.
	16-20	JJ	I	Number of groups molecule divided into.
	21-25	ICM	I	A 1 punch in column 25 if crystal, otherwise blank.
	26-30	MN	I	A 1 punch gives $\tilde{S}$ matrix instead of $\tilde{D}$, otherwise blank.
	31-35	LL	I	A 1 punch if $\tilde{D}$ or $\tilde{S}$ matrix is to be generated on tape, otherwise blank.

*NOTE: The product of MI, J and M should not exceed 2400 unless the dimensions are changed.

3*	3-5	I Atoms	I	Number of atoms in group 1.
	8-10	I Atoms	I	Number of atoms in group 2.
	13-15	I Atoms	I	Number of atoms in group 3.
	.	.	.	
	.	.	.	
	.	.	.	

*Omit this card type if crystal.

4*	1-10	Cell x (1)	F	x component of 1st lattice vector.
	11-20	Cell y (1)	F	y component of 1st lattice vector.
	21-30	Cell z (1)	F	z component of 1st lattice vector.
	1-10	Cell x (2)	F	x component of 2nd lattice vector.
	11-20	Cell y (2)	F	y component of 2nd lattice vector.

Type	Columns	Mnemonic Name	Format	Meaning
4	21-30	Cell z (2)	F	z component of 2nd lattice vector. /
	1-10	Cell x (3)	F	x component of 3rd lattice vector.
	11-20	Cell y (3)	F	y component of 3rd lattice vector.
	21-30	Cell z (3)	F	z component of 3rd lattice vector.

*Omit this card type if molecule.

5*	1-3	L1 (1)	I	Multiplier of α_1 for cell 1.
	4-6	L2 (1)	I	Multiplier of α_2 for cell 1.
	7-9	L3 (1)	I	Multiplier of α_3 for cell 1.
	.	.	.	
	.	.	.	
	.	.	.	
	75-78	L2 (9)	I	Multiplier of α_2 for cell 9.
	1-3	L3 (9)	I	Multiplier of α_3 for cell 9.
	4-6	L1 (10)	I	Multiplier of α_1 for cell 10.
	.	.	.	
	.	.	.	
	.	.	.	

*Omit this card type if molecule.

6	1-10	A Mass (1)	F	Mass in atomic units of Atom 1.
	11-20	x (1)	F	x coordinates of Atom 1.
	21-30	y (1)	F	y coordinates of Atom 1.
	31-40	z (1)	F	z coordinates of Atom 1.
	41-50	A Mass (2)	F	Mass of Atom 2.
	.	.	.	
	.	.	.	
	.	.	.	

Type	Columns	Mnemonic Name	Format	Meaning
6	1-10	A Mass (3)	F	Mass of Atom 3.
	.	.	.	
	.	.	.	
	.	.	.	
7*	1-5	N1	I	Identification number of 1st atom in group 1.
	6-10	N2	I	Identification number of 2nd atom in group 1.
	.	.	.	
	.	.	.	
	.	.	.	
	21-25	N5	I	Identification number of 5th atom in group 1.
	1-5	N1	I	Identification number of 1st atom in group 2.
	.	.	.	
	.	.	.	
	.	.	.	
	21-25	N5	I	Identification number of 5th atom in group 2.
	1-5	N1	I	Identification number of 1st atom in group 3.
	.	.	.	
	.	.	.	
	.	.	.	
	21-25	N5	I	Identification number of 5th atom in group 3
	.	.	.	
	.	.	.	
	.	.	.	

*Omit this card type if crystal or if there is only one group in the molecule. Maximum of 5 in any group.

Type	Columns	Mnemonic Name	Format	Meaning
8	1-3	I	I	Row of $\underline{D}$ matrix to be calculated.
	3-6	Itype	I	Type of calculation to be performed (see next page).
	7-9	I1	I	Cell No. - corresponds to indexing of multipliers. Leave blank for molecule.
	10-12	N1	I	Atom number in cell or molecule.
	13-15	I2	I	Cell number. Leave blank for molecule.
	16-18	N2	I	Atom number. Apex atom for angle bending.
	.	.	.	
	.	.	.	
	.	.	.	
	37-39	I5	I	Cell number. Leave blank for molecule.
	40-42	N5	I	Atom number.
	43-54	Ro	F	Gives dimensions to bending coordinates. Required only for valence angle bending, dihedral torsion. If it is equal to zero, it is set = 1.0.
	55-62	Wx	F	x component of unit vector about which torsional rotation takes place.
	63-70	Wy	F	y component.
	71-78	Wz	F	z component.
	79-80	NTOR	I	Numbers of atoms involved in torsional rotation (NTOR > 3).

I TYPE = 1 for bond stretch

= 2 for valence angle bend

= 3 for torsional rotation

= 4 for dihedral torsion

= 5 for change of angle between a bond and plane defined
by two other bonds.

For valence angle bending I2, N2 are indexes of apex atom.

For dihedral torsional, (I1, N1), (I2, N2), (I3, N3), (I4, N4) are the indices of atom 1, 2, 3, 4, respectively.

For type 5, (I1, N1) are indices of end atom.

(I2, N2) are indices of an anchor atom.

(I3, N3) are indices of an anchor atom.

(I4, N4) are indices of an apex atom.

Type	Columns	Mnemonic Name	Format	Meaning
9*	1-3	I6	I	Cell number.
	4-6	N6	I	Atom number.
	7-9	I7	I	Cell number.
	10-12	N7	I	Atom number.
	13-15	I8	I	Cell number.
	16-18	N8	I	Atom number.

*This card used only if NTOR > 6 and is inserted directly behind the type

8 card to which it corresponds.

V. REFERENCES

1. H. L. McMurry, A Simplified Group Vibration Method for Calculating Normal Vibrations of Large Molecules, Spectrochimica Acta, 21 2091 (1965).
2. E. B. Wilson, Jr., J. C. Decius and P. C. Cross, Molecular Vibrations, McGraw-Hill, New York (1955). The sign between the terms in Equation 22 should be positive (F. Herman, Phys. J. Chem. of Solids, 8, 403 (1959)).

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

APPENDIX A

Diamond as a Test Example

1. The input for the diamond problem

0000000001	111111112	222222223	333333334	444444445	555555556	666666667	777777778
1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890
D. MATR IX. F.P.R. DIAMOND.							
0.0	1.78348	0.0	1.78348	0.0	1.78348	0.0	1.78348
1.78348	0.0	1.78348	0.0	1.78348	0.0	1.78348	0.0
1.78348	0.0	1.78348	0.0	1.78348	0.0	1.78348	0.0
1	1	1	1	1	1	1	1
12.0039	0.0	0.0	0.0	12.0039	0.89174	0.89174	0.89174
1	1	1	1	1	1	1	1
2	1	2	1	2	1	2	1
3	1	2	2	1	2	2	1
4	1	2	3	1	2	3	1
5	2	2	2	1	2	2	1
6	2	2	2	1	2	2	1
7	2	2	2	1	2	2	1
8	2	2	2	1	2	2	1
9	2	2	2	1	2	2	1
10	2	2	2	1	2	2	1
11	2	2	2	1	2	2	1
12	2	2	2	1	2	2	1
13	2	2	2	1	2	2	1
14	2	2	2	1	2	2	1
15	2	2	2	1	2	2	1
16	2	2	2	1	2	2	1
17	3	1	2	1	2	1	2
18	3	1	2	1	2	1	2
19	3	1	2	1	2	1	2
20	3	1	2	1	2	1	2
21	3	1	2	1	2	1	2
22	3	1	2	1	2	1	2
23	3	1	2	1	2	1	2
24	3	1	2	1	2	1	2

2. The program output

```

      D MATRIX FOR DIAMOND

      MI      JJ      M      JJ      CM      MN      LL
      24      13      2      0      1      0      0

      CELLX      CELLY      CELLZ
      0.000000      1.783480      1.783480
      1.783480      0.000000      1.783480
      1.783480      1.783480      0.000000

      N      L1(N)      L2(N)      L3(N)
      1      1      0      0
      2      0      1      0
      3      0      0      1
      4      0      1      -1
      5      -1      1      0
      6      -1      0      1
      7      0      0      0
      8      -1      0      0
      9      0      1      0
      10      0      0      -1
      11      0      -1      1
      12      1      -1      0
      13      1      0      -1

      NU      MASS(NU)      X(NU)      Y(NU)      Z(NU)
      1      12.00390      0.00000      0.00000      0.00000
      2      12.00390      0.89174      0.89174      0.89174

      UNCORRECTED CENTER OF MASS.
      XBAR = 0.445870      YBAR = 0.445870      ZBAR = 0.445870

      CORRECTED COORDINATES OF ATOM NU
      NU      X      Y      Z
      1      -0.44587      -0.44587      -0.44587
      2      0.44587      0.44587      0.44587

```

GERMAN SCRIPT B MATRIX

```

0.000000 1.544790 -1.544790 0.000000 -1.544790 1.544790
-1.544790 0.000000 1.544790 1.544790 0.000000 -1.544790
1.544790 -1.544790 0.000000 -1.544790 1.544790 0.000000

```


CELL MULTIPLIERS (0 1 0)

```

0, 0, 0, 0,
0, 0, 0, 0,
0,16664E 00=0,16664E 00 0,16664E 00 0,
0, 0, 0, 0,
0, 0, 0, 0,
0, 0, 0, 0,
0, 0, 0, 0,
0,11783E 00 0,23566E 00 0,11783E 00 0,
0, 0, 0, 0,
0, 0, 0, 0,
0, 0, 0, 0,
0,11783E 00=0,11783E 00=0,23566E 00 0,
0, 0, 0, 0,
-0,23566E 00=0,11783E 00 0,11783E 00 0,
0,29836E 00 0, -0,29836E 00 0,
0, 0, 0, 0,
-0,29836E 00=0,29836E 00 0,21588E=08 0,
0, 0, 0, 0,
-0,21588E=08 0,29836E 00 0,29836E 00 0,
0, 0, 0, 0,
0, 0, 0, 0,
0, 0, 0, 0,
0, 0, 0, 0,

```

```

0, 0, 1 16 D
0, 0, 2 16 D
0, 0, 3 16 D
0, 0, 4 16 D
0, 0, 5 16 D
0, 0, 6 16 D
0, 0, 7 16 D
0, 0, 8 16 D
0, 0, 9 16 D
0, 0, 10 16 D
0, 0, 11 16 D
0, 0, 12 16 D
0, 0, 13 16 D
0, 0, 14 16 D
0, 0, 15 16 D
0, 0, 16 16 D
0, 0, 17 16 D
0, 0, 18 16 D
0, 0, 19 16 D
0, 0, 20 16 D
0, 0, 21 16 D
0, 0, 22 16 D
0, 0, 23 16 D
0, 0, 24 16 D

```

CELL MULTIPLIERS (0 0 1)

```

0, 0, 0, 0,
0, 0, 0, 0,
0,16664E 00 0,16664E 00=0,16664E 00 0,
0, 0, 0, 0,
0, 0, 0, 0,
0, 0, 0, 0,
0, 0, 0, 0,
0,11783E 00 0,11783E 00 0,23566E 00 0,
0, 0, 0, 0,
0, 0, 0, 0,
0, 0, 0, 0,
0,11783E 00=0,23566E 00=0,11783E 00 0,
-0,23566E 00 0,11783E 00=0,11783E 00 0,
-0,29836E 00 0,29836E 00 0,
0, 0, 0, 0,
0,29836E/00=0,21588E=08 0,29836E 00 0,
0,21588E=08=0,29836E 00=0,29836E 00 0,
0, 0, 0, 0,
0, 0, 0, 0,
0, 0, 0, 0,
0, 0, 0, 0,

```

```

0, 0, 1 16 D
0, 0, 2 16 D
0, 0, 3 16 D
0, 0, 4 16 D
0, 0, 5 16 D
0, 0, 6 16 D
0, 0, 7 16 D
0, 0, 8 16 D
0, 0, 9 16 D
0, 0, 10 16 D
0, 0, 11 16 D
0, 0, 12 16 D
0, 0, 13 16 D
0, 0, 14 16 D
0, 0, 15 16 D
0, 0, 16 16 D
0, 0, 17 16 D
0, 0, 18 16 D
0, 0, 19 16 D
0, 0, 20 16 D
0, 0, 21 16 D
0, 0, 22 16 D
0, 0, 23 16 D
0, 0, 24 16 D

```

CELL MULTIPLIERS (0 1 -1)

0.	0.	0.	0.	0.	0.	1 16 D
0.	0.	0.	0.	0.	0.	2 16 D
0.	0.	0.	0.	0.	0.	3 16 D
0.	0.	0.	0.	0.	0.	4 16 D
0.	0.	0.	0.	0.	0.	5 16 D
0.	0.	0.	0.	0.	0.	6 16 D
0.	0.	0.	0.	0.	0.	7 16 D
0.	0.	0.	0.	0.	0.	8 16 D
0.	0.	0.	0.	0.	0.	9 16 D
0.	0.	0.	0.	0.	0.	10 16 D
0.	0.	0.	0.	0.	0.	11 16 D
0.	0.	0.	0.	0.	0.	12 16 D
0.	0.	0.	0.	0.	0.	13 16 D
0.	0.	0.	0.	0.	0.	14 16 D
0.	0.	0.	0.	0.	0.	15 16 D
0.	0.	0.	0.	0.	0.	16 16 D
0.	0.	0.	0.	0.	0.	17 16 D
0.	0.	0.	0.	0.	0.	18 16 D
0.	0.	0.	0.	0.	0.	19 16 D
0.	0.	0.	0.	0.	0.	20 16 D
0.	0.	0.	0.	0.	0.	21 16 D
0.	0.	0.	0.	0.	0.	22 16 D
0.	0.	0.	0.	0.	0.	23 16 D
0.	0.	0.	0.	0.	0.	24 16 D

CELL MULTIPLIERS (-1 1 0)

0.	0.	0.	0.	0.	0.	1 16 D
0.	0.	0.	0.	0.	0.	2 16 D
0.	0.	0.	0.	0.	0.	3 16 D
0.	0.	0.	0.	0.	0.	4 16 D
0.	0.	0.	0.	0.	0.	5 16 D
0.	0.	0.	0.	0.	0.	6 16 D
0.	0.	0.	0.	0.	0.	7 16 D
0.	0.	0.	0.	0.	0.	8 16 D
0.	0.	0.	0.	0.	0.	9 16 D
0.	0.	0.	0.	0.	0.	10 16 D
0.	0.	0.	0.	0.	0.	11 16 D
0.	0.	0.	0.	0.	0.	12 16 D
0.	0.	0.	0.	0.	0.	13 16 D
0.	0.	0.	0.	0.	0.	14 16 D
0.	0.	0.	0.	0.	0.	15 16 D
0.	0.	0.	0.	0.	0.	16 16 D
0.	0.	0.	0.	0.	0.	17 16 D
0.	0.	0.	0.	0.	0.	18 16 D
0.	0.	0.	0.	0.	0.	19 16 D
0.	0.	0.	0.	0.	0.	20 16 D
0.	0.	0.	0.	0.	0.	21 16 D
0.	0.	0.	0.	0.	0.	22 16 D
0.	0.	0.	0.	0.	0.	23 16 D
0.	0.	0.	0.	0.	0.	24 16 D

CELL MULTIPLIERS (=1 0 1)

```
0, 0, 0, 0, 0, 0, 1 16 D
0, 0, 0, 0, 0, 0, 2 16 D
0, 0, 0, 0, 0, 0, 3 16 D
0, 0, 0, 0, 0, 0, 4 16 D
0, 0, 0, 0, 0, 0, 5 16 D
0, 0, 0, 0, 0, 0, 6 16 D
0, 0, 0, 0, 0, 0, 7 16 D
0, 0, 0, 0, 0, 0, 8 16 D
0, 0, 0, 0, 0, 0, 9 16 D
0, 0, 0, 0, 0, 0, 10 16 D
0, 0, 0, 0, 0, 0, 11 16 D
0, 0, 0, 0, 0, 0, 12 16 D
0, 0, 0, 0, 0, 0, 13 16 D
0, 0, 0, 0, 0, 0, 14 16 D
0, 0, 0, 0, 0, 0, 15 16 D
0, 0, 0, 0, 0, 0, 16 16 D
0, 0, 0, 0, 0, 0, 17 16 D
0, 0, 0, 0, 0, 0, 18 16 D
0, 0, 0, 0, 0, 0, 19 16 D
0, 0, 0, 0, 0, 0, 20 16 D
0, 0, 0, 0, 0, 0, 21 16 D
0, 0, 0, 0, 0, 0, 22 16 D
0, 0, 0, 0, 0, 0, 23 16 D
0, 0, 0, 0, 0, 0, 24 16 D
-0,16664E 00-0,16664E 00-0,16664E 00 0,16664E 00 0,16664E 00 0,16664E 00 1 16 D
0, 0, 0, 0, 0, 0, 0,16664E 00-0,16664E 00-0,16664E 00 2 16 D
0, 0, 0, 0, 0, 0, -0,16664E 00 0,16664E 00-0,16664E 00 3 16 D
0, 0, 0, 0, 0, 0, -0,16664E 00-0,16664E 00 0,16664E 00 4 16 D
0,47133E 00 0,21504E-08 0,21504E-08-0,23566E 00 0,11783E 00 0,11783E 00 5 16 D
0,21504E-08 0,47133E 00 0,21504E-08 0,11783E 00-0,23566E 00 0,11783E 00 6 16 D
0,21504E-08 0,21504E-08 0,47133E 00 0,11783E 00 0,11783E 00-0,23566E 00 7 16 D
0,23566E 00-0,11783E 00-0,11783E 00-0,47133E 00-0,21504E-08-0,21504E-08 8 16 D
-0,11783E 00 0,23566E 00-0,11783E 00-0,21504E-08-0,47133E 00-0,21504E-08 9 16 D
-0,11783E 00-0,11783E 00 0,23566E 00-0,21504E-08-0,21504E-08-0,47133E 0010 16 D
0,21504E-08 0,21504E-08-0,47133E 00 0, 0, 0, 11 16 D
0,21504E-08-0,47133E 00 0,21504E-08 0, 0, 0, 12 16 D
-0,47133E 00 0,21504E-08 0,21504E-08 0, 0, 0, 13 16 D
0, 0, 0, 0, -0,21504E-08-0,21504E-08 0,47133E 0014 16 D
0, 0, 0, 0, -0,21504E-08 0,47133E 00-0,21504E-0815 16 D
0, 0, 0, 0, 0,47133E 00-0,21504E-08-0,21504E-0816 16 D
0, 0, 0, 0, 0, 0, 0, 17 16 D
-0, 0, 0, 0, 0, 0, 0, 18 16 D
0, 0, 0,29836E 00-0,29836E 00-0,29836E 00-0,27312E-05 0,27312E-0519 16 D
-0,29836E 00 0,29836E 00 0,29836E 00 0,27312E-05-0,27312E-0520 16 D
0,29836E 00-0,29836E 00 0, -0,27525E-05 0,27525E-05-0, 21 16 D
-0,55050E-06-0,49545E-05 0,44040E-05-0,10794E-08 0,29836E 00-0,29836E 0022 16 D
0,49545E-05 0,55050E-06-0,44040E-05-0,29836E 00 0,10794E-08 0,29836E 0023 16 D
-0,48423E-05 0,43043E-05-0,53803E-06 0,29836E 00-0,29836E 00-0,10794E-0824 16 D
0, 0, 0, 0, 0, 0, 1 16 D
0, 0, 0, 0, 0, 0, 2 16 D
0, 0, 0, 0, 0, 0, 3 16 D
0, 0, 0, 0, 0, 0, 4 16 D
0, 0, 0, 0, 0, 0, 5 16 D
0, 0, 0, 0, 0, 0, 6 16 D
0, 0, 0, 0, 0, 0, 7 16 D
0, 0, 0, 0, 0, 0, 8 16 D
0, 0, 0, 0, 0, 0, 9 16 D
0, 0, 0, 0, 0, 0, 10 16 D
```

0.	0.	0.	0.	0.11783E 00	0.11783E 00	0.23566E 00	11	16	D
0.	0.	0.	0.	0.11783E 00	0.23566E 00	0.11783E 00	12	16	D
0.	0.	0.	0.	0.	0.	0.	13	16	D
0.	0.	0.	0.	0.	0.	0.	14	16	D
0.	0.	0.	0.	0.	0.	0.	15	16	D
0.	0.	0.	0.	0.	0.	0.	16	16	D
0.	0.	0.	0.	0.	0.	0.	17	16	D
0.	0.	0.	0.	0.	0.29836E 00	0.29836E 00	18	16	D
0.	0.	0.	0.	0.	0.	0.	19	16	D
0.	0.	0.	0.	0.	0.	0.	20	16	D
0.	0.	0.	0.	0.	0.	0.	21	16	D
0.	0.	0.	0.	0.	0.	0.	22	16	D
0.	0.	0.	0.	0.29836E 00	0.29836E 00	0.32382E 00	23	16	D
0.	0.	0.	0.	0.29836E 00	0.32382E 00	0.29836E 00	24	16	D
0.	0.	0.	0.	0.	0.	0.	1	16	D
0.	0.	0.	0.	0.	0.	0.	2	16	D
0.	0.	0.	0.	0.	0.	0.	3	16	D
0.	0.	0.	0.	0.	0.	0.	4	16	D
0.	0.	0.	0.	0.	0.	0.	5	16	D
0.	0.	0.	0.	0.11783E 00	0.23566E 00	0.11783E 00	6	16	D
0.	0.	0.	0.	0.	0.	0.	7	16	D
0.	0.	0.	0.	0.	0.	0.	8	16	D
0.	0.	0.	0.	0.	0.	0.	9	16	D
0.	0.	0.	0.	0.	0.	0.	10	16	D
0.	0.	0.	0.	0.11783E 00	0.11783E 00	0.23566E 00	11	16	D
0.	0.	0.	0.	0.	0.	0.	12	16	D
0.	0.	0.	0.	0.23566E 00	0.11783E 00	0.11783E 00	13	16	D
0.	0.	0.	0.	0.	0.	0.	14	16	D
0.	0.	0.	0.	0.	0.	0.	15	16	D
0.	0.	0.	0.	0.	0.	0.	16	16	D
0.	0.	0.	0.	0.	0.	0.	17	16	D
0.	0.	0.	0.	0.29836E 00	0.	0.29836E 00	18	16	D
0.	0.	0.	0.	0.	0.	0.	19	16	D
0.	0.	0.	0.	0.	0.	0.	20	16	D
0.	0.	0.	0.	0.	0.	0.	21	16	D
0.	0.	0.	0.	0.29836E 00	0.29836E 00	0.32382E 00	22	16	D
0.	0.	0.	0.	0.	0.	0.	23	16	D
0.	0.	0.	0.	0.43177E 00	0.29836E 00	0.29836E 00	24	16	D
0.	0.	0.	0.	0.	0.	0.	1	16	D
0.	0.	0.	0.	0.	0.	0.	2	16	D
0.	0.	0.	0.	0.	0.	0.	3	16	D
0.	0.	0.	0.	0.	0.	0.	4	16	D
0.	0.	0.	0.	0.	0.	0.	5	16	D
0.	0.	0.	0.	0.	0.	0.	6	16	D
0.	0.	0.	0.	0.11783E 00	0.11783E 00	0.23566E 00	7	16	D
0.	0.	0.	0.	0.	0.	0.	8	16	D
0.	0.	0.	0.	0.	0.	0.	9	16	D
0.	0.	0.	0.	0.	0.	0.	10	16	D
0.	0.	0.	0.	0.	0.	0.	11	16	D
0.	0.	0.	0.	0.11783E 00	0.23566E 00	0.11783E 00	12	16	D
0.	0.	0.	0.	0.23566E 00	0.11783E 00	0.11783E 00	13	16	D
0.	0.	0.	0.	0.	0.	0.	14	16	D
0.	0.	0.	0.	0.	0.	0.	15	16	D
0.	0.	0.	0.	0.	0.	0.	16	16	D
0.	0.	0.	0.	0.	0.	0.	17	16	D
0.	0.	0.	0.	0.29836E 00	0.29836E 00	0.	18	16	D
0.	0.	0.	0.	0.	0.	0.	19	16	D
0.	0.	0.	0.	0.	0.	0.	20	16	D
0.	0.	0.	0.	0.	0.	0.	21	16	D
0.	0.	0.	0.	0.29836E 00	0.43177E 00	0.29836E 00	22	16	D
0.	0.	0.	0.	0.43177E 00	0.29836E 00	0.29836E 00	23	16	D
0.	0.	0.	0.	0.	0.	0.	24	16	D
0.	0.	0.	0.	0.	0.	0.	1	16	D
0.	0.	0.	0.	0.	0.	0.	2	16	D
0.	0.	0.	0.	0.	0.	0.	3	16	D
0.	0.	0.	0.	0.	0.	0.	4	16	D

APPENDIX B

Propane as a Test Example

1. The input for the propane problem

0000000001	1111111112	2222222223	3333333334	4444444445	5555555556	6666666667	7777777778
1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890
D. NATRIX FOR PROPANE							
30	1	11	3				
4	3	4					
1.0081	2.1617		-0.22298	1.0081	1.29124	0.88096	-1.49207
1.0081	1.29124	-0.88096	-1.49207	1.2.0039	1.26810	-0.848914	
1.0081		0.87588	0.65883	1.0081		-0.87588	0.65883
1.2.0039				1.0081	-2.16170		-0.22298
1.0081	-1.29124	0.88096	-1.49207	1.0081	-1.29124	-0.88096	-1.49207
1.2.0039	-1.26810		-0.848914				
1	3	4					
5	6	7					
8	9	10	11				
1	1	1	4				
2	1	2	4				
3	1	3	4				
4	2	1	4	2	1.091		
5	2	2	4	3	1.091		
6	2	1	4	3	1.091		
7	1	5	7				
8	1	6	7				
9	2	5	7	6	1.096		
10	1	8	11				
11	1	9	11				
12	1	10	11				
13	2	8	11	9	1.091		
14	2	9	11	10	1.091		
15	2	8	11	10	1.091		
16	2	1	4	7	1.091		
17	2	2	4	7	1.091		
18	2	3	4	7	1.091		
19	2	8	11	7	1.091		
20	2	9	11	7	1.091		
21	2	10	11	7	1.091		
22	2	5	7	11	1.096		
23	2	6	7	11	1.096		
0000000001	1111111112	2222222223	3333333334	4444444445	5555555556	6666666667	7777777778
1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	1234567890

28

2. The program output

```

      D MATRIX FOR PROPANE
MI      J      H      JJ      JCH      MN      LL
30      1      11      3      0      0      0

      ATOMS IN GROUP NUMBER 1 = 4
      ATOMS IN GROUP NUMBER 2 = 3
      ATOMS IN GROUP NUMBER 3 = 4

NU      MASS(NU)      X(NU)      Y(NU)      Z(NU)
1      1.00810      -2.16170      0.00000      =0.22298
2      1.00810      1.29124      0.88096      =1.49207
3      1.00810      1.29124      =0.88096      =1.49207
4      12.00390      1.26810      0.00000      =0.84891
5      1.00810      0.00000      0.87588      0.65883
6      1.00810      0.00000      =0.87588      0.65883
7      12.00390      0.00000      0.00000      0.00000
8      1.00810      =2.16170      0.00000      =0.22298
9      1.00810      =1.29124      0.88096      =1.49207
10     1.00810      =1.29124      =0.88096      =1.49207
11     12.00390      =1.26810      0.00000      =0.84891

      UNCORRECTED CENTER OF MASS
XBAR = =0.000000      YBAR = 0.000000      ZBAR = =0.578957

      CORRECTED COORDINATES OF ATOM NU
NU      X      Y      Z
1      2.16170      =0.00000      0.35598
2      1.29124      0.88096      =0.91311
3      1.29124      =0.88096      =0.91311
4      1.26810      =0.00000      =0.26996
5      0.00000      0.87588      1.23779
6      0.00000      =0.87588      1.23779
7      0.00000      =0.00000      0.57896
8      =2.16170      =0.00000      0.35598
9      =1.29124      0.88096      =0.91311
10     =1.29124      =0.88096      =0.91311
11     =1.26810      =0.00000      =0.26996

```

GERMAN SCRIPT B MATRIX

```

0,000000 -0,357416 -0,000000 0,000000 0,916803 0,884521 0,000000 0,916803 -0,884521 0,000000 0,935309 -0,000000
0,000000 -1,242790 0,879420 0,000000 -1,242790 -0,879420 0,000000 -2,005893 -0,000000 0,000000 -0,357416 -0,000000
0,000000 0,916803 0,884521 0,000000 0,916803 -0,884521 0,000000 0,935309 -0,000000
0,357416 0,000000 -2,170437 -0,916803 0,000000 -1,296459 -0,916803 0,000000 -1,296459 -0,935309 0,000000 -4,393541
1,242790 0,000000 -0,000000 1,242790 0,000000 -0,000000 2,005893 0,000000 -0,000000 0,357416 0,000000 2,170437
-0,916803 0,000000 1,296459 -0,916803 0,000000 1,296459 -0,935309 0,000000 4,393541
0,000000 2,170437 0,000000 -0,884521 1,296459 0,000000 0,884521 1,296459 0,000000 0,000000 4,393541 0,000000
-0,879420 0,000000 0,000000 0,879420 0,000000 0,000000 0,000000 0,000000 0,000000 0,000000 -2,170437 0,000000
-0,884521 -1,296459 0,000000 0,884521 -1,296459 0,000000 0,000000 -4,393541 0,000000

```

```

GROUP NUMBER      N1  N2  N3  N4  N5

```

```

1                1  2  3  4  0

```

```

XBAR(I)          YBAR(I)          ZBAR(I)

```

```

1,331148 -0,000000 -0,314255

```

```

GROUP NUMBER      N1  N2  N3  N4  N5

```

```

2                5  6  7  0  0

```

```

XBAR(I)          YBAR(I)          ZBAR(I)

```

```

0,000000 -0,000000 0,673702

```

```

GROUP NUMBER      N1  N2  N3  N4  N5

```

```

3                8  9 10 11  0

```

```

XBAR(I)          YBAR(I)          ZBAR(I)

```

```

-1,331148 -0,000000 0,314255

```

B SUB J MATRIX

```

0,000000 -0,672941 0,000000 0,000000 0,601278 0,884521 0,000000 0,601278 -0,884521 0,000000 0,153480 0,000000
0,000000 -0,566365 0,879420 0,000000 -0,566365 -0,879420 0,000000 0,328259 0,000000 0,000000 -0,672941 0,000000
0,000000 0,601278 0,884521 0,000000 0,601278 -0,884521 0,000000 -0,153480 0,000000
0,672941 0,000000 -0,833909 -0,601278 0,000000 0,040069 -0,601278 0,000000 0,040069 0,153480 0,000000 0,218439
0,566365 0,000000 -0,000000 0,566365 0,000000 -0,000000 -0,328259 0,000000 -0,000000 0,672941 0,000000 0,833909
-0,601278 0,000000 -0,040069 -0,601278 0,000000 -0,040069 0,153480 0,000000 -0,218439
-0,000000 0,833909 0,000000 -0,884521 -0,040069 0,000000 0,884521 -0,040069 0,000000 -0,000000 -0,218439 0,000000
-0,879420 0,000000 0,000000 0,879420 0,000000 0,000000 -0,000000 0,000000 0,000000 -0,000000 -0,833909 0,000000
-0,884521 0,040069 0,000000 0,884521 0,040069 0,000000 -0,000000 0,218439 0,000000

```

I	ITYPE	I1	N1	I2	N2	I3	N3	I4	N4	I5	N5	I6	N6	RO	OMEGAX	OMEGAY	OMEGAZ	NTOR
1	1	-0	1	-0	4	-0	-0	-0	-0	-0	-0	-0	-0	-0	0.00000	0.00000	0.00000	-0
2	1	-0	2	-0	4	-0	-0	-0	-0	-0	-0	-0	-0	-0	0.00000	0.00000	0.00000	-0
3	1	-0	3	-0	4	-0	-0	-0	-0	-0	-0	-0	-0	-0	0.00000	0.00000	0.00000	-0
4	2	-0	1	-0	4	-0	2	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
5	2	-0	2	-0	4	-0	3	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
6	2	-0	1	-0	4	-0	3	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
7	1	-0	5	-0	7	-0	-0	-0	-0	-0	-0	-0	-0	-0	0.00000	0.00000	0.00000	-0
8	1	-0	6	-0	7	-0	-0	-0	-0	-0	-0	-0	-0	-0	0.00000	0.00000	0.00000	-0
9	2	-0	5	-0	7	-0	-0	-0	-0	-0	-0	-0	-0	-0	1.09600	0.00000	0.00000	-0
10	1	-0	8	-0	11	-0	-0	-0	-0	-0	-0	-0	-0	-0	0.00000	0.00000	0.00000	-0
11	1	-0	9	-0	11	-0	-0	-0	-0	-0	-0	-0	-0	-0	0.00000	0.00000	0.00000	-0
12	1	-0	10	-0	11	-0	-0	-0	-0	-0	-0	-0	-0	-0	0.00000	0.00000	0.00000	-0
13	2	-0	8	-0	11	-0	9	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
14	2	-0	9	-0	11	-0	10	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
15	2	-0	8	-0	11	-0	10	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
16	2	-0	1	-0	4	-0	7	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
17	2	-0	2	-0	4	-0	7	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
18	2	-0	3	-0	4	-0	7	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
19	2	-0	8	-0	11	-0	7	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
20	2	-0	9	-0	11	-0	7	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
21	2	-0	10	-0	11	-0	7	-0	-0	-0	-0	-0	-0	-0	1.09100	0.00000	0.00000	-0
22	2	-0	5	-0	7	-0	11	-0	-0	-0	-0	-0	-0	-0	1.09600	0.00000	0.00000	-0
23	2	-0	6	-0	7	-0	11	-0	-0	-0	-0	-0	-0	-0	1.09600	0.00000	0.00000	-0
24	2	-0	5	-0	7	-0	4	-0	-0	-0	-0	-0	-0	-0	1.09600	0.00000	0.00000	-0
25	2	-0	6	-0	7	-0	4	-0	-0	-0	-0	-0	-0	-0	1.09600	0.00000	0.00000	-0
26	2	-0	4	-0	7	-0	11	-0	-0	-0	-0	-0	-0	-0	1.52600	0.00000	0.00000	-0
27	1	-0	7	-0	11	-0	-0	-0	-0	-0	-0	-0	-0	-0	0.00000	0.00000	0.00000	-0
28	1	-0	4	-0	7	-0	-0	-0	-0	-0	-0	-0	-0	-0	0.00000	0.00000	0.00000	-0
29	3	-0	1	-0	2	-0	3	-0	4	-0	-0	-0	-0	-0	0.00000	0.83100	0.00000	55630
30	3	-0	8	-0	9	-0	10	-0	11	-0	-0	-0	-0	-0	0.00000	0.83100	0.00000	55630
															0.81576E 00	0.	0.	1 16 D
															0.	0.	0.	1 76 D
															0.	0.	0.	1136 D
															0.	0.	0.	1196 D
															0.	0.	0.	1256 D
															0.	0.	0.	1313 D
															0.	0.	0.	2 16 D
															0.	0.	0.	2 76 D
															0.	0.	0.	2136 D
															0.	0.	0.	2196 D
															0.	0.	0.	2256 D
															0.	0.	0.	2313 D
															0.	0.	0.	3 16 D
															0.	0.	0.	3 76 D
															0.	0.	0.	3136 D
															0.	0.	0.	3196 D
															0.	0.	0.	3256 D
															0.	0.	0.	3313 D
															0.	0.	0.	4 16 D
															0.	0.	0.	4 76 D
															0.	0.	0.	4136 D
															0.	0.	0.	4196 D
															0.	0.	0.	4256 D
															0.	0.	0.	4313 D
															0.	0.	0.	5 16 D
															0.	0.	0.	5 76 D
															0.	0.	0.	5136 D
															0.	0.	0.	5196 D
															0.	0.	0.	5256 D
															0.	0.	0.	5313 D

```

-0,29864E 00 0,84911E 00 0,42634E 00 0, 0, 0, 6 16 D
-0,86849E 00 0,27243E 00-0,40441E 00 0,33822E 00-0,32502E 00-0,63556E-02 6 76 D
0, 0, 0, 0, 0, 0, 6136 D
0, 0, 0, 0, 0, 0, 6196 D
0, 0, 0, 0, 0, 0, 6256 D
0, 0, 0, 0, 0, 0, 6313 D
0, 0, 0, 0, 0, 0, 7 16 D
0, 0, 0, 0, 0, 0, 7 76 D
0, 0, 0, 0, 0, 0, 7136 D
0, 0, 0, 0, 0, 0, 7196 D
-0, 0, 0, 0, 0, 0, 7256 D
0, 0, 0, 0, 0, 0, 7313 D
0, 0, 0, 0, 0, 0, 8 16 D
0, 0, 0, 0, 0, 0, 8 76 D
0, 0, 0, 0, 0, 0, 8136 D
-0, 0, 0, 0, 0, 0, 8196 D
0, 0, 0, 0, 0, 0, 8256 D
0, 0, 0, 0, 0, 0, 8313 D
0, 0, 0, 0, 0, 0, 9 16 D
0, 0, 0, 0, 0, 0, 9 76 D
-0, 0, 0, 0, 0, 0, 9136 D
0, 0, 0, 0, 0, 0, 9196 D
0, 0, 0, 0, 0, 0, 9256 D
0, 0, 0, 0, 0, 0, 9313 D
0, 0, 0, 0, 0, 0, 10 16 D
0, 0, 0, 0, 0, 0, 10 76 D
0, 0, 0, 0, 0, 0, 10136 D
0, 0, 0, 0, 0, 0, 10196 D
0, 0, 0, 0, 0, 0, 10256 D
0, 0, 0, 0, 0, 0, 10313 D
0, 0, 0, 0, 0, 0, 11 16 D
0, 0, 0, 0, 0, 0, 11 76 D
0, 0, 0, 0, 0, 0, 11136 D
0, 0, 0, 0, 0, 0, 11196 D
-0, 0, 0, 0, 0, 0, 11256 D
0, 0, 0, 0, 0, 0, 11313 D
0, 0, 0, 0, 0, 0, 12 16 D
0, 0, 0, 0, 0, 0, 12 76 D
0, 0, 0, 0, 0, 0, 12136 D
0, 0, 0, 0, 0, 0, 12196 D
0, 0, 0, 0, 0, 0, 12256 D
0, 0, 0, 0, 0, 0, 12313 D
0, 0, 0, 0, 0, 0, 13 16 D
0, 0, 0, 0, 0, 0, 13 76 D
0, 0, 0, 0, 0, 0, 13136 D
0, 0, 0, 0, 0, 0, 13196 D
0, 0, 0, 0, 0, 0, 13256 D
-0, 0, 0, 0, 0, 0, 13313 D
0, 0, 0, 0, 0, 0, 14 16 D
0, 0, 0, 0, 0, 0, 14 76 D
0, 0, 0, 0, 0, 0, 14136 D
0, 0, 0, 0, 0, 0, 14196 D
0, 0, 0, 0, 0, 0, 14256 D
-0, 0, 0, 0, 0, 0, 14313 D
0, 0, 0, 0, 0, 0, 15 16 D
0, 0, 0, 0, 0, 0, 15 76 D
0, 0, 0, 0, 0, 0, 15136 D
0, 0, 0, 0, 0, 0, 15196 D
0, 0, 0, 0, 0, 0, 15256 D
-0, 0, 0, 0, 0, 0, 15313 D

```

```

0,57140E 00=0,      -0,81575E 00 0,      0,      0,      16 16 D
0,      0,      0,      -0,50798E=01 0,      0,40787E 0016 76 D
0,      0,      0,      0,      0,      0,      16136 D
-0,11479E 00 0,      -0,17147E 00 0,      0,      0,      16196 D
0,      0,      0,      0,      0,      0,      16256 D
0,      0,      0,      0,      0,      0,      16313 D
0,      0,      0,      0,87420E 00=0,29616E 00=0,37421E 0017 16 D
0,      0,      0,      -0,31182E 00 0,26339E 00 0,21085E=0117 76 D
0,      0,      0,      0,      0,      0,      17136 D
0,58482E=01=0,17756E 00 0,87359E=01 0,      0,      17196 D
0,      0,      0,      0,      0,      0,      17256 D
0,      0,      0,      0,      0,      0,      17313 D
0,      0,      0,      0,      0,      0,      18 16 D
0,87420E 00 0,29616E 00=0,37421E 00=0,31182E 00=0,26339E 00 0,21085E=0118 76 D
0,      0,      0,      0,      0,      0,      18136 D
0,58482E=01 0,17756E 00 0,87359E=01 0,      0,      18196 D
0,      0,      0,      0,      0,      0,      -18256 D
0,      0,      0,      0,      0,      0,      18313 D
0,      0,      0,      0,      0,      0,      19 16 D
0,      0,      0,      0,      0,      0,      19 76 D
0,      0,      0,      0,      0,      0,      19136 D
0,11479E 00 0,      -0,17147E 00=0,57140E 00=0,      -0,81575E 0019196 D
0,      0,      0,      0,      0,      0,      19256 D
0,50798E=01 0,      0,40787E 00 0,      0,      0,      19313 D
0,      0,      0,      0,      0,      0,      20 16 D
0,      0,      0,      0,      0,      0,      20 76 D
0,      0,      0,      0,      0,      0,      20136 D
-0,58482E=01=0,17756E 00 0,87359E=01 0,      0,      20196 D
-0,87420E 00=0,29616E 00=0,37421E 00 0,      0,      20256 D
0,31182E 00 0,26339E 00 0,21085E=01 0,      0,      20313 D
0,      0,      0,      0,      0,      0,      21 16 D
0,      0,      0,      0,      0,      0,      21 76 D
0,      0,      0,      0,      0,      0,      21136 D
-0,58482E=01 0,17756E 00 0,87359E=01 0,      0,      21196 D
0,      0,      0,      0,      0,      0,      21256 D
0,31182E 00=0,26339E 00 0,21085E=01 0,      0,      21313 D
0,      0,      0,      0,      0,      0,      22 16 D
0,      0,      0,      0,      0,      0,      22 76 D
0,87819E 00=0,28242E 00 0,37546E 00 0,      0,      22136 D
-0,31562E 00 0,25763E 00=0,17503E=01 0,      0,      22196 D
0,      0,      0,      0,      0,      0,      22256 D
0,61122E=01=0,17578E 00=0,91304E=01 0,      0,      22313 D
0,      0,      0,      0,      0,      0,      23 16 D
0,      0,      0,      0,      0,      0,      23 76 D
-0,31562E 00=0,25763E 00=0,17503E=01 0,      0,      23136 D
0,      0,      0,      0,      0,      0,      23196 D
0,      0,      0,      0,      0,      0,      23256 D
0,61122E=01 0,17578E 00=0,91304E=01 0,      0,      23313 D
0,      0,      0,      0,      0,      0,      24 16 D
0,      0,      0,      0,      0,      0,      24 76 D
-0,87819E 00=0,28242E 00 0,37546E 00 0,      0,      24136 D
0,31562E 00 0,25763E 00=0,17503E=01 0,      0,      24196 D
0,      0,      0,      0,      0,      0,      24256 D
0,      0,      0,      0,      0,      0,      24313 D
0,      0,      0,      0,      0,      0,      25 16 D
0,      0,      0,      0,      0,      0,      25 76 D
-0,61122E=01 0,17578E 00=0,91304E=0125 76 D
0,87819E 00 0,28242E 00 0,37546E 0025136 D
0,31562E 00=0,25763E 00=0,17503E=01 0,      0,      25196 D
0,      0,      0,      0,      0,      0,      25256 D
0,      0,      0,      0,      0,      0,      25313 D

```

0,	0,	0,	0,	0,	0,	26 16	D
0,	0,	0,	0,16056E 00	0,	0,23984E 00	26 76	D
0,	0,	0,	0,	0,	0,	26136	D
-0,	0,	-0,47969E 00	0,	0,	0,	26196	D
0,	0,	0,	0,	0,	0,	26256	D
-0,16056E 00	0,	0,23984E 00	0,	0,	0,	26313	D
0,	0,	0,	0,	0,	0,	27 16	D
0,	0,	0,	0,	0,	0,	27 76	D
0,	0,	0,	0,	0,	0,	27136	D
0,23985E 00	0,	0,16056E 00	0,	0,	0,	27196	D
0,	0,	0,	0,	0,	0,	27256	D
-0,23985E 00	0,	0,16056E 00	0,	0,	0,	27313	D
0,	0,	0,	0,	0,	0,	28 16	D
0,	0,	0,23985E 00	0,	-0,16056E 00	28 76	D	D
0,	0,	0,	0,	0,	0,	28136	D
-0,23985E 00	0,	0,16056E 00	0,	0,	0,	28196	D
0,	0,	0,	0,	0,	0,	28256	D
0,	0,	0,	0,	0,	0,	28313	D
0,	0,	0,	0,50866E 00	0,53956E 00	0,75984E 00	29 16	D
-0,50866E 00	0,53956E 00	0,75984E 00	0,	-0,22942E-01	0,	29 76	D
0,	0,	0,	0,	0,	0,	29136	D
0,	0,	0,	0,	0,	0,	29196	D
0,	0,	0,	0,	0,	0,	29256	D
0,	0,	0,	0,	0,	0,	29313	D
0,	0,	0,	0,	0,	0,	30 16	D
0,	0,	0,	0,	0,	0,	30 76	D
0,	0,	0,	0,	0,	0,	30136	D
0,	0,	0,	0,	0,	0,	30196	D
0,51976E 00	0,50424E 00	0,77641E 00	0,51976E 00	-0,16650E 01	0,77641E 00	30256	D
-0,	-0,22240E-01	0,	0,	0,	0,	30313	D

A Test Example With a Dihedral Torsional Coordinate

0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 5 5 5 5 5 5 5 5 5 6 6 6 6 6 6 6 6 6 7 7 7 7 7 7 7 7 7 8 8 8 8 8 8 8 8 8 9 9 9 9 9 9 9 9 9 0									
1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0									
A. PROBLEM WITH A. DINE DRAL. TORSIONAL. COORDINATE.									
6 1 4 1									
4 1.0 -0.866 -0.500 1.0 0.433 -0.750 1.5									
1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0									
1 4 1 2 3 4 1 0 0.433 -0.750 1.5									
2 1 1 2 3 4 1 0 0.433 -0.750 1.5									
3 1 1 2 3 4 1 0 0.433 -0.750 1.5									
4 1 1 2 3 4 1 0 0.433 -0.750 1.5									
5 1 1 2 3 4 1 0 0.433 -0.750 1.5									
6 2 2 3 4 1 0 0.433 -0.750 1.5									

2. The program output

```

A  PROBLEM WITH A  DIHEDRAL  TORSIONAL  COORDINATE
M1      J      H      JJ      JCM      MN      LL
6        1        4        1        0        0        0

  ATOMS IN GROUP NUMBER 1 : 4
  NU      MASS(NU)      X(NU)      Y(NU)      Z(NU)
  1        1,00000      0,00000      -0,86600      -0,50000
  2        1,00000      0,00000      -0,00000      0,00000
  3        1,00000      0,00000      0,00000      1,00000
  4        1,00000      0,43300      -0,75000      1,50000

  UNCORRECTED CENTER OF MASS
  XBAR = 0,108250      YBAR = -0,404000      ZBAR = 0,500000

  CORRECTED COORDINATES OF ATOM NU
  NU      X      Y      Z
  1      -0,10825      -0,46200      -1,00000
  2      -0,10825      0,40400      -0,50000
  3      -0,10825      0,40400      0,50000
  4      0,32475      -0,34600      1,00000

  GERMAN SCRIPT B MATRIX

  0,000000  1,000000  -0,462000  0,000000  0,500000  0,404000  0,000000  -0,500000  0,404000  0,000000  -1,000000  -0,346000
 -1,000000  0,000000  0,108250  -0,500000  0,000000  0,108250  0,500000  0,000000  0,108250  1,000000  0,000000  -0,324750
  0,462000  -0,108250  0,000000  -0,404000  -0,108250  0,000000  -0,404000  -0,108250  0,000000  0,346000  0,324750  0,000000

```


I	ITYPE	I1	N1	I2	N2	I3	N3	I4	N4	I5	N5	I6	N6	R0	OMEGAX	OMEGAY	OMEGAZ	NTOR
1	4	-0	1	-0	2	-0	3	-0	4	-0	-0	-0	-0	1.00000	-0.00000	-0.00000	-0.00000	-0
2	1	-0	1	-0	2	-0	-0	-0	-0	-0	-0	-0	-0	-0.00000	-0.00000	-0.00000	-0.00000	-0
3	1	-0	2	-0	3	-0	-0	-0	-0	-0	-0	-0	-0	-0.00000	-0.00000	-0.00000	-0.00000	-0
4	1	-0	3	-0	4	-0	-0	-0	-0	-0	-0	-0	-0	-0.00000	-0.00000	-0.00000	-0.00000	-0
5	2	-0	1	-0	2	-0	3	-0	-0	-0	-0	-0	-0	1.00000	-0.00000	-0.00000	-0.00000	-0
6	2	-0	2	-0	3	-0	4	-0	-0	-0	-0	-0	-0	1.00000	-0.00000	-0.00000	-0.00000	-0
-0.11547E	01	-0.												0.22321E	01	0.28867E	00	-0.
-0.20774E	01	-0.	0.86601E	00	0.									0.10000E	01	0.57734E	00	-0.
-0.		-0.	0.86602E	00	-0.50001E	00	0.							0.86602E	00	0.50001E	00	2.16 D
0.		0.		0.	0.		0.							0.		0.		1.76 D
0.		0.		0.	0.		0.							0.		0.		2.76 D
0.		-0.		0.	0.10000E	01	0.							-0.10000E	01	3.16 D		3.76 D
0.		0.		0.	0.		0.							0.		0.		4.16 D
-0.43300E	00	0.75000E	00	-0.50000E	00	0.43300E	00	-0.75000E	00	0.50000E	00	0.43300E	00	0.75000E	00	0.50000E	00	4.76 D
0.		0.50002E	00	-0.86604E	00	-0.								-0.15000E	01	0.86604E	00	5.16 D
-0.		0.10000E	01	-0.										0.		0.		5.76 D
0.		0.		0.										-0.49999E	00	0.86603E	00	6.16 D
0.74999E	00	-0.12991E	01	-0.86603E	00	-0.25000E	00	0.43302E	00	0.86603E	00	0.43302E	00	0.86603E	00	0.86603E	00	6.76 D

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

APPENDIX D

A Test Example With a Coordinate Which is the Change in the

Angle Between a Bond and a Plane Defined by Two Bonds

1. The input to the program

[illegible]

2. The program output

A COORDINATE WHICH IS THE ANGLE BETWEEN A BOND AND A PLANE DEFINED BY TWO BONDS

MJ	J	M	JJ	JM	MN	LL
6	1	4	1	0	0	0

ATOMS IN GROUP NUMBER 1 = 4

NU	MASS(NU)	X(NU)	Y(NU)	Z(NU)
1	1.00800	0.00000	0.93530	0.54000
2	12.01100	0.00000	0.00000	-1.39000
3	12.01100	0.00000	-1.20370	0.69500
4	12.01100	0.00000	0.00000	0.00000

UNCORRECTED CENTER OF MASS

XBAR = 0.000000 YBAR = -0.364862 ZBAR = -0.210667

NU	X	Y	Z
1	-0.00000	1.30016	0.75067
2	-0.00000	0.36486	-1.17033
3	-0.00000	-0.83884	0.90967
4	-0.00000	0.36486	0.21067

GERMAN SCRIPT B MATRIX

0.000000	-0.753664	1.305352	0.000000	4.087201	1.264499	0.000000	-3.138761	-2.907151	0.000000	-0.730107	1.264499
0.753664	0.000000	0.000000	-4.087201	0.000000	0.000000	3.138761	0.000000	0.000000	0.730107	0.000000	0.000000
-1.305352	0.000000	0.000000	-1.264499	0.000000	0.000000	2.907151	0.000000	0.000000	-1.264499	0.000000	0.000000

I	ITYPE	I1	N1	I2	N2	I3	N3	I4	N4	I5	N5	I6	N6	R0	OMEGAX	OMEGAY	OMEGAZ	NTOR	
1	1	-0	1	-0	4	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0,00000	-0,00000	-0,00000	-0,00000	-0
2	1	-0	2	-0	4	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0,00000	-0,00000	-0,00000	-0,00000	-0
3	1	-0	3	-0	4	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0,00000	-0,00000	-0,00000	-0,00000	-0
4	2	-0	2	-0	4	-0	3	-0	-0	-0	-0	-0	-0	-0	-0,39000	-0,00000	-0,00000	-0,00000	-0
5	2	-0	1	-0	4	-0	3	-0	-0	-0	-0	-0	-0	-0	-0,39000	-0,00000	-0,00000	-0,00000	-0
6	5	-0	1	-0	2	-0	3	-0	4	-0	-0	-0	-0	-0	-0,00000	-0,00000	-0,00000	-0,00000	-0
0,			0,86258E	00	0,	49801E	00	0,										1 16	D
0,			0,		0,	-0,		-0,						-0,24988E	00	-0,14427E	00	1 76	D
0,			0,		0,	0,		0,						0,		-0,28854E	00	2 16	D
0,			0,		0,	0,		0,						-0,		0,28854E	00	2 76	D
0,			0,		0,	0,		0,						0,		0,		3 16	D
0,			-0,24988E	00	0,14428E	00	-0,							0,24988E	00	-0,14428E	00	3 76	D
0,			0,		0,	0,		0,						0,28854E	00	0,		4 16	D
0,			0,14428E	00	0,24989E	00	0,							-0,43283E	00	-0,24989E	00	4 76	D
0,			0,64097E	00	-0,11102E	01	0,							0,		0,		5 16	D
0,			-0,14428E	00	-0,24989E	00	0,							-0,41400E	-01	0,57191E	00	5 76	D
0,99602E	00	0,			0,			0,22420E	00	-0,				-0,				6 16	D
0,22420E	00	-0,			-0,			-0,73694E	00	-0,				-0,				6 76	D