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MACS C
A COMPUTING PROGRAM FOR CRYSTAL VIBRATIONS WHICH
INCLUDES LONG-RANGE COULOMB INTERACTIONS

IDAHO NUCLEAR CORPORATION
NATIONAL REACTOR TESTING STATION
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A B S T R A C T

The program described here is one of a collection of computer programs aimed at giving maximum capability for calculating the slow-neutron scattering by moderators.

The program calculates crystal vibrations when the potential energy is a sum of parts arising from short-range forces and long-range Coulomb interactions. It also calculates and punches Jacobian matrices for use in determining adjustments in force constants and ionic charge which can lead to improved agreement with data. Finally, structure factors for neutron inelastic scattering can be calculated.

The program is a modification of earlier programs which cannot easily include the contribution of Coulomb interactions, and are limited to calculating Jacobian matrices for only valence force potential functions.

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I. INTRODUCTION

The program described in this report removes some limitations which have hampered the use of our earlier programs for calculating crystal vibrations. A review of the earlier programs will exhibit the need for the changes introduced into the new program.

The first program⁽¹⁾, called MACS M (number 40*0650, described in IN-1125) can calculate a dynamical matrix and from this the frequencies and normal coordinates for a crystal assuming either a valence force potential function or a Cartesian potential (see below). The program also calculates structure factors for neutron inelastic scattering.

When a valence force potential is used MACS M permits adjusting the force constants in any desired way between successive calculations. This feature has been used to construct Jacobian matrices whose elements contain the changes in frequencies $\partial v_k / \partial f_j$ with changes in force constants. Jacobians involving changes in "raw" eigenvalues which are proportional to squared frequencies can be obtained also. The Jacobian matrix is useful in calculating alterations in force constants which tend toward a least squares fit of calculated⁽²⁾ to observed frequencies.

For practical reasons the use of the MACS M program is limited to short-range interactions. In particular, it is not possible to include the long-range interactions between charges which characterize ionic crystals.

The first modification in MACS M came when it was realized that simple changes would make the computer calculate and punch Jacobian matrices. This led to the production of MACS J⁽³⁾ which modified

MACS M to compute Jacobians and punch them on cards in a format suited to another program⁽⁴⁾ which calculates adjusted force constants (program 40*0930, see IN-1148).

The program described in this work was developed when it was realized that MACS J could not be used to adjust force constants when interactions between Cartesian displacements were used. This was because MACS J fails to deal properly with force constants which occur with both positive and negative signs. In addition, it had become evident that the inability to include long-range Coulomb interactions in MACS M or MACS J was a serious deficiency which needed to be removed.

II. THEORY

This discussion is to assist in identifying the meanings of the pieces of input data for the program. Much more complete details will be found in Ref. (1) and in published work⁽⁵⁾.

A. The Short-Range Valence Force and Cartesian Potential Energies

To calculate the crystal vibrations the potential energy must be given in some convenient coordinate system. Two procedures are in common use for expressing the effects of short-range interactions. The valence force potential is in terms of interactions between valence coordinates which are changes in bond distances, interbond angles, etc. The Cartesian potential is in terms of interactions between the displacements of the atoms along suitably chosen Cartesian axes.

Let $\underline{H}(\ell)$ be a column vector whose elements are the valence coordinates for the ℓ th cell in the crystal. This is the cell at location $\underline{r}_\ell = \ell_1 \underline{a}_1 + \ell_2 \underline{a}_2 + \ell_3 \underline{a}_3$ relative to some origin cell in the crystal. The ℓ_1, ℓ_2, ℓ_3 are integers and $\underline{a}_1, \underline{a}_2$ and $\underline{a}_3$ are primitive displacement vectors for the crystals. Procedures for choosing the valence coordinates so they are the same for every cell, and no coordinate is assigned to more than one cell, are discussed in Ref. (5). The potential energy V in terms of these coordinates has the form:

$$2V = \sum_{\ell, \ell'} \underline{H}^T(\ell) \underline{F}_{\ell, \ell'} \underline{H}(\ell'). \quad (1)$$

Here $\underline{F}_{\ell, \ell'}$ is a matrix which contains the valence force constants which show the interactions between the coordinates in cells ℓ' and ℓ . The $\underline{F}_{\ell, \ell'}$ are square matrices of dimension $N \times N$ where N is the number of elements in each $\underline{H}(\ell)$. The translational symmetry of the crystal is such that $\underline{r}_{\ell'} = \underline{r}_\ell + \underline{r}_t$ where $\underline{r}_t$ is a translation of the lattice. Therefore, the PE can be written as:

$$\begin{aligned} 2V &= \sum_{\ell, t} \underline{H}^T(\ell) \underline{F}_{\ell, \ell+t} \underline{H}(\ell+t) \\ &= \sum_{\ell, t} \underline{H}^T(\ell) \underline{F}_{0, t} \underline{H}(\ell+t) . \end{aligned} \quad (2)$$

Here, $\underline{F}_{0, t}$ denotes the matrix associated with the reference or origin cell. Use is made of the fact that every cell is in a similar environment so that $\underline{F}_{\ell, \ell+t} = \underline{F}_{0, t}$.

The real matrices $F_{o,t}$ are part of the input to MACS M, MACS J and this program.

In making calculations, the $H(\ell)$ must be expressed in terms of the Cartesian displacements of the atoms in cell ℓ and surrounding cells. It is convenient to use mass adjusted displacements in which Δr_v , the displacement of atom v , is replaced by $\sqrt{m_v} \Delta r_v = q_v$. The kinetic energy is then just a sum of the squared velocities $\dot{q}_v^2$. The $H(\ell)$ is related to the q_v quantities by the matrix equation

$$\begin{aligned} H(\ell) &= \sum_t D_{\ell, \ell+t} q_{\ell+t} \\ &= \sum_t D_{o,t} q_{\ell+t} \end{aligned} \quad (3)$$

Here $q_{\ell+t}$ is a column vector containing as elements the mass adjusted Cartesian displacements of the atoms in the cell at $r_\ell + r_t$. The matrices $D_{\ell, \ell+t}$ are such that they express the way the elements in $H(\ell)$ depend on the mass adjusted Cartesian displacements in the cell at $r_\ell + r_t$. Translational symmetry requires that $D_{\ell, \ell+t} = D_{o,t}$.

The real matrices $D_{o,t}$ are part of the input to MACS M, MACS J and the present program.

When a Cartesian potential is used the potential energy is given by

$$2V = \sum_{\ell, \ell'} \Delta r^T(\ell) F_{\ell, \ell'} \Delta r(\ell'). \quad (4)$$

In this relation $F_{\ell, \ell'}$ is a Cartesian force matrix which expresses the interaction between the Cartesian displacements $\Delta r(\ell)$ of atoms in cell ℓ and displacements $\Delta r(\ell')$ of the atoms in cell ℓ' . Every

Cartesian $\underline{F}_{\ell,\ell}$ is of dimension $3N \times 3N$ where N is the number of atoms in a primitive cell.

As before, it is convenient to use:

$$\begin{aligned} 2V &= \sum_{\ell, \ell+t} \Delta \underline{r}^T(\ell) \underline{F}_{\ell, \ell+t} \Delta \underline{r}(\ell+t) \\ &= \sum_{\ell, \ell+t} \Delta \underline{r}^T(\ell) \underline{F}_{\underline{O}, t} \Delta \underline{r}(\ell+t). \end{aligned} \quad (5)$$

The expression for $\Delta \underline{r}(\ell)$ in terms of the $\underline{q}(\ell+t)$ is

$$\begin{aligned} \Delta \underline{r}(\ell) &= \sum_t \underline{D}_{\underline{O}, t} \underline{q}(\ell+t) \\ &= \underline{D}_{\underline{C}} \underline{q}(\ell). \end{aligned} \quad (6)$$

Eq. (6) results because the $\underline{D}_{\underline{O}, t}$ matrices for a Cartesian potential function have zero elements when $t \neq 0$. The $\underline{D}_{\underline{O}, 0}$ matrix, which is denoted by $\underline{D}_{\underline{C}}$, is the following diagonal matrix:

$$\underline{D}_{\underline{C}} = \begin{bmatrix} 1/\sqrt{m_1} & & & & & & \\ & 1/\sqrt{m_1} & & & & & \\ & & 1/\sqrt{m_1} & & & & \\ & & & \ddots & & & \\ & & & & \ddots & & \\ & & & & & 1/\sqrt{m_v} & \\ & & & & & & 1/\sqrt{m_v} \\ & & & & & & & 1/\sqrt{m_v} \end{bmatrix} \quad (7)$$

When Cartesian potentials are used the appropriate $\underline{F}_{\underline{O}, \ell}$ matrices are entered in MACS M, MACS J and in this program in the same way as the valence force matrices are entered when a valence force potential

is used. Also, the $\underline{D}_{0,\ell}$ matrices are entered as is done in a valence force treatment. However, all $\underline{D}_{0,\ell}$ for $\ell \neq 0$ are entered as zero matrices. The diagonal matrix $\underline{D}_{0,0} \equiv \underline{D}_C$ is entered as defined by Eq. (7).

When the Born-Von Karman boundary conditions are introduced, Eqs. (2), (3) and (5) are simplified. These boundary conditions amount to stating that the normal modes can be associated with values of a wave vector $\underline{k}$. When a mode with wave vector $\underline{k}$ is excited the displacements of the atoms in cell ℓ can be related to the displacements in the origin cell by

$$\Delta \underline{r}(\ell, \underline{k}) = \Delta \underline{r}(0, \underline{k}) e^{-i\underline{k} \cdot \underline{r}_\ell}. \quad (8)$$

The BVK boundary conditions lead to dynamical matrices which involve sums of the form

$$\underline{F}(\underline{k}) = \sum_t \underline{F}_{0,t} e^{-i\underline{k} \cdot \underline{r}_t} \quad (9)$$

$$\underline{D}(\underline{k}) = \sum_t \underline{D}_{0,t} e^{-i\underline{k} \cdot \underline{r}_t}. \quad (10)$$

The $\underline{F}_{0,t}$ and $\underline{D}_{0,t}$ can be either valence force or Cartesian force matrices as the problem requires. The machine computes these sums from the input data which includes the information needed to define $\underline{k}$ and the position $\underline{r}_t$.

B. The Long-Range Coulomb Interactions

When ionic charges are present, the potential energy required to assemble the charges in the crystal is given by

$$2V^{(C)} = \sum_{v,v'} \frac{Z_v Z_{v'}}{|r_v - r_{v'}|} |e|^2. \quad (v' \neq v) \quad (11)$$

In this equation Z_v is the fraction of one electron which is on atom v and is positive or negative. The $|e|$ is the electronic charge in esu so that $Z_v |e| = e_v$ is the charge on atom v in esu. The statements for atom v also apply to atom v' . The sum in Eq. (11) is over all atoms in the crystal. Eq. (11) can be written also as a sum over atoms in the cells, and a sum over cells. Thus,

$$2V^{(C)} = \sum_{l,l'} \sum_{v,v'} \frac{Z_v Z_{v'} |e|^2}{|r_v^{(l)} - r_{v'}^{(l')}|} \cdot (l) \neq (l') \quad (12)$$

In Eq. (12), the sum on v, v' is over the atoms in a primitive cell, and the sum on l, l' is over all cells in the crystal.

When the atoms move about during vibrational motions the $r_v^{(l)}$ vary. The interaction between any atom v and all other atoms in the crystal can be calculated if the motions are assumed to be restricted by the BVK boundary conditions. When the variation in the $r_v^{(l)}$ is expressed by Eq. (8), and account of this is taken in Eqs. (11,12), the Coulomb potential energy per unit volume is found to be

$$2V^{(C)} = \Delta r^T(0, \kappa) F_C(\kappa) \Delta r(0, \kappa). \quad (13)$$

The matrix $F_C(\kappa)$ is expressible in terms of 3×3 sub matrices $F_{Cvv'}(\kappa)$ which give the interactions between atoms v and v' . The $F_{Cvv'}(\kappa)$ are calculated from

$$F_{C,vv'}(\kappa) = \sum_{\ell} F_{\nu}^{(0)}(\ell, \nu') e^{-i\kappa \cdot r_{\ell}}. \quad (14)$$

Here $F_{\nu}^{(0)}(\ell, \nu')$ is a matrix obtained by expanding Eq. (11) or Eq. (12) and noting the Coulomb interaction between atom ν in some reference cell and atom ν' in a cell at $r_{\ell} = \ell_1 a_1 + \ell_2 a_2 + \ell_3 a_3$ relative to the reference cell.

However, the matrix generated by the usual Coulomb interaction calculation is built of 3×3 sub matrices $\psi_{C,vv'}(\kappa)$ which are defined using a different phase factor than that used in Eq. (14). The relation is

$$\psi_{C,vv'}(\kappa) = \sum_{\ell} F_{\nu}^{(0)}(\ell, \nu') e^{i\kappa \cdot [r_{\ell} + r_{\nu} - r_{\nu'}]}. \quad (15)$$

Thus, $\psi_{C,vv'}(\kappa)$ involves the same Coulomb coupling matrices $F_{\nu}^{(0)}(\ell, \nu')$ as does $F_{C,vv'}(\kappa)$ but the exponentials use the opposite sign and carry an additional factor $e^{i\kappa \cdot (r_{\nu} - r_{\nu'})}$ where r_{ν} and $r_{\nu'}$ are the equilibrium positions of atoms ν and ν' within a primitive cell. It is readily established that

$$F_{C,vv'}(\kappa) = \psi_{C,vv'}^c(\kappa) e^{i\kappa \cdot (r_{\nu} - r_{\nu'})} = \left[\psi_{C,vv'} e^{i\kappa \cdot (r_{\nu} - r_{\nu'})} \right]^c. \quad (16)$$

The superscript c denotes complex conjugate.

Finally, the matrices $\psi_{C,vv'}(\kappa)$ are not the ones usually tabulated. Instead the tabulations give charge-independent matrices $\chi_{C,vv'}$ related to $\psi_{C,vv'}(\kappa)$ by

$$\chi_{C,vv'}(\kappa) = \left(\psi_{C,vv'}(\kappa) \right) \frac{V}{e_{\nu} e_{\nu'}} = (\psi_{C,vv'}) \frac{V}{z_{\nu} z_{\nu'}} |e^2| \quad (17)$$

Here V is the volume of a unit cell (usually in cm^3) and e_v and $e_{v'}$ are the charges on atoms v and v' in esu. If the elements in $\underline{F}_C(\underline{\kappa})$ are to be in millidynes/ $\text{\AA}$, the $\underline{F}_{C,vv'}(\underline{\kappa})$ are computed from the $\chi_{C,vv'}(\underline{\kappa})$ by

$$\underline{F}_{C,vv'}(\underline{\kappa}) = \frac{2.307}{V} Z_v Z_{v'} \chi_{C,vv'}^c(\underline{\kappa}) e^{i\underline{\kappa} \cdot (\underline{r}_v - \underline{r}_{v'})}. \quad (18)$$

In this equation, the factor 2.307 is chosen so that the elements in $\underline{F}_{C,vv'}(\underline{\kappa})$ are in millidynes/ $\text{\AA}$ when V is in $\text{\AA}^3$ and $e_v = Z_v |e|$, $e_{v'} = Z_{v'} |e|$ where $|e|$ is the charge on the electron in esu and Z_v and $Z_{v'}$ are fractional numbers which can be negative or positive as the case requires.

Thus, the input information required to give $\underline{F}_C(\underline{\kappa})$ must include:

1. The volume V in $\text{\AA}^3$.
2. The fractional electron charges Z_v of the atoms.
3. The position vectors $\underline{r}_v$ of the atoms in the unit cell.
4. The elements of the matrices $\chi_{C,vv'}(\underline{\kappa})$ in the charge-independent form as computed from the Coulomb coupling coefficient equations and tabulated according to established convention.

The dynamical matrix which results when the long-range Coulomb interactions are added to the short-range interactions has the form

$$\underline{M} = \underline{D}^{cT} \underline{F} \underline{D} + \underline{D}_C \underline{F}_C \underline{D}_C.$$

In this equation $\underline{F}$ and $\underline{D}$ are defined by Eqs. (9,10) and will involve either valence force matrices and associated $\underline{D}_{o,l}$ matrices or their corresponding Cartesian counterparts. (Actually, mixtures of valence force and Cartesian potential functions could be employed

provided the size of the $F_{o,t}$ and $D_{o,t}$ matrices do not exceed the limits imposed by machine storage. See Sect. V for limitations.) The D_C matrix appears on each side of $F_C(\underline{x})$ because mass adjusted coordinates are used.*

All of these programs provide for multiplying M from the left by a real rectangular matrix A , and from the right by A^T . The dynamical matrix can be factored in this way (see Refs. (1,5) for more details).

*The program also prints out a matrix labeled $[(2.307)/V]$
 $D_C Z \text{ CCCZ } D_C$. This is just $D_C \psi D_C$. The Z denotes the diagonal matrix

$$Z = \begin{bmatrix} Z_1 & & & & & \\ & Z_1 & & & & \\ & & Z_1 & & & \\ & & & \ddots & & \\ & & & & Z_v & \\ & & & & & Z_v \\ & & & & & & Z_v \\ & & & & & & & \ddots \end{bmatrix}$$

III. PROGRAM ALTERATIONS FROM MACS M AND MACS J

A. The Changes From MACS M and MACS J

1. relate to the means for altering force constants between passes through the computer.
2. provide for adding dynamical matrices computed from short-range valence force or Cartesian interactions and the long-range Coulomb interaction.
3. provides for calculating Jacobian elements $\frac{-\partial v_k}{\partial f_j}$ for potential constants f_j which occur with both positive and negative sign in the $F_{o,l}$ matrices. This happens only for Cartesian potential constants. "Raw" Jacobian elements $\frac{-\partial \omega_k}{\partial f_j}$ are also calculated. A "raw" eigenvalue ω_k is related to v_k by $v_k (\text{cm}^{-1}) = 1303.61 \sqrt{\omega_k}$.
4. provides for calculating Jacobian elements $\frac{-\partial v_k}{\partial (Z_i^2)}$ and $\frac{-\partial \omega_k}{\partial (Z_i^2)}$ where i refers to the first atom in the list on card 13 which undergoes a change in charge. It is assumed that $\sum_v Z_v = 0$ before and after the charge alteration.

The input format closely parallels that used in MACS M and MACS J but cards 3 through 6 are significantly different. The format is presented in the following pages. However, it is useful to discuss some of the new features at this point.

B. Mechanism for Changing Force Constants

First we consider the problem of how to alter a force constant which appears in the $F_{o,t}$ matrices with both positive and negative signs, and how to compute the Jacobian elements for such force constant. The procedure must work for constants which appear always

with the same sign (positive or negative) and must allow for decreasing as well as increasing the value of any constant. The general technique for changing an arbitrary number of force constants (up to a maximum of 15) is first presented. Then the way this procedure is used to calculate Jacobian elements is given.

Let $|f_k^{(i)}|$ be the initial magnitude of force constant f_k . This force constant f_k may occur with only one sign, or it may occur with both positive and negative sign in the $F_{o,t}$ matrices. The input data card 5 will include the initial value $f_k^{(i)}$ of f_k . If f_k appears with both positive and negative sign, it can be entered on card 5 as either a positive or a negative quantity, but not both ways. The input format designates $f_k^{(i)}$ (including sign) as X_k . Suppose the value to be assumed by f_k after the change is $f_k^{(f)}$. This quantity is not entered as input. Instead a quantity, denoted in a format by Y_k is entered. The $Y_k = f_k^{(f)} * (\text{sign of } X_k)$.^(a)

With this as input the computation proceeds as follows:

1. The machine scans the elements in the $F_{o,t}$ matrices for quantities of magnitude $|X_k|$.
2. When an $f_k^{(i)}$ with $|X_k|$ is found, it replaces this element by

$$\begin{aligned} f_k^{(f)} &= X_k + \Delta f_k = X_k + \left\{ Y_k * (\text{sign of } X_k) - X_k \right\} \\ &= f_k^{(f)} * (\text{sign of } X_k)^2. \end{aligned}$$

^(a) The * denotes multiplication. This notation follows that used in FORTRAN programming.

To see why this procedure is adopted consider a case where $f_k^{(i)}$ occurs with values -0.16 and $+0.16$, i.e., it appears with both signs. Suppose we want these values to be changed to -0.06 and $+0.06$, respectively. Suppose we choose to insert $X_k = -0.16$ as the input on card 5. The desired value for the $f_k^{(f)}$ associated with $X_k = -0.16$ is $f_k^{(f)} = -0.06$. This means we must put on card 6 the quantity

$$Y_k = \underset{f_k^{(f)}}{\overset{\text{Sign of } X_i}{(-0.06)}} * (-1) = 0.06 .$$

Suppose that in scanning the $F_{o,t}$ for matrix elements with the magnitude $|X_k| = 0.16$, the machine finds an $f_k^{(i)} = -0.16$. It then replaces this with

$$\begin{aligned} f_k^{(f)} &= X_k + \left\{ Y_k * (\text{sign of } X_k) - X_k \right\} \\ &= -0.16 + \left\{ 0.06 * (-1) - (-0.16) \right\} \\ &= -0.16 + 0.10 = -0.06. \end{aligned}$$

On the other hand, if it finds an element with $f_k^{(i)} = 0.16$ it replaces it by

$$\begin{aligned} f_k^{(f)} &= 0.16 + \left\{ 0.06 * (+1) - 0.16 \right\} \\ &= 0.06. \end{aligned}$$

If the initial input had used $X_k = 0.16$ and $f_k^{(f)} = 0.06$, the input on card 6 would use $Y_k = 0.06 * (+1) - 0.06$. If the scan picks up an $f_k^{(i)} = -0.16$, it calculates

$$f_k^{(f)} = -0.16 + \left\{ 0.06 * (-1) - (-0.16) \right\}$$

$$= -0.06.$$

Again, if with this X_k and Y_k input, it picks up $f_k^{(i)} = 0.16$ it calculates

$$f_k^{(f)} = 0.16 + \left\{ 0.06 * (+1) - 0.16 \right\}$$

$$= 0.06.$$

The procedure works also when $f_k^{(f)}$ changes sign from $f_k^{(i)}$. For example, suppose $f_k^{(1)}$ occurs with values -0.16 and 0.16 and we want these changed to 0.04 and -0.04 , respectively. Suppose we insert $X_k = -0.16$ on card 5. Then on card 6, $Y_k = (0.04) * (-1) = -0.04$. If the machine finds an $f_k^{(i)} = -0.16$, it changes it to

$$f_k^{(f)} = -0.16 + \left\{ (-0.04) * (-1) - (-0.16) \right\}$$

$$= 0.04.$$

If, with this X_k and Y_k input, it picks up an $f_k^{(i)} = 0.16$, it changes it to

$$f_k^{(f)} = 0.16 + \left\{ (-0.04) * (+1) - 0.16 \right\}$$

$$= -0.04.$$

Since the force constant changer works for constants which appear with both signs, it will work if they appear with only one sign.

C. Calculation of Jacobian Elements for Force Constants

The elements in the Jacobian matrices are calculated as follows. On pass 0 (the initial pass) a desired initial set of force constants is entered and a set of frequencies $\nu_1^{(0)}, \nu_2^{(0)} \dots \nu_3^{(0)} \dots$ (in cm^{-1} , eV and cycles/sec $\times 10^{12}$) and an associated set of "raw" eigenvalues are calculated. (A "raw" eigenvalue ω_m is related to the frequency ν_m in cm^{-1} or in eV by $\nu_m(\text{cm}^{-1}) = 1303.061 \sqrt{\omega_m}$ and $\nu_m(\text{eV}) = 0.16155 \sqrt{\omega_m}$.) On succeeding passes, only one constant is changed (a different constant on each pass). Suppose constant f_k is altered by $\Delta f_k^{(j)}$ on the j th pass. The machine computes $\Delta f_k^{(j)}$ as described above using

$$\Delta f_k^{(j)} = Y_k^{(j)} * (\text{sign of } X_k^{(j)}) - X_k^{(j)}.$$

It then calculates the Jacobian column for this force constant from the equation

$$-J_{m,f_k} \equiv \frac{\nu_m^{(j)} - \nu_m^{(0)}}{f_k^{(j)} - f_k^{(0)}} \equiv \frac{\nu_m^{(j)} - \nu_m^{(0)}}{\Delta f_k^{(j)}}.$$

(The Jacobians are calculated for ν_m in eV units.)

Here $\nu_m^{(j)}$ is the value of ν_m when all constants except f_k have their initial values, and f_k has the value $f_k^{(j)}$. The $\nu_m^{(0)}$ is the value of ν_m on pass 0. Jacobian elements which involve $\omega_m^{(j)} - \omega_m^{(0)}$ are also computed.

D. Calculation of Jacobian Elements for a Change in Z_i^2

Let i denote the first atom in the list on card 13 for which the charge is altered. The Jacobian column for the change in Z_i^2 is computed on

some pass, j , by putting a 1 in column 70 of control card 1 to tell the machine to use new data for the charges (also cell volume, atom positions and atomic masses). Control card 4 has a 0 in column 5 telling the machine that there are to be no changes in the force constants. (Cards 5,6 which give the force constant changes are to be omitted when card 4 has a 0 in column 5.) Data cards 11-13 carry the new values of cell volume, atom positions, masses and charges Z_v (the $\sum_v Z_v = 0$ before and after the change). Let $Z_i^{(j)}$ and $Z_i^{(0)}$ be the fractional charge on atom i . The machine calculates

$$-I_{v_m, Z_i^2} = \frac{v_m^{(j)} - v_m^{(0)}}{Z_i^2(j) - Z_i^2(0)}.$$

Here j denotes the pass on which Z_i^2 is given its new value. Jacobians with $v_m^{(j)} - v_m^{(0)}$ are also obtained.

The program operates so that after a calculation in which $IJAC = 1$ (on card 4) and any charges have been changed, all charges are restored to their original values.

IV. COMMENTS ON INPUT-OUTPUT

A. General

The information on the input format sheets shows what input data can be printed, and what calculated quantities (aside from eigenvalues, etc.) can be printed out. Eigenvalues and eigenvectors are always printed according to the format described in Ref. (1).

Jacobian elements calculated on any pass are printed. To obtain a punched Jacobian a 1 is inserted in column 25 of card 4. All

Jacobian elements up through that pass are then printed and punched. The format of the punched card output for the J matrix is discussed in Sect. 3, p 8 of Ref. (3).

This program accepts A, D and F matrices with up to 40 rows and/or columns. (The MACS M and MACS J are limited to 32 rows and/or columns.)

The sum check described on pages 7 and 8 of Ref. (3) is valid if all non-zero constants (including charge) are varied in forming the Jacobian.

In this program the $D(\kappa)$ matrix is computed on every pass in a Jacobian calculation.

B. Format of Input Matrices

The matrices (A , $D_{o,t}$, $F_{o,t}$) are in the following format (WRIM format). Each card contains six twelve-digit numbers in E format (example: 1.03E+01) or F format (example: 10.3). Card columns 73-74 indicate the row that the values on the card are to occupy. Card columns 75-76 indicate the column of the matrix that the value in word one of the card is to occupy. The remaining values on the card will occupy successive column locations in the given row of the matrix. Card column 77 indicates the total number of values on the card. Card columns 78-80 are not used by this sub-routine, so these columns can be used for identification or not as the user sees fit. Before a matrix is called into core, the complete areas that it will occupy is set to zero; consequently, it is necessary

to enter only nonzero values into the computer.* If a card contains one or more zero matrix elements, such elements may be represented by a 0.0 or by no punches at all. Since each card contains its own input information, values may be entered in any order.*

The output format for real matrices corresponds to the WRIM input format, except that meaningless "junk" numbers may appear at the end of matrix rows. (Example: A real 3 x 3 matrix will occupy only the first three positions of each printed line, and the last three positions may contain meaningless "junk".)

Except for the Coulomb coupling coefficient matrices (denoted by $\underline{\underline{CCC}}$, or sometimes $\underline{\underline{X_C}}$), all input matrices must be real. The $\underline{\underline{CCC}}$ matrices are in WRIMC format which closely corresponds to WRIM format except that each row contains three complex numbers in "x,y" form. Two successive words are used for the real (x) and imaginary (y) parts of a complex number, respectively.

Any $\underline{\underline{CCC}}$ matrix is composed of sub matrices $\underline{\underline{X_{C,vv'}}}$ which contain the (complex) Cartesian couplings between atoms v and v' (see Eqs. (17,18)). The ordering of atoms must be the same as the ordering on cards 11-13.

Complex matrices ($\underline{\underline{F}}$, $\underline{\underline{D}}$ and $\underline{\underline{M}}$) are printed as output in WRIMC format.

* Exception: The loading of a matrix is terminated by the subroutine WRIM storing the final value of the highest numbered row. For example, in a 24 x 27 matrix, when the element (24,27) is stored, the loading process is terminated and the matrix is assumed to be complete. This last element must be entered even if it has value zero.

Table I gives the input format for this program. Except for features associated with inserting the CCC matrices, it is like MACS J.

TABLE I

INPUT FORMAT FOR MACS C

<u>Card Type</u>	<u>Columns</u>	<u>Mnemonic</u>	<u>Format</u>		<u>Remarks</u>
1	1-5	ILTAPE	I	ℓ indices and $\underline{D}_{0,\ell}$ matrices	0: quantity read from tape
	6-10	IFTAPE	I	$\underline{F}_{0,\ell}$ matrices*	1: quantity read from cards
	11-15	IVTAPE	I	CCC matrix	The notation CCC denotes Coulomb Coupling Coefficient. It is a mnemonic for the matrix $\chi_C(\kappa)$ in Eq. (17).
	16-20	IATAPE	I	A matrix	
	21-25	KLTAPE	I	ℓ indices and $\underline{D}_{0,\ell}$ matrices	0: quantity not stored on tape
	26-30	KFTAPE	I	$\underline{F}_{0,\ell}$ matrices	1: quantity stored on tape
	31-35	KVTAPE	I	CCC matrix	
	36-40	KATAPE	I	A matrix	
	41-45	N2	I	Number of columns in A (= number of columns in $\underline{D} = 3N$, where N = number of atoms per primitive cell)	
	46-50	N3	I	Number of rows in $\underline{F}$ (= number of columns in $\underline{F}$ = number of rows in $\underline{D}$)	

* Since $\underline{F}_{0,0} = \underline{F}_{0,0}^T$, only the diagonal and superdiagonal elements of $\underline{F}_{0,0}$ need to be entered as data. The program takes the diagonal and superdiagonal elements and constructs a symmetric $\underline{F}_{0,0}$ from these entries. However, the print out of $\underline{F}_{0,0}$ will show only what was inserted on the input cards. Only the $\underline{F}_{0,\ell}$ matrices with $\ell \geq 0$ are given as input data to the program because $\underline{F}_{0,-\ell} = \underline{F}_{0,\ell}^T$.

TABLE I (CONT)

<u>Card Type</u>	<u>Columns</u>	<u>Mnemonic</u>	<u>Format</u>	<u>Remarks</u>
1	51-55	N5	I	Number of rows in A
	56-60	NUMAT	I	Number of $D_{0,\ell}$ matrices with $\ell > 0$. $\ell \geq 1$ required.
	61-65	ICCC	I	$\left\{ \begin{array}{l} 0: \text{ no Coulomb coupling coefficients} \\ \text{in calculation} \\ 1: \text{ Coulomb coupling coefficients} \\ \text{in calculation} \end{array} \right.$
	66-70	ICIN	I	0: use previous data (volume, mass, positions and charge) for CCC calculation 1: read new data (volume, mass, positions and charge) for CCC calculation
	71-75	IFSTRU	I	0: structure factor input is not read from cards and no structure factors computed 1: structure factor input is read from cards and structure factors computed

<u>Card Type</u>	<u>Columns</u>	<u>Mnemonic</u>	<u>Format</u>	<u>Remarks</u>
				0: Quantity is printed 1: Quantity is not printed
2	1-5	IØP1	I	$D_{0,1}, D_{0,2}, \dots, D_{0,NUMAT}$
	6-10	IØP2	I	$D_{0,0}$
	11-15	IØP3	I	$D_{0,0}, D_{0,-1}, D_{0,-2}, \dots, D_{0,-NUMAT}$
	16-20	IØP4	I	D
	21-25	IØP5	I	$F_{0,1}, F_{0,2}, \dots, F_{0,NUMAT}$ $F_{0,0}$
				Only the changed $F_{0,\ell}, F_{0,0}$ are printed (see card type 4). The changed $F_{0,\ell}$ remain on tape for use as desired.
	31-35	IØP7	I	F

TABLE I (CONT)

Card Type	Columns	Mnemonic	Format	Remarks	0: Quantity is printed
					1: Quantity is not printed
2	36-40	IØP8	I	$\underline{A}$	
	41-45	IØP9	I	$\underline{A}$ (Normalized)	
	46-50	IØP10	I	$\underline{A}^*$ = Orthonormalized $\underline{A}$	
	51-55	IØP11	I	$\underline{FD}$	
	56-60	IØP12	I	$\underline{D}^{cT} \underline{FD}$	
	61-65	IØP13	I	$\underline{A}^* [\underline{D}^{cT} \underline{FD} + \underline{D}_C^F \underline{D}_C]$; $\underline{D}_C^F \underline{D}_C$ is added if ICCC = 1	
	66-70	IØP14	I	$\underline{M}$ (Raw) = $\underline{A}^* [\underline{D}^{cT} \underline{FD} + \underline{D}_C^F \underline{D}_C] \underline{A}^{*T}$ $\underline{M}$ (Hermitian, except that some diagonal elements may have small nonzero imaginary part) $\underline{M}$ (Expanded; Real; Symmetric, see Ref. (1))	
3 ^{*†}	1-5	IØP15	I	Cell Volume, Atom Masses, Positions Fractional Charges Z_v	
	6-10	IØP16	I	CCC. This is the same as $\chi_C(\kappa)$ as defined from Eq. (17).	
	11-15	IØP17	I	$[(2.307)/V] \underline{D}_C^Z \underline{X}_C^Z \underline{D}_C = \underline{D}_C^{\psi} \underline{D}_C$, see footnote on page 10.	
	16-20	IØP18	I	$\underline{D}_C^F \underline{D}_C$	
	21-25	IØP19	I	$\underline{D}^{cT} \underline{FD} + \underline{D}_C^F \underline{D}_C$	

* This card is included only if ICCC $\neq$ 0.

[†] A superscript * does not denote a complex conjugate. The superscript c is used for this, and superscript T is for transposed. Thus, $\underline{D}^{cT}$ means the conjugate transpose of $\underline{D}$.

TABLE I (CONT)

Card Type	Columns	Mnemonic	Format	Remarks	0: Quantity is printed	1: Quantity is not printed
4	1-5	NØCH	I	The number of force constants to be changed in the $F_{0,l}$ matrices. These changes are read from card types 5 and 6. Changes are limited to 15 force constants. When Jacobian elements are calculated from a change in Z_i^2 , put a zero here and follow instructions in text. Z_i is the electronic charge on the first atom listed on card 13 whose charge is altered.		
	6-10	KBASIS	I	If KBASIS $\neq$ 0, a transformation matrix A_1 is read from cards and EA_1 is computed where the rows of E are the eigenvectors.		
	11-15	N8	I	The number of columns in A_1 . Note that the number of rows in A_1 = Number of rows in A .		
	16-20	IJAC	I	Put 0 for first pass and 1 for subsequent passes when columns in J are calculated and printed.		
	21-25	NUSAVE1	I	If NUSAVE1 $\neq$ 0 and IJAC $\neq$ 0, the Jacobians calculated up to that point are printed and punched.		
5 [†]	1-10	X ₁	F	Each $F_{0,l}$ matrix is scanned and if the absolute value of any element is equal to $ X_k $, then this element is replaced by the sign of that element		
	11-20	X ₂	F			
	.	.	.			
	.	.	.			

[†]Cards 5,6 are not needed when there are no force constant changes (0 in col. 5, card 4).

TABLE I (CONT)

Card				0: Quantity is printed
Type	Columns	Mnemonic	Format	Remarks 1: Quantity is not printed
6 [†]	1-10	Y ₁	F	times Y _k (see card 6). To compute a column in J put X _k = old force constant with sign and Y _k = new constant times sign of X _k (see Sect. IIC). Notice that the number of X _k 's = number of Y _k 's = NOCH of card type 4. If NOCH = 0, then card type 5 and 6 are omitted. If NOCH > 8, more than one card type 5 and card type 6 are used.
	11-20	Y ₂	F	
	.	.	.	
	.	.	.	
7	1-10	f ₁	F	These are the kappa components. This card is <u>always</u> USED. (Note change from MACS M and MACS J.)
	11-20	f ₂	F	
	21-30	f ₃	F	
8*	1-5	l _{1,1}	F	$r_i = l_{1i}a_1 + l_{2i}a_2 + l_{3i}a_3$ where l_{1i} , l_{2i} and l_{3i} are integers. There are l_i and $D_{0,i}$ cards for each cell i .
	6-10	l _{2,1}	F	
	11-15	l _{3,1}	F	
9*		D _{0,1}	WRIM	
8*	1-5	l _{1,2}	F	
	6-10	l _{2,2}	F	
	11-15	l _{3,2}	F	
9*		D _{0,2}	WRIM	
.		.		
.		.		
.		.		

* All l_i and $D_{0,i}$ are punched by 40*0720 to be inserted here. See report IN-1076, "D Matrix" by J. K. Boyter and H. L. McMurry.

[†]Cards 5,6 are not needed when there are no force constant changes (0 in col. 5, card 4).

TABLE I (CONT)

Card Type	Columns	Mnemonic	Format	Remarks
8*	1-5	ℓ_1, NUMAT	F	$r_{\text{NUMAT}} = \ell_1, \text{NUMAT}^{a_1} + \ell_2, \text{NUMAT}^{a_2} + \ell_3, \text{NUMAT}^{a_3}$. NUMAT denotes the highest ℓ index. See mnemonic on card 1, cols. 56-60. Note: In calculating vibrations for a molecule, put $\ell = 1$ in col. 60, card 1, insert $\ell_1 = 0$, $\ell_2 = 0$, $\ell_3 = 0$ on card 8 and put in null matrices for D_{01} , D_{0-1} and F_{01} (cards 9,10).
	6-10	ℓ_2, NUMAT	F	
	11-15	ℓ_3, NUMAT	F	
9*		$D_{0, \text{NUMAT}}$	WRIM	
9*		$D_{0,0}$	WRIM	
9*		$D_{0,-1}$		
.		.		
.		.		
.		.		
9*		$D_{0,-\text{NUMAT}}$	WRIM	
10		$F_{0,1}$	WRIM	
10		$F_{0,2}$	WRIM	
.		.		
.		.		
.		.		
10		$F_{0, \text{NUMAT}}$	WRIM	
10		$F_{0,0}$	WRIM	
11 [†]	1-10	VOLUME	F	Volume of primitive cell (direct lattice) in $\text{\AA}^3$
12 ^{†*}	1-10	MASS ₁	F	Mass of first atom (AMU)
	11-20	R_{11}	F	
	21-30	R_{21}	F	$R_v = R_{1v}a_1 + R_{2v}a_2 + R_{3v}a_3$.
	31-40	R_{31}	F	$R_{iv}a_i$ is component of R_v along a_i in $\text{\AA}$.
	41-50	MASS ₂	F	The subscript v is for the v th atom.
	51-60	R_{12}	F	

[†]The cards are used only if ICC = 0 and ICIN = 1.

*As many cards as needed.

TABLE I (CONT)

Card Type	Columns	Mnemonic	Format	Remarks
12 ^{†*}	61-70	R ₂₂	F	
	71-80	R ₃₂	F	
13	1-10	Z ₁	F	Z _v is the charge on atom v in fraction of the electron charge ($e_v = e Z_v$ where e is the electronic charge in esu and e _v is the charge on atom v in esu).
	11-20	Z ₂	F	$\sum_v Z_v = 0$ Note: This is not checked by the program.
	.	.		
	.	.		
	.	.		
14		CCC	WRIMC	Note that WRIMC format is necessary for the CCC matrix.
15		A	WRIM	

The remaining input is identical to MACS M. It concerns the structure factor input and cards are needed only if there is a 1 in column 75 of Control Card 1 (INSTRU $\neq$ 0).

Card Type S1 contains the first $\underline{t}$ -vector.

Columns 1-10	t_1	(F format)
11-20	t_2	
21-30	t_3	

Card Type S2

Columns 1-5	NTAU = number of $\underline{t}$ vectors to be read in (integer format)
-------------	---

[†]The cards are used only if ICCC $\neq$ 0 and ICIN = 1.

* As many cards as needed.

Card Type S3

Columns 1-10 m_1 (F format)
 11-20 m_2
 .
 .
 . ($m_k, k = 1, \dots, N$)

Card Type S4

Columns 1-10 b_1 (F format)
 11-20 b_2
 .
 .
 . ($b_k, k = 1, \dots, N$)

Card Type S5

B matrix (3 x 3) (WRIM Format)

Card Type S6

R matrix (N rows and 3 columns) (WRIM Format)

Card Type S7

Remaining t-vectors (if the punch in column 1-5 of Card
Type S3, NTAU, > 1).

Card Type A₁ (WRIM Format)

The A₁ matrix is entered next (if KBASIS*NB+0) as the
final set of cards in the input of a given problem. This
matrix is not stored on tape; it must be entered anew for
each problem which calls for it. If there is another
problem, then another Control Card 1 comes next in the
deck.

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APPENDIX

ILLUSTRATIVE INPUT FOR THE Mg_2Sn CRYSTAL

This crystal is face centered cubic with three atoms per unit cell. The basis vectors $\underline{a}_1$, $\underline{a}_2$ and $\underline{a}_3$ are all of length $\sqrt{2} a$ where $2a$ is the distance between the second neighbor Sn atoms which lie along the cube edges.

The vectors $\underline{a}_1$, $\underline{a}_2$, $\underline{a}_3$ are related to the unit vectors $\underline{i}$, $\underline{j}$, $\underline{k}$ along the Cartesian directions by

$$\begin{bmatrix} \underline{a}_1 \\ \underline{a}_2 \\ \underline{a}_3 \end{bmatrix} = a \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} \underline{i} \\ \underline{j} \\ \underline{k} \end{bmatrix}$$

$$\begin{bmatrix} \underline{i} \\ \underline{j} \\ \underline{k} \end{bmatrix} = \frac{1}{2a} \begin{bmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} \begin{bmatrix} \underline{a}_1 \\ \underline{a}_2 \\ \underline{a}_3 \end{bmatrix}$$

$$a = 3.3775 \text{ \AA} \text{ for } \text{Mg}_2\text{Sn}$$

$$|\underline{a}_1| = |\underline{a}_2| = |\underline{a}_3| = \sqrt{2} a$$

$$\text{cell volume} = \underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3) = 2a^3 = 77.058 \text{ \AA}^3$$

The position of any atom v is given by

$$\begin{aligned} \underline{r}(\underline{\ell}) &= \ell_1 \underline{a}_1 + \ell_2 \underline{a}_2 + \ell_3 \underline{a}_3 + \underline{r}_v \\ &= \underline{r}_{\underline{\ell}} + \underline{r}_v \end{aligned}$$

Here $\underline{\ell}$ is an index which designates the set of integers ℓ_1, ℓ_2, ℓ_3 which locate the cell in which atom v lies. The $\underline{r}_v$ gives the position of atom v within any primitive cell. The theory⁽⁵⁾ is set up so that

$\bar{r}_\ell = -\bar{r}_{-\ell}$. This means the indices ℓ must be chosen so that if ℓ is used to designate the set for $\bar{r}_\ell$ then $-\ell$ designates the set for $-\bar{r}_\ell$. This is seen in Table A1 which gives the indexing used in this work. It is the same as for diamond⁽⁵⁾ except for one additional cell which was not needed in the diamond work.

TABLE A1

CELL INDEXING FOR Mg_2Sn

Theor. ℓ	Proj. ℓ	ℓ_1	ℓ_2	ℓ_3	x_ℓ	y_ℓ	z_ℓ
1	1	1	0	0	0	a	a
2	2	0	1	0	a	0	a
3	3	0	0	1	a	a	0
4	4	0	1	-1	0	-a	a
5	5	-1	1	0	-a	-a	0
6	6	-1	0	1	a	0	-a
7	7	1	1	-1	0	0	2a
0	8	0	0	0	0	0	0
-1	9	-1	0	0	0	-a	-a
-2	10	0	-1	0	-a	0	-a
-3	11	0	0	-1	-a	-a	0
-4	12	0	-1	1	0	a	-a
-5	13	1	-1	0	a	a	0
-6	14	1	0	-1	-a	0	a
-7	15	-1	-1	1	0	0	-2a

It is convenient to order the atoms as Mg-Sn-Mg so that the Mg atoms are numbers 1 and 3 in the list of atoms, and the Sn atom is number 2. This reflects the fact that there are primary bonds from 1-2 and 2-3 but not 1-3.

Each Sn atom is at the origin of a primitive cell, e.g.,
 $\underline{r}_2 = 0$.

The first Mg atom which is number 1 in the listing, has

$$\underline{r}_1 = \frac{\underline{a}_1 + \underline{a}_2 + \underline{a}_3}{4} = \frac{a(\underline{i} + \underline{j} + \underline{k})}{2}.$$

The other Mg atom, number 3 in the listing, is at

$$\underline{r}_3 = \frac{-\underline{a}_1 - \underline{a}_2 + 3\underline{a}_3}{4} = \frac{a(\underline{i} + \underline{j} - \underline{k})}{2}.$$

To illustrate the use of the program a long-range Coulomb matrix is added to a short-range Cartesian matrix. T. Worlton provided the Cartesian interaction matrix which is just a preliminary one. The long-range Coulomb contribution to the dynamical matrix is for $\underline{\kappa} = \frac{\pi}{a} \times 0.4 \underline{i}$ (or $.4, 0, 0$). The self interactions and Mg-Mg interactions are from Kellermann⁽⁷⁾ and the Mg-Sn interactions are from Whitten et al.⁽⁸⁾

The input shown in this appendix does not show the $\underline{D}_{0\ell}$ (all zero in this case for $\ell \neq 0$) matrices, or the $\underline{F}_{0\ell}$ matrices for the short-range Cartesian couplings. However, these matrices are printed in the output which is in the WRIM form. The output also gives several matrices (notably $\underline{F}_C$ and $\underline{\chi}_C$) which are complex and are in WRIMC format.

The input data which is shown are as follows:

1. First Problem

Card 1 designates that all matrices $D_{O\ell}$, $F_{O\ell}$, χ_C and A (a matrix which defines symmetry coordinates suited to factoring the dynamical matrix along $\xi, 0, 0$), as well as the cell volume, atom positions r_v^* and atom charges Z_v , are read in from cards. All these data designated to be stored on tape for subsequent use.

Card 2 calls for printing all the $D_{O\ell}$, $F_{O\ell}$ matrices and certain sums of these, as well as A , the A with normalized rows and the orthonormalized A .

Card 3 calls for printing the cell volume, atom positions r_v and atom charges Z_v and the χ_C matrix.

Card 4 instructs the machine to update all 9 constants in the short-range Cartesian force matrix. This illustrates the force constant change feature. The updated $F_{O\ell}$ matrices will be stored and printed if this is called for on card 2.

Card 4 has 0 in cols. 10,15 so there will be no basis change, and zero in cols. 20,25 so no Jacobians are to be calculated, punched and printed.

Cards 5 and 6 tell the changes to be made in the force constants.

Card 7 gives the f_i values corresponding to k at 0.4, 0, 0 (cf. Ref. (5)).

* Only the coefficients for a_1 , a_2 and a_3 are needed. These vectors are not used as input because use is made of the relation $b_i \cdot a_j = \delta_{ij}$ where b_i is a reciprocal space basis vector.

Cards 8 through 10 are not shown. They are matrices in WRIM format in the print-out.

Cards 11, 12, 13 give the cell volume and atom masses, positions and charges.

Cards 14, 15 are omitted. Their contents are shown in the print-out.

2. Second Problem

In this problem the Jacobian for a change in charge Z_1 is computed.

Card 1 is altered to show that all matrices are read from tape and are returned to tape. However, there is a 1 in col. 70 to show that new charge data, etc., are to come from a new set of 11, 12, 13 cards.

Cards 2 and 3 call for printing only new quantities.

Card 4 says there are no force constant changes and Cards 5 and 6 are omitted. The 1 in col. 20 calls for a Jacobian and the 1 in col. 25 calls for printing and punching.

Card 7 repeats the f_i which define κ .

Cards 11, 12, 13 give new data on cell volume, atom positions and charge. (Actually only the Z_v change, but all the data are needed again.)

The succeeding problems are like the first, the only difference being that three different A matrices are used. These correspond to different vibrational symmetries which do not interact with each other. In solving these problems the set of charges Z_v used in the first problem are used.

Table A-2

Input Format for Mg₂Sn Frequencies at $k = 2\pi(0.2b_2 + 0.2b_3) = \frac{\pi}{2}(0.4i)$

Card	0 0 0 0 0 0 0 0 1 1 2 3 4 5 6 7 8 9 0	1 1 1 1 1 1 1 1 2 1 2 3 4 5 6 7 8 9 0	2 2 2 2 2 2 2 2 3 1 2 3 4 5 6 7 8 9 0	3 3 3 3 3 3 3 3 4 1 2 3 4 5 6 7 8 9 0	4 4 4 4 4 4 4 4 5 1 2 3 4 5 6 7 8 9 0	5 5 5 5 5 5 5 5 6 1 2 3 4 5 6 7 8 9 0	6 6 6 6 6 6 6 6 7 1 2 3 4 5 6 7 8 9 0	7 7 7 7 7 7 7 7 8 1 2 3 4 5 6 7 8 9 0
1	1	1	1	1	9	9	7	1
2	0	0	0	0	0	0	0	0
3	0	0	0	0				
4	9	0	0	0				
5	0.5392	0.1381	0.132	0.007175	0.06775	1.1992	0.02	0.0518
6	0.4144	0.1036	0.1314	0.0	0.0	1.600	0.04132	0.07574
7	0.0343							
8	0.0	0.2	0.2					
9	SEE PRINT -	OUT FOR	VALUES					
10	SEE PRINT -	OUT FOR	D MATRICES					
11	SEE PRINT -	OUT FOR	F MATRICES					
12	7.7.058							
13	2.4.31	0.25	0.25	0.25	1.18.7	0.0	0.0	0.0
14	2.4.31	0.25	0.25	0.75				
15	0.5	1.0	0.5					
16	SEE PRINT -	OUT FOR	COMB. SCUP	ING MATR IX				
17	SEE PRINT -	OUT FOR	A MATRIX					
18	0	0	0	0	9	9	7	1
19	1	1	1	1	1	1	1	1
20	0	1	1	1				
21	0	0	1					
22	0.0	0.2	0.2					
23	7.7.058							
24	2.4.31	0.25	0.25	0.25	1.18.7	0.0	0.0	0.0
25	2.4.31	0.25	0.25	0.75				
26	0.48	1.04	0.48					
27	0	0	0	0	9	9	7	1
28	1	1	1	1	1	1	1	1
29	0	1	1	1	0	0	0	0
30	0	0	0					
31	0	0	0					
32	0.0	0.2	0.2					
33	SEE PRINT -	OUT FOR	A					
34								
35								
36								
37								
38								
39								
40								
41								
42								
43								
44								
45								
46								
47								
48								
49								
50								

Table A-2 (Continued)

[illegible]

ILTAPE= 1 IFTAPE= 1 IVTAPE= 1 IATAPE= 1

KLTAPE= 1 KFTAPE= 1 KVTAPE= 1 KATAPE= 1

NUMBER OF COLUMNS IN D,N2= 9

NUMBER OF ROWS IN D,N3= 9

NUMBER OF ROWS IN A,N5= 9

NUMBER OF D MATRICES WITH POSITIVE SUBSCRIPTS,NUMAT 7

INITIAL FORCE CONSTANTS

5.39200E-01	1.03100E-01	1.32000E-01	-7.17500E-03	6.77500E-02	1.19920E 00	-2.00000E-02	5.18000E-02
3.18000E-02							

Y(I)

4.14400E-01	1.03600E-01	1.31400E-01	0.	0.	1.60000E 00	-4.13200E-02	7.57400E-02
3.44300E-02							

F = (0.000000, 0.200000, 0.200000)

Mg₂Sn at 0.4, 0, 0

Adds Coulomb matrix to
short range Cartesian matrix

[illegible]

L(2)=(0.0000, 1.0000, 0.0000)

D+ 2

0.	0.	0.	0.	0.	0.	1	1	6	D-
0.	0.	0.	0.	0.	0.	1	7	3	D-
0.	0.	0.	0.	0.	0.	2	1	6	D-
0.	0.	0.	0.	0.	0.	2	7	3	D-
0.	0.	0.	0.	0.	0.	3	1	6	D-
0.	0.	0.	0.	0.	0.	3	7	3	D-
0.	0.	0.	0.	0.	0.	4	1	6	D-
0.	0.	0.	0.	0.	0.	4	7	3	D-
0.	0.	0.	0.	0.	0.	5	1	6	D-
0.	0.	0.	0.	0.	0.	5	7	3	D-
0.	0.	0.	0.	0.	0.	6	1	6	D-
0.	0.	0.	0.	0.	0.	6	7	3	D-
0.	0.	0.	0.	0.	0.	7	1	6	D-
0.	0.	0.	0.	0.	0.	7	7	3	D-
0.	0.	0.	0.	0.	0.	8	1	6	D-
0.	0.	0.	0.	0.	0.	8	7	3	D-
0.	0.	0.	0.	0.	0.	9	1	6	D-
0.	0.	0.	0.	0.	0.	9	7	3	D-

L(3)=(0.0000, 0.0000, 1.0000)

D+ 3

0.	0.	0.	0.	0.	0.	1	1	6	D-
0.	0.	0.	0.	0.	0.	1	7	3	D-
0.	0.	0.	0.	0.	0.	2	1	6	D-
0.	0.	0.	0.	0.	0.	2	7	3	D-
0.	0.	0.	0.	0.	0.	3	1	6	D-
0.	0.	0.	0.	0.	0.	3	7	3	D-
0.	0.	0.	0.	0.	0.	4	1	6	D-
0.	0.	0.	0.	0.	0.	4	7	3	D-
0.	0.	0.	0.	0.	0.	5	1	6	D-
0.	0.	0.	0.	0.	0.	5	7	3	D-
0.	0.	0.	0.	0.	0.	6	1	6	D-
0.	0.	0.	0.	0.	0.	6	7	3	D-
0.	0.	0.	0.	0.	0.	7	1	6	D-
0.	0.	0.	0.	0.	0.	7	7	3	D-
0.	0.	0.	0.	0.	0.	8	1	6	D-
0.	0.	0.	0.	0.	0.	8	7	3	D-
0.	0.	0.	0.	0.	0.	9	1	6	D-
0.	0.	0.	0.	0.	0.	9	7	3	D-

L(4)=(0.0000, 1.0000, -1.0000)

D+ 4

0.	0.	0.	0.	0.	0.	1	1	6	D-
0.	0.	0.	0.	0.	0.	1	7	3	D-
0.	0.	0.	0.	0.	0.	2	1	6	D-
0.	0.	0.	0.	0.	0.	2	7	3	D-
0.	0.	0.	0.	0.	0.	3	1	6	D-
0.	0.	0.	0.	0.	0.	3	7	3	D-
0.	0.	0.	0.	0.	0.	4	1	6	D-
0.	0.	0.	0.	0.	0.	4	7	3	D-
0.	0.	0.	0.	0.	0.	5	1	6	D-
0.	0.	0.	0.	0.	0.	5	7	3	D-
0.	0.	0.	0.	0.	0.	6	1	6	D-
0.	0.	0.	0.	0.	0.	6	7	3	D-
0.	0.	0.	0.	0.	0.	7	1	6	D-
0.	0.	0.	0.	0.	0.	7	7	3	D-
0.	0.	0.	0.	0.	0.	8	1	6	D-
0.	0.	0.	0.	0.	0.	8	7	3	D-
0.	0.	0.	0.	0.	0.	9	1	6	D-
0.	0.	0.	0.	0.	0.	9	7	3	D-

L(5)=(-1.0000, 1.0000, 0.0000)

D+ 5

0.	0.	0.	0.	0.	0.	1	1	6	D-
0.	0.	0.	0.	0.	0.	1	7	3	D-
0.	0.	0.	0.	0.	0.	2	1	6	D-
0.	0.	0.	0.	0.	0.	2	7	3	D-
0.	0.	0.	0.	0.	0.	3	1	6	D-
0.	0.	0.	0.	0.	0.	3	7	3	D-
0.	0.	0.	0.	0.	0.	4	1	6	D-
0.	0.	0.	0.	0.	0.	4	7	3	D-
0.	0.	0.	0.	0.	0.	5	1	6	D-
0.	0.	0.	0.	0.	0.	5	7	3	D-
0.	0.	0.	0.	0.	0.	6	1	6	D-
0.	0.	0.	0.	0.	0.	6	7	3	D-
0.	0.	0.	0.	0.	0.	7	1	6	D-
0.	0.	0.	0.	0.	0.	7	7	3	D-
0.	0.	0.	0.	0.	0.	8	1	6	D-
0.	0.	0.	0.	0.	0.	8	7	3	D-
0.	0.	0.	0.	0.	0.	9	1	6	D-
0.	0.	0.	0.	0.	0.	9	7	3	D-

L(6)=(-1.0000, 0.0000, 1.0000)

D+ 6									
0.	0.	0.	0.	0.	0.	1	1	6	0-
0.	0.	0.	0.	0.	0.	1	7	3	0-
0.	0.	0.	0.	0.	0.	2	1	6	0-
0.	0.	0.	0.	0.	0.	2	7	3	0-
0.	0.	0.	0.	0.	0.	3	1	6	0-
0.	0.	0.	0.	0.	0.	3	7	3	0-
0.	0.	0.	0.	0.	0.	4	1	6	0-
0.	0.	0.	0.	0.	0.	4	7	3	0-
0.	0.	0.	0.	0.	0.	5	1	6	0-
0.	0.	0.	0.	0.	0.	5	7	3	0-
0.	0.	0.	0.	0.	0.	6	1	6	0-
0.	0.	0.	0.	0.	0.	6	7	3	0-
0.	0.	0.	0.	0.	0.	7	1	6	0-
0.	0.	0.	0.	0.	0.	7	7	3	0-
0.	0.	0.	0.	0.	0.	8	1	6	0-
0.	0.	0.	0.	0.	0.	8	7	3	0-
0.	0.	0.	0.	0.	0.	9	1	6	0-
0.	0.	0.	0.	0.	0.	9	7	3	0-

L(7)=(1.0000, 1.0000, -1.0000)

D+ 7

0.	0.	0.	0.	0.	0.	1	1	6	D-
0.	0.	0.	0.	0.	0.	1	7	3	D-
0.	0.	0.	0.	0.	0.	2	1	6	D-
0.	0.	0.	0.	0.	0.	2	7	3	D-
0.	0.	0.	0.	0.	0.	3	1	6	D-
0.	0.	0.	0.	0.	0.	3	7	3	D-
0.	0.	0.	0.	0.	0.	4	1	6	D-
0.	0.	0.	0.	0.	0.	4	7	3	D-
0.	0.	0.	0.	0.	0.	5	1	6	D-
0.	0.	0.	0.	0.	0.	5	7	3	D-
0.	0.	0.	0.	0.	0.	6	1	6	D-
0.	0.	0.	0.	0.	0.	6	7	3	D-
0.	0.	0.	0.	0.	0.	7	1	6	D-
0.	0.	0.	0.	0.	0.	7	7	3	D-
0.	0.	0.	0.	0.	0.	8	1	6	D-
0.	0.	0.	0.	0.	0.	8	7	3	D-
0.	0.	0.	0.	0.	0.	9	1	6	D-
0.	0.	0.	0.	0.	0.	9	7	3	D-
2.02819E-01	0.	0.	0.	0.	0.	1	1	6	D-0
0.	0.	0.	0.	0.	0.	1	7	3	D-0
0.	2.02819E-31	0.	0.	0.	0.	2	1	6	D-0
0.	0.	0.	0.	0.	0.	2	7	3	D-0
0.	0.	2.02819E-01	0.	0.	0.	3	1	6	D-0
0.	0.	0.	0.	0.	0.	3	7	3	D-0
0.	0.	0.	9.17852E-02	0.	0.	4	1	6	D-0
0.	0.	0.	0.	0.	0.	4	7	3	D-0
0.	0.	0.	0.	9.17852E-02	0.	5	1	6	D-0
0.	0.	0.	0.	0.	0.	5	7	3	D-0
0.	0.	0.	0.	0.	9.17852E-02	6	1	6	D-0
0.	0.	0.	0.	0.	0.	6	7	3	D-0
2.02819E-01	0.	0.	0.	0.	0.	7	1	6	D-0
0.	0.	0.	0.	0.	0.	7	7	3	D-0
0.	2.02819E-01	0.	0.	0.	0.	8	1	6	D-0
0.	0.	0.	0.	0.	0.	8	7	3	D-0
0.	0.	0.	0.	0.	0.	9	1	6	D-0
0.	0.	2.02819E-01	0.	0.	0.	9	7	3	D-0

D- 1

0.	0.	0.	0.	0.	0.	1	1	6	D+
0.	0.	0.	0.	0.	0.	1	7	3	D+
0.	0.	0.	0.	0.	0.	2	1	6	D+
0.	0.	0.	0.	0.	0.	2	7	3	D+
0.	0.	0.	0.	0.	0.	3	1	6	D+
0.	0.	0.	0.	0.	0.	3	7	3	D+
0.	0.	0.	0.	0.	0.	4	1	6	D+
0.	0.	0.	0.	0.	0.	4	7	3	D+
0.	0.	0.	0.	0.	0.	5	1	6	D+
0.	0.	0.	0.	0.	0.	5	7	3	D+
0.	0.	0.	0.	0.	0.	6	1	6	D+
0.	0.	0.	0.	0.	0.	6	7	3	D+
0.	0.	0.	0.	0.	0.	7	1	6	D+
0.	0.	0.	0.	0.	0.	7	7	3	D+
0.	0.	0.	0.	0.	0.	8	1	6	D+
0.	0.	0.	0.	0.	0.	8	7	3	D+
0.	0.	0.	0.	0.	0.	9	1	6	D+
0.	0.	0.	0.	0.	0.	9	7	3	D+

0.	0.	0.	0.	0.	0.	1	1	6	D+
0.	0.	0.	0.	0.	0.	1	7	3	D+
0.	0.	0.	0.	0.	0.	2	1	6	D+
0.	0.	0.	0.	0.	0.	2	7	3	D+
0.	0.	0.	0.	0.	0.	3	1	6	D+
0.	0.	0.	0.	0.	0.	3	7	3	D+
0.	0.	0.	0.	0.	0.	4	1	6	D+
0.	0.	0.	0.	0.	0.	4	7	3	D+
0.	0.	0.	0.	0.	0.	5	1	6	D+
0.	0.	0.	0.	0.	0.	5	7	3	D+
0.	0.	0.	0.	0.	0.	6	1	6	D+
0.	0.	0.	0.	0.	0.	6	7	3	D+
0.	0.	0.	0.	0.	0.	7	1	6	D+
0.	0.	0.	0.	0.	0.	7	7	3	D+
0.	0.	0.	0.	0.	0.	8	1	6	D+
0.	0.	0.	0.	0.	0.	8	7	3	D+
0.	0.	0.	0.	0.	0.	9	1	6	D+
0.	0.	0.	0.	0.	0.	9	7	3	D+

D- 3

[illegible]

D- 4

0.	0.	0.	0.	0.	0.	1	1	6	D+
0.	0.	0.	0.	0.	0.	1	7	3	D+
0.	0.	0.	0.	0.	0.	2	1	6	D+
0.	0.	0.	0.	0.	0.	2	7	3	D+
0.	0.	0.	0.	0.	0.	3	1	6	D+
0.	0.	0.	0.	0.	0.	3	7	3	D+
0.	0.	0.	0.	0.	0.	4	1	6	D+
0.	0.	0.	0.	0.	0.	4	7	3	D+
0.	0.	0.	0.	0.	0.	5	1	6	D+
0.	0.	0.	0.	0.	0.	5	7	3	D+
0.	0.	0.	0.	0.	0.	6	1	6	D+
0.	0.	0.	0.	0.	0.	6	7	3	D+
0.	0.	0.	0.	0.	0.	7	1	6	D+
0.	0.	0.	0.	0.	0.	7	7	3	D+
0.	0.	0.	0.	0.	0.	8	1	6	D+
0.	0.	0.	0.	0.	0.	8	7	3	D+
0.	0.	0.	0.	0.	0.	9	1	6	D+

0.	0.	0.	0.	0.	0.	9	7	3	D+
D- 5									
0.	0.	0.	0.	0.	0.	1	1	6	D+
0.	0.	0.	0.	0.	0.	1	7	3	D+
0.	0.	0.	0.	0.	0.	2	1	6	D+
0.	0.	0.	0.	0.	0.	2	7	3	D+
0.	0.	0.	0.	0.	0.	3	1	6	D+
0.	0.	0.	0.	0.	0.	3	7	3	D+
0.	0.	0.	0.	0.	0.	4	1	6	D+
0.	0.	0.	0.	0.	0.	4	7	3	D+
0.	0.	0.	0.	0.	0.	5	1	6	D+
0.	0.	0.	0.	0.	0.	5	7	3	D+
0.	0.	0.	0.	0.	0.	6	1	6	D+
0.	0.	0.	0.	0.	0.	6	7	3	D+
0.	0.	0.	0.	0.	0.	7	1	6	D+
0.	0.	0.	0.	0.	0.	7	7	3	D+
0.	0.	0.	0.	0.	0.	8	1	6	D+
0.	0.	0.	0.	0.	0.	8	7	3	D+
0.	0.	0.	0.	0.	0.	9	1	6	D+
0.	0.	0.	0.	0.	0.	9	7	3	D+

0.	0.	0.	0.	0.	0.	1	1	6	D+
D- 6									
0.	0.	0.	0.	0.	0.	1	7	3	D+
0.	0.	0.	0.	0.	0.	2	1	6	D+
0.	0.	0.	0.	0.	0.	2	7	3	D+
0.	0.	0.	0.	0.	0.	3	1	6	D+
0.	0.	0.	0.	0.	0.	3	7	3	D+
0.	0.	0.	0.	0.	0.	4	1	6	D+
0.	0.	0.	0.	0.	0.	4	7	3	D+
0.	0.	0.	0.	0.	0.	5	1	6	D+
0.	0.	0.	0.	0.	0.	5	7	3	D+
0.	0.	0.	0.	0.	0.	6	1	6	D+
0.	0.	0.	0.	0.	0.	6	7	3	D+
0.	0.	0.	0.	0.	0.	7	1	6	D+
0.	0.	0.	0.	0.	0.	7	7	3	D+
0.	0.	0.	0.	0.	0.	8	1	6	D+
0.	0.	0.	0.	0.	0.	8	7	3	D+
0.	0.	0.	0.	0.	0.	9	1	6	D+
0.	0.	0.	0.	0.	0.	9	7	3	D+

0.	0.	0.	0.	0.	0.	1	1	6	D+
D- 7									
0.	0.	0.	0.	0.	0.	1	7	3	D+
0.	0.	0.	0.	0.	0.	2	1	6	D+
0.	0.	0.	0.	0.	0.	2	7	3	D+
0.	0.	0.	0.	0.	0.	3	1	6	D+
0.	0.	0.	0.	0.	0.	3	7	3	D+
0.	0.	0.	0.	0.	0.	4	1	6	D+
0.	0.	0.	0.	0.	0.	4	7	3	D+
0.	0.	0.	0.	0.	0.	5	1	6	D+
0.	0.	0.	0.	0.	0.	5	7	3	D+
0.	0.	0.	0.	0.	0.	6	1	6	D+
0.	0.	0.	0.	0.	0.	6	7	3	D+
0.	0.	0.	0.	0.	0.	7	1	6	D+
0.	0.	0.	0.	0.	0.	7	7	3	D+
0.	0.	0.	0.	0.	0.	8	1	6	D+
0.	0.	0.	0.	0.	0.	8	7	3	D+

0.	0.	0.	0.	0.	0.	9	1	6	D+
0.	0.	0.	0.	0.	0.	9	7	3	D+
D									
2.0281870E-01	0.	0.	0.	0.	0.			1	1 3 0
0.	0.	0.	0.	0.	0.			1	4 3 0
0.	0.	0.	0.	0.	0.			1	7 3 0
0.	0.	2.0281870E-01	0.	0.	0.			2	1 3 0
0.	0.	0.	0.	0.	0.			2	4 3 0
0.	0.	0.	0.	0.	0.			2	7 3 0
0.	0.	0.	0.	2.0281870E-01	0.			3	1 3 0
0.	0.	0.	0.	0.	0.			3	4 3 0
0.	0.	0.	0.	0.	0.			3	7 3 0
0.	0.	0.	0.	0.	0.			4	1 3 0
9.1785200E-02	0.	0.	0.	0.	0.			4	4 3 0
0.	0.	0.	0.	0.	0.			4	7 3 0
0.	0.	0.	0.	0.	0.			5	1 3 0
0.	0.	9.1785200E-02	0.	0.	0.			5	4 3 0
0.	0.	0.	0.	0.	0.			5	7 3 0
0.	0.	0.	0.	0.	0.			6	1 3 0
0.	0.	0.	0.	0.	9.1785200E-02			6	4 3 0
0.	0.	0.	0.	0.	0.			6	7 3 0
0.	0.	0.	0.	0.	0.			7	1 3 0
0.	0.	0.	0.	0.	0.			7	4 3 0
2.0281870E-01	0.	0.	0.	0.	0.			7	7 3 0
0.	0.	0.	0.	0.	0.			8	1 3 0
0.	0.	0.	0.	0.	0.			8	4 3 0
0.	0.	2.0281870E-01	0.	0.	0.			8	7 3 0
0.	0.	0.	0.	0.	0.			9	1 3 0
0.	0.	0.	0.	0.	0.			9	4 3 0
0.	0.	0.	0.	0.	2.0281870E-01			9	7 3 0

F- 1									
0.	0.	0.	-1.03600E-01	1.31400E-01	1.31400E-01	1	1	6	F-
0.	-0.	-0.	0.	0.	0.	1	7	3	F-
0.	0.	0.	1.31400E-01	-1.03600E-01	-1.31400E-01	2	1	6	F-
-0.	-0.	-0.	0.	0.	0.	2	7	3	F-
0.	0.	0.	1.31400E-01	-1.03600E-01	-1.03600E-01	3	1	6	F-
-0.	-0.	0.	0.	0.	0.	3	7	3	F-
0.	0.	0.	-4.13200E-02	-0.	-0.	4	1	6	F-
0.	0.	0.	0.	0.	0.	4	7	3	F-
0.	0.	0.	-0.	-7.57400E-02	-3.44300E-02	5	1	6	F-
0.	0.	0.	0.	0.	0.	5	7	3	F-
0.	0.	0.	-0.	-3.44300E-02	-7.57400E-02	6	1	6	F-
0.	0.	0.	0.	0.	0.	6	7	3	F-
0.	0.	0.	0.	0.	0.	7	1	6	F-
0.	0.	0.	0.	0.	0.	7	7	3	F-
0.	0.	0.	0.	0.	0.	8	1	6	F-
0.	0.	0.	0.	0.	0.	8	7	3	F-
0.	0.	0.	0.	0.	0.	9	1	6	F-
0.	0.	0.	0.	0.	0.	9	7	3	F-

F- 2									
0.	0.	0.	-1.03600E-01	1.31400E-01	-1.31400E-01	1	1	6	F-
-0.	-0.	-0.	0.	0.	0.	1	7	3	F-
0.	0.	0.	1.31400E-01	-1.03600E-01	1.31400E-01	2	1	6	F-
-0.	0.	-0.	0.	0.	0.	2	7	3	F-
0.	0.	0.	-1.31400E-01	1.31400E-01	-1.03600E-01	3	1	6	F-
-0.	-0.	0.	0.	0.	0.	3	7	3	F-

0.	0.	0.	-7.57400E-02	-0.	-3.44300E-02	4	1	6	F-
0.	0.	0.	0.	0.	0.	4	7	3	F-
0.	0.	0.	-0.	-4.13200E-02	-0.	5	1	6	F-
0.	0.	0.	0.	0.	0.	5	7	3	F-
0.	0.	0.	-3.44300E-02	-0.	-7.57400E-02	6	1	6	F-
0.	0.	0.	0.	0.	0.	6	7	3	F-
0.	0.	0.	0.	0.	0.	7	1	6	F-
0.	0.	0.	0.	0.	0.	7	7	3	F-
0.	0.	0.	0.	0.	0.	8	1	6	F-
0.	0.	0.	0.	0.	0.	8	7	3	F-
0.	0.	0.	0.	0.	0.	9	1	6	F-
0.	0.	0.	0.	0.	0.	9	7	3	F-

F- 3									
0.	0.	0.	-1.03600E-01	-1.31400E-01	1.31400E-01	1	1	6	F-
0.	0.	0.	0.	0.	0.	1	7	3	F-
0.	0.	0.	-1.31400E-01	-1.03600E-01	1.31400E-01	2	1	6	F-
0.	0.	0.	0.	0.	0.	2	7	3	F-
0.	0.	0.	1.31400E-01	1.31400E-01	-1.03600E-01	3	1	6	F-
0.	0.	0.	0.	0.	0.	3	7	3	F-
0.	0.	0.	-7.57400E-02	-3.44300E-02	-0.	4	1	6	F-
0.	0.	0.	0.	0.	0.	4	7	3	F-
0.	0.	0.	-3.44300E-02	-7.57400E-02	-0.	5	1	6	F-
0.	0.	0.	0.	0.	0.	5	7	3	F-
0.	0.	0.	-0.	-0.	-4.13200E-02	6	1	6	F-
0.	0.	0.	0.	0.	0.	6	7	3	F-
0.	0.	0.	-1.03600E-01	-1.31400E-01	-1.31400E-01	7	1	6	F-
0.	0.	0.	0.	0.	0.	7	7	3	F-
0.	0.	0.	-1.31400E-01	-1.03600E-01	-1.31400E-01	8	1	6	F-
0.	0.	0.	0.	0.	0.	8	7	3	F-
0.	0.	0.	-1.31400E-01	-1.31400E-01	-1.03600E-01	9	1	6	F-
0.	0.	0.	0.	0.	0.	9	7	3	F-

F- 4									
0.	0.	0.	0.	0.	0.	1	1	6	F-
0.	-0.	-0.	0.	0.	0.	1	7	3	F-
0.	0.	0.	0.	0.	0.	2	1	6	F-
-0.	-0.	-0.	0.	0.	0.	2	7	3	F-
0.	0.	0.	0.	0.	0.	3	1	6	F-
-0.	-0.	0.	0.	0.	0.	3	7	3	F-
0.	0.	0.	-4.13200E-02	-0.	-0.	4	1	6	F-
-1.03600E-01	1.31400E-01	-1.31400E-01	0.	0.	0.	4	7	3	F-
0.	0.	0.	-0.	-7.57400E-02	3.44300E-02	5	1	6	F-
1.31400E-01	-1.03600E-01	1.31400E-01	0.	0.	0.	5	7	3	F-
0.	0.	0.	-0.	3.44300E-02	-7.57400E-02	6	1	6	F-
-1.31400E-01	1.31400E-01	-1.03600E-01	0.	0.	0.	6	7	3	F-
0.	0.	0.	0.	0.	0.	7	1	6	F-
0.	0.	0.	0.	0.	0.	7	7	3	F-
0.	0.	0.	0.	0.	0.	8	1	6	F-
0.	0.	0.	0.	0.	0.	8	7	3	F-
0.	0.	0.	0.	0.	0.	9	1	6	F-
0.	0.	0.	0.	0.	0.	9	7	3	F-

F- 5									
0.	0.	0.	0.	0.	0.	1	1	6	F-
0.	0.	0.	0.	0.	0.	1	7	3	F-
0.	0.	0.	0.	0.	0.	2	1	6	F-
0.	0.	0.	0.	0.	0.	2	7	3	F-
0.	0.	0.	0.	0.	0.	3	1	6	F-

0.	0.	0.	0.	0.	0.	3	7	3	F-
0.	0.	0.	-7.57400E-02	3.44300E-02	-0.	4	1	6	F-
0.	0.	0.	0.	0.	0.	4	7	3	F-
0.	0.	0.	3.44300E-02	-7.57400E-02	-0.	5	1	6	F-
0.	0.	0.	0.	0.	0.	5	7	3	F-
0.	0.	0.	-0.	-0.	-4.13200E-02	6	1	6	F-
0.	0.	0.	0.	0.	0.	6	7	3	F-
0.	0.	0.	0.	0.	0.	7	1	6	F-
0.	0.	0.	0.	0.	0.	7	7	3	F-
0.	0.	0.	0.	0.	0.	8	1	6	F-
0.	0.	0.	0.	0.	0.	8	7	3	F-
0.	0.	0.	0.	0.	0.	9	1	6	F-
0.	0.	0.	0.	0.	0.	9	7	3	F-

F- 6

0.	0.	0.	0.	0.	0.	1	1	6	F-
0.	0.	0.	0.	0.	0.	1	7	3	F-
0.	0.	0.	0.	0.	0.	2	1	6	F-
0.	0.	0.	0.	0.	0.	2	7	3	F-
0.	0.	0.	0.	0.	0.	3	1	6	F-
0.	0.	0.	0.	0.	0.	3	7	3	F-
0.	0.	0.	-7.57400E-02	-0.	3.44300E-02	4	1	6	F-
0.	0.	0.	0.	0.	0.	4	7	3	F-
0.	0.	0.	-0.	-4.13200E-02	-0.	5	1	6	F-
0.	0.	0.	0.	0.	0.	5	7	3	F-
0.	0.	0.	3.44300E-02	-0.	-7.57400E-02	6	1	6	F-
0.	0.	0.	0.	0.	0.	6	7	3	F-
-0.	-0.	-0.	-1.03600E-01	1.31400E-01	-1.31400E-01	7	1	6	F-
0.	0.	0.	0.	0.	0.	7	7	3	F-
-0.	0.	-0.	1.31400E-01	-1.03600E-01	-1.31400E-01	8	1	6	F-
0.	0.	0.	0.	0.	0.	8	7	3	F-
-0.	-0.	0.	1.31400E-01	-1.31400E-01	-1.03600E-01	9	1	6	F-
0.	0.	0.	0.	0.	0.	9	7	3	F-

F- 7

0.	0.	0.	0.	0.	0.	1	1	6	F-
0.	-0.	-0.	0.	0.	0.	1	7	3	F-
0.	0.	0.	0.	0.	0.	2	1	6	F-
-0.	0.	-0.	0.	0.	0.	2	7	3	F-
0.	0.	0.	0.	0.	0.	3	1	6	F-
-0.	-0.	-0.	0.	0.	0.	3	7	3	F-
0.	0.	0.	0.	0.	0.	4	1	6	F-
0.	0.	0.	0.	0.	0.	4	7	3	F-
0.	0.	0.	0.	0.	0.	5	1	6	F-
0.	0.	0.	0.	0.	0.	5	7	3	F-
0.	0.	0.	0.	0.	0.	6	1	6	F-
0.	0.	0.	0.	0.	0.	6	7	3	F-
0.	0.	0.	0.	0.	0.	7	1	6	F-
0.	0.	0.	0.	0.	0.	7	7	3	F-
0.	0.	0.	0.	0.	0.	8	1	6	F-
0.	0.	0.	0.	0.	0.	8	7	3	F-
0.	0.	0.	0.	0.	0.	9	1	6	F-
0.	0.	0.	0.	0.	0.	9	7	3	F-
4.14400E-01	-0.	-0.	-1.03600E-01	-1.31400E-01	-1.31400E-01	1	1	6	F-0
0.	-0.	-0.	0.	0.	0.	1	7	3	F-0
-0.	4.14400E-01	-0.	-1.31400E-01	-1.03600E-01	-1.31400E-01	2	1	6	F-0
-0.	0.	-0.	0.	0.	0.	2	7	3	F-0
-0.	-0.	-0.	4.14400E-01	-1.31400E-01	-1.03600E-01	3	1	6	F-0
-0.	-0.	-0.	0.	0.	0.	3	7	3	F-0

0.	0.	0.	1.60000E 00	-0.	-0.	4	1	6	F-0
-1.03600E-01	-1.31400E-01	1.31400E-01	0.	0.	0.	4	7	3	F-0
0.	0.	0.	-0.	1.60000E 00	-0.	5	1	6	F-0
-1.31400E-01	-1.03600E-01	1.31400E-01	0.	0.	0.	5	7	3	F-0
0.	0.	0.	-0.	-0.	1.60000E 00	6	1	6	F-0
1.31400E-01	1.31400E-01	-1.03600E-01	0.	0.	0.	6	7	3	F-0
0.	0.	0.	0.	0.	0.	7	1	6	F-0
4.14400E-01	-0.	-0.	0.	0.	0.	7	7	3	F-0
0.	0.	0.	0.	0.	0.	8	1	6	F-0
-0.	4.14400E-01	-0.	0.	0.	0.	8	7	3	F-0
0.	0.	0.	0.	0.	0.	9	1	6	F-0
-0.	-0.	4.14400E-01	0.	0.	0.	9	7	3	F-0
4.1440000E-01	-0.	-0.	-0.	-0.	-0.				
-2.7122832E-01	1.9705891E-01	-1.8626451E-09	-0.	-1.8626451E-09	-0.	1	1	3	F
0.	-0.	0.	0.	0.	0.	1	4	3	F
-0.	-0.	4.1440000E-01	-0.	-0.	-0.	2	1	3	F
-1.8626451E-09	-0.	-2.7122832E-01	1.9705891E-01	-1.8159033E-01	-2.4993765E-01	2	4	3	F
0.	0.	0.	-0.	0.	0.	2	7	3	F
-0.	-0.	-0.	-0.	4.1440000E-01	-0.	3	1	3	F
-1.8626451E-09	-0.	-1.8159033E-01	-2.4993765E-01	-2.7122832E-01	1.9705891E-01	3	4	3	F
0.	0.	0.	0.	0.	0.	3	7	3	F
-2.7122832E-01	-1.9705891E-01	-1.8626451E-09	-0.	-1.8626451E-09	-0.	4	1	3	F
1.2474804E 00	-0.	-0.	-0.	-0.	-0.	4	4	3	F
-2.7122832E-01	-1.9705891E-01	-1.8626451E-09	-0.	1.8626451E-09	-0.	4	7	3	F
-1.8626451E-09	-0.	-2.7122832E-01	-1.9705891E-01	-1.8159033E-01	2.4993765E-01	5	1	3	F
-0.	-0.	1.1523459E 00	-0.	-0.	-0.	5	4	3	F
-1.8626451E-09	-0.	-2.7122832E-01	-1.9705891E-01	1.8159033E-01	-2.4993765E-01	5	7	3	F
-1.8626451E-09	-0.	-1.8159033E-01	-2.4993765E-01	-2.7122832E-01	-1.9705891E-01	6	1	3	F
-0.	-0.	-0.	-0.	1.1523459E 00	-0.	6	4	3	F
1.8626451E-09	-0.	1.8159033E-01	-2.4993765E-01	-2.7122832E-01	-1.9705891E-01	6	7	3	F
0.	-0.	0.	-0.	0.	-0.	7	1	3	F
-2.7122832E-01	1.9705891E-01	-1.8626451E-09	-0.	1.8626451E-09	-0.	7	4	3	F
4.1440000E-01	-0.	-0.	-0.	-0.	-0.	7	7	3	F
0.	-0.	0.	-0.	0.	-0.	8	1	3	F
-1.8626451E-09	-0.	-2.7122832E-01	1.9705891E-01	1.8159033E-01	2.4993765E-01	8	4	3	F
-0.	-0.	4.1440000E-01	-0.	-0.	-0.	8	7	3	F
0.	-0.	0.	-0.	0.	-0.	9	1	3	F
1.8626451E-09	-0.	1.8159033E-01	2.4993765E-01	-2.7122832E-01	1.9705891E-01	9	4	3	F
-0.	-0.	-0.	-0.	4.1440000E-01	-0.	9	7	3	F
8.4048068E-02	0.	0.	0.	0.	0.	1	1	3	F*D
-2.4894745E-02	1.8087091E-02	-1.7096326E-10	0.	-1.7096326E-10	0.	1	4	3	F*D
0.	0.	0.	0.	0.	0.	1	7	3	F*D
0.	0.	8.4048068E-02	0.	0.	0.	2	1	3	F*D
-1.7096326E-10	0.	-2.4894745E-02	1.8087091E-02	-1.6667305E-02	-2.2940577E-02	2	4	3	F*D
0.	0.	0.	0.	0.	0.	2	7	3	F*D
0.	0.	0.	0.	8.4048068E-02	0.	3	1	3	F*D
-1.7096326E-10	0.	-1.6667305E-02	-2.2940577E-02	-2.4894745E-02	1.8087091E-02	3	4	3	F*D
0.	0.	0.	0.	0.	0.	3	7	3	F*D
-5.5010174E-02	-3.9967231E-02	-3.7777926E-10	-0.	-3.7777926E-10	-0.	4	1	3	F*D
1.1450024E-01	-0.	0.	-0.	0.	-0.	4	4	3	F*D
-5.5010174E-02	-3.9967231E-02	-3.7777926E-10	-0.	3.7777926E-10	-0.	4	7	3	F*D
-3.7777926E-10	-0.	-5.5010174E-02	-3.9967231E-02	-3.6829914E-02	5.0692029E-02	5	1	3	F*D
0.	-0.	1.0576830E-01	-0.	0.	-0.	5	4	3	F*D
-3.7777926E-10	-0.	-5.5010174E-02	-3.9967231E-02	3.6829914E-02	-5.0692029E-02	5	7	3	F*D
-3.7777926E-10	-0.	-3.6829914E-02	5.0692029E-02	-5.5010174E-02	-3.9967231E-02	6	1	3	F*D
0.	-0.	0.	-0.	1.0576830E-01	-0.	6	4	3	F*D
3.7777926E-10	-0.	3.6829914E-02	-5.0692029E-02	-5.5010174E-02	-3.9967231E-02	6	7	3	F*D
0.	-0.	0.	-0.	0.	-0.	7	1	3	F*D
-2.4894745E-02	1.8087091E-02	-1.7096326E-10	-0.	1.7096326E-10	-0.	7	4	3	F*D

8.4048068E-02	-0.	0.	-0.	0.	-0.	7	7	3	F*D
0.	-0.	0.	-0.	0.	-0.	8	1	3	F*D
-1.7096326E-10	-0.	-2.4E94745E-02	1.8087091E-02	1.6667305E-02	2.2940577E-02	8	4	3	F*D
0.	-0.	8.4C48068E-02	-0.	0.	-0.	8	7	3	F*D
0.	-0.	0.	-0.	0.	-0.	9	1	3	F*D
1.7096326E-10	-0.	1.6667305E-02	2.2940577E-02	-2.4E94745E-02	1.8087091E-02	9	4	3	F*D
0.	-0.	0.	-0.	8.4C48068E-02	-0.	9	7	3	F*D
1.7046520E-02	-0.	0.	-0.	0.	-0.	1	1	3	DFD
-5.0491198E-03	3.6684003E-03	-3.4674545E-11	-0.	-3.4674545E-11	0.	1	4	3	DFD
0.	-0.	0.	-0.	0.	-0.	1	7	3	DFD
0.	-0.	1.7046520E-02	-0.	0.	-0.	2	1	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	3.6684003E-03	-3.3804410E-03	-4.6527779E-03	2	4	3	DFD
0.	-0.	0.	-0.	0.	-0.	2	7	3	DFD
0.	-0.	0.	-0.	1.7046520E-02	-0.	3	1	3	DFD
-3.4674545E-11	-0.	-3.3804410E-03	-4.6527779E-03	-5.0491198E-03	3.6684003E-03	3	4	3	DFD
0.	-0.	0.	-0.	0.	-0.	3	7	3	DFD
-5.0491198E-03	-3.6684003E-03	-3.4674545E-11	-0.	-3.4674545E-11	-0.	4	1	3	DFD
1.0509427E-02	-0.	0.	-0.	0.	-0.	4	4	3	DFD
-5.0491198E-03	-3.6684003E-03	-3.4674545E-11	-0.	3.4674545E-11	-0.	4	7	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	-3.6684003E-03	-3.3804410E-03	4.6527779E-03	5	1	3	DFD
0.	-0.	9.7079642E-03	-0.	0.	0.	5	4	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	-3.6684003E-03	3.3804410E-03	-4.6527779E-03	5	7	3	DFD
-3.4674545E-11	-0.	-3.3804410E-03	4.6527779E-03	-5.0491198E-03	-3.6684003E-03	6	1	3	DFD
0.	-0.	0.	-0.	9.7079642E-03	0.	6	4	3	DFD
3.4674545E-11	-0.	3.3804410E-03	-4.6527779E-03	-5.0491198E-03	-3.6684003E-03	6	7	3	DFD
0.	-0.	0.	-0.	0.	-0.	7	1	3	DFD
-5.0491198E-03	3.6684003E-03	-3.4674545E-11	-0.	3.4674545E-11	0.	7	4	3	DFD
1.7046520E-02	-0.	0.	-0.	0.	-0.	7	7	3	DFD
0.	-0.	0.	-0.	0.	-0.	8	1	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	3.6684003E-03	3.3804410E-03	4.6527779E-03	8	4	3	DFD
0.	-0.	1.7046520E-02	-0.	0.	-0.	8	7	3	DFD
0.	-0.	0.	-0.	0.	-0.	9	1	3	DFD
3.4674545E-11	-0.	3.3804410E-03	4.6527779E-03	-5.0491198E-03	3.6684003E-03	9	4	3	DFD
0.	-0.	0.	-0.	1.7046520E-02	-0.	9	7	3	DFD

CELL VOLUME OF DIRECT SPACE = 77.05800

ATOM MASSES AND POSITIONS

1	M(1)	L1(1)	L2(1)	L3(1)
1	2.43100E 01	2.50000E-01	2.50000E-01	2.50000E-01
2	1.18700E 02	0.	0.	0.
3	2.43100E 01	2.50000E-01	2.50000E-01	7.50000E-01

FRACTIONAL CHARGE ON ATOMS

1	-5.00000E-01
2	1.00000E 00
3	-5.00000E-01

COULOMB COUPLING COEFFICIENT MATRIX

7.0380200E 00	-0.	-0.	-0.	-0.	-0.	1	1	3	CCC
6.7498400E 00	-0.	-0.	-0.	-0.	-0.	1	4	3	CCC
1.0626260E 01	-0.	-0.	-0.	-0.	-0.	1	7	3	CCC
-0.	-0.	-3.5190100E 00	-0.	-0.	-0.	2	1	3	CCC
-0.	-0.	-3.3749200E 00	-0.	-0.	6.0225400E 00	2	4	3	CCC
-0.	-0.	-5.3131300E 00	-0.	-0.	-0.	2	7	3	CCC

-0.	-0.	-0.	-0.	-3.5190100E 00	-0.	3	1	3	CCC
-0.	-0.	-0.	6.0225400E 00	-3.3749200E 00	-0.	3	4	3	CCC
-0.	-0.	-0.	-0.	-5.3131300E 00	-0.	3	7	3	CCC
6.7498400E 00	-0.	-0.	-0.	-0.	-0.	4	1	3	CCC
7.0380200E 00	-0.	-0.	-0.	-0.	-0.	4	4	3	CCC
6.7498400E 00	-0.	-0.	-0.	-0.	-0.	4	7	3	CCC
-0.	-0.	-3.3749200E 00	-0.	-0.	-6.0225400E 00	5	1	3	CCC
-0.	-0.	-3.5190100E 00	-0.	-0.	-0.	5	4	3	CCC
-0.	-0.	-3.3749200E 00	-0.	-0.	6.0225400E 00	5	7	3	CCC
-0.	-0.	-0.	-6.0225400E 00	-3.3749200E 00	-0.	6	1	3	CCC
-0.	-0.	-0.	-0.	-3.5190100E 00	-0.	6	4	3	CCC
-0.	-0.	-0.	6.0225400E 00	-3.3749200E 00	-0.	6	7	3	CCC
1.0626260E 01	-0.	-0.	-0.	-0.	-0.	7	1	3	CCC
6.7498400E 00	-0.	-0.	-0.	-0.	-0.	7	4	3	CCC
7.0380200E 00	-0.	-0.	-0.	-0.	-0.	7	7	3	CCC
-0.	-0.	-5.3131300E 00	-0.	-0.	-0.	8	1	3	CCC
-0.	-0.	-3.3749200E 00	-0.	-0.	-6.0225400E 00	8	4	3	CCC
-0.	-0.	-3.5190100E 00	-0.	-0.	-0.	8	7	3	CCC
-0.	-0.	-0.	-0.	-5.3131300E 00	-0.	9	1	3	CCC
-0.	-0.	-0.	-6.0225400E 00	-3.3749200E 00	-0.	9	4	3	CCC
-0.	-0.	-0.	-0.	-3.5190100E 00	-0.	9	7	3	CCC

2.307/V*D(C)*Z*CCC*Z*D(C)

2.1668827E-03	-0.	-0.	-0.	-0.	-0.	1	1	3	DCD
-1.8809424E-03	0.	0.	0.	0.	-0.	1	4	3	DCD
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	1	7	3	DCD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	2	1	3	DCD
0.	0.	9.4047122E-04	0.	0.	-1.6782696E-03	2	4	3	DCD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	2	7	3	DCD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	3	1	3	DCD
0.	0.	0.	-1.6782696E-03	9.4047122E-04	0.	3	4	3	DCD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	DCD
-1.8809424E-03	0.	0.	0.	0.	0.	4	1	3	DCD
1.7751279E-03	-0.	-0.	-0.	-0.	-0.	4	4	3	DCD
-1.8809424E-03	0.	0.	0.	0.	0.	4	7	3	DCD
0.	0.	9.4047122E-04	0.	0.	1.6782696E-03	5	1	3	DCD
-0.	-0.	-8.8756394E-04	-0.	-0.	-0.	5	4	3	DCD
0.	0.	9.4047122E-04	0.	0.	-1.6782696E-03	5	7	3	DCD
0.	0.	0.	1.6782696E-03	9.4047122E-04	0.	6	1	3	DCD
-0.	-0.	-0.	-0.	-8.8756394E-04	-0.	6	4	3	DCD
0.	0.	0.	-1.6782696E-03	9.4047122E-04	0.	6	7	3	DCD
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	7	1	3	DCD
-1.8809424E-03	0.	0.	0.	0.	0.	7	4	3	DCD
2.1668827E-03	-0.	-0.	-0.	-0.	-0.	7	7	3	DCD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	8	1	3	DCD
0.	0.	9.4047122E-04	0.	0.	1.6782696E-03	8	4	3	DCD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	8	7	3	DCD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	9	1	3	DCD
0.	0.	0.	1.6782696E-03	9.4047122E-04	0.	9	4	3	DCD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	9	7	3	DCD

D(C)*F(C)*D(C)

2.1668827E-03	0.	-0.	-0.	-0.	-0.	1	1	3	DMD
-1.5217144E-03	1.1055902E-03	0.	-0.	0.	-0.	1	4	3	DMD
3.2716388E-03	0.	-0.	-0.	-0.	-0.	1	7	3	DMD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	2	1	3	DMD
0.	-0.	7.6085719E-04	-5.5279510E-04	9.8646208E-04	1.3577486E-03	2	4	3	DMD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	2	7	3	DMD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	3	1	3	DMD

0.	-0.	9.8646208E-04	1.3577486E-03	7.6085719E-04	-5.5279510E-04	3	4	3	DMD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	DMD
-1.5217144E-03	-1.1055902E-03	0.	0.	0.	0.	4	1	3	DMD
1.7751279E-03	0.	-0.	-0.	-0.	-0.	4	4	3	DMD
-1.5217144E-03	-1.1055902E-03	0.	0.	0.	0.	4	7	3	DMD
0.	0.	7.6085719E-04	5.5279510E-04	9.8646208E-04	-1.3577486E-03	5	1	3	DMD
-0.	-0.	-8.8756394E-04	-0.	-0.	-0.	5	4	3	DMD
0.	0.	7.6085719E-04	5.5279510E-04	-9.8646208E-04	1.3577486E-03	5	7	3	DMD
0.	0.	9.8646208E-04	-1.3577486E-03	7.6085719E-04	5.5279510E-04	6	1	3	DMD
-0.	-0.	-0.	-0.	-8.8756394E-04	-0.	6	4	3	DMD
0.	0.	-9.8646208E-04	1.3577486E-03	7.6085719E-04	5.5279510E-04	6	7	3	DMD
3.2716388E-03	-0.	-0.	0.	-0.	0.	7	1	3	DMD
-1.5217144E-03	1.1055902E-03	0.	-0.	0.	-0.	7	4	3	DMD
2.1668827E-03	0.	-0.	-0.	-0.	-0.	7	7	3	DMD
-0.	0.	-1.6358194E-03	0.	-0.	0.	8	1	3	DMD
0.	-0.	7.6085719E-04	-5.5279510E-04	-9.8646208E-04	-1.3577486E-03	8	4	3	DMD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	8	7	3	DMD
-0.	0.	-0.	0.	-1.6358194E-03	0.	9	1	3	DMD
0.	-0.	-9.8646208E-04	-1.3577486E-03	7.6085719E-04	-5.5279510E-04	9	4	3	DMD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	9	7	3	DMD

D(TRANPOSE)*F*D + D(C)*F(C)*D(C)									
1.9213402E-02	-0.	-0.	-0.	-0.	-0.	1	1	3	FFM
-6.5708342E-03	4.7739905E-03	-3.4674545E-11	-0.	-3.4674545E-11	0.	1	4	3	FFM
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	1	7	3	FFM
-0.	-0.	1.5963078E-02	-0.	-0.	-0.	2	1	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	3.1156052E-03	-2.3939790E-03	-3.2950294E-03	2	4	3	FFM
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	2	7	3	FFM
-0.	-0.	-0.	-0.	1.5963078E-02	-0.	3	1	3	FFM
-3.4674545E-11	-0.	-2.3939790E-03	-3.2950294E-03	-4.2882626E-03	3.1156052E-03	3	4	3	FFM
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	FFM
-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	-0.	-3.4674545E-11	-0.	4	1	3	FFM
1.2284555E-02	-0.	-0.	-0.	-0.	0.	4	4	3	FFM
-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	-0.	3.4674545E-11	-0.	4	7	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	-3.1156052E-03	-2.3939790E-03	3.2950294E-03	5	1	3	FFM
-0.	-0.	8.8204002E-03	-0.	-0.	0.	5	4	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	-3.1156052E-03	2.3939790E-03	-3.2950294E-03	5	7	3	FFM
-3.4674545E-11	-0.	-2.3939790E-03	3.2950294E-03	-4.2882626E-03	-3.1156052E-03	6	1	3	FFM
-0.	-0.	-0.	-0.	8.8204002E-03	0.	6	4	3	FFM
3.4674545E-11	-0.	-2.3939790E-03	-3.2950294E-03	-4.2882626E-03	-3.1156052E-03	6	7	3	FFM
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	7	1	3	FFM
-6.5708342E-03	4.7739905E-03	-3.4674545E-11	-0.	3.4674545E-11	0.	7	4	3	FFM
1.9213402E-02	-0.	-0.	-0.	-0.	-0.	7	7	3	FFM
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	8	1	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	3.1156052E-03	2.3939790E-03	-3.2950294E-03	8	4	3	FFM
-0.	-0.	1.5963078E-02	-0.	-0.	-0.	8	7	3	FFM
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	9	1	3	FFM
3.4674545E-11	-0.	2.3939790E-03	3.2950294E-03	-4.2882626E-03	3.1156052E-03	9	4	3	FFM
-0.	-0.	-0.	-0.	1.5963078E-02	-0.	9	7	3	FFM

A									
1.000000E 00	-0.	-0.	-0.	-0.	-0.	1	1	6	A
1.000000E 00	-0.	-0.	0.	0.	0.	1	7	3	A
-0.	-0.	-0.	1.000000E 00	-0.	-0.	2	1	6	A
-0.	-0.	0.	0.	0.	0.	2	7	3	A
1.000000E 00	-0.	-0.	-0.	-0.	-0.	3	1	6	A
-1.000000E 00	-0.	-0.	0.	0.	0.	3	7	3	A
-0.	1.000000E 00	-0.	-0.	-0.	-0.	4	1	6	A
-	1.000000E 00	-0.	0.	0.	0.	4	7	3	A

-0.	-0.	1.00000E 00	-0.	-0.	-0.	5	1	6	A
-0.	-0.	-1.00000E 00	0.	0.	0.	5	7	3	A
-0.	-0.	0.	-0.	1.00000E 00	-0.	6	1	6	A
-0.	-0.	0.	0.	0.	0.	6	7	3	A
-0.	-0.	1.00000E 00	-0.	-0.	-0.	7	1	6	A
-0.	-0.	1.00000E 00	0.	0.	0.	7	7	3	A
-0.	1.00000E 00	-0.	-0.	-0.	-0.	8	1	6	A
-0.	-1.00000E 00	-0.	0.	0.	0.	8	7	3	A
-0.	-0.	-0.	-0.	-0.	1.00000E 00	9	1	6	A
-0.	-0.	0.	0.	0.	0.	9	7	3	A

NORMALIZED A

7.07107E-01	-0.	-0.	-0.	-0.	-0.	1	1	6	A N
7.07107E-01	-0.	0.	0.	0.	0.	1	7	3	A N
-0.	-0.	-0.	1.00000E 00	-0.	-0.	2	1	6	A N
-0.	-0.	0.	0.	0.	0.	2	7	3	A N
7.07107E-01	-0.	-0.	-0.	-0.	-0.	3	1	6	A N
-7.07107E-01	-0.	-0.	0.	0.	0.	3	7	3	A N
-0.	7.07107E-01	-0.	-0.	-0.	-0.	4	1	6	A N
-0.	7.07107E-01	-0.	0.	0.	0.	4	7	3	A N
-0.	-0.	7.07107E-01	-0.	-0.	-0.	5	1	6	A N
-0.	-0.	-7.07107E-01	0.	0.	0.	5	7	3	A N
-0.	-0.	-0.	-0.	1.00000E 00	-0.	6	1	6	A N
-0.	-0.	0.	0.	0.	0.	6	7	3	A N
-0.	-0.	7.07107E-01	-0.	-0.	-0.	7	1	6	A N
-0.	-0.	7.07107E-01	0.	0.	0.	7	7	3	A N
-0.	7.07107E-01	-0.	-0.	-0.	-0.	8	1	6	A N
-0.	-7.07107E-01	-0.	0.	0.	0.	8	7	3	A N
-0.	-0.	-0.	-0.	-0.	1.00000E 00	9	1	6	A N
-0.	-0.	0.	0.	0.	0.	9	7	3	A N

A(STAR)

7.07107E-01	-0.	-0.	-0.	-0.	0.	1	1	6	A S
7.07107E-01	-0.	0.	0.	0.	0.	1	7	3	A S
0.	0.	0.	1.00000E 00	0.	-0.	2	1	6	A S
0.	0.	-0.	0.	0.	0.	2	7	3	A S
7.07107E-01	-0.	-0.	-0.	-0.	0.	3	1	6	A S
-7.07107E-01	-0.	0.	0.	0.	0.	3	7	3	A S
-0.	7.07107E-01	-0.	-0.	-0.	0.	4	1	6	A S
-0.	7.07107E-01	0.	0.	0.	0.	4	7	3	A S
-0.	-0.	7.07107E-01	-0.	-0.	0.	5	1	6	A S
-0.	-0.	-7.07107E-01	0.	0.	0.	5	7	3	A S
0.	0.	0.	0.	1.00000E 00	-0.	6	1	6	A S
0.	0.	-0.	0.	0.	0.	6	7	3	A S
0.	0.	7.07107E-01	0.	0.	-0.	7	1	6	A S
0.	0.	7.07107E-01	0.	0.	0.	7	7	3	A S
-0.	7.07107E-01	-0.	-0.	-0.	0.	8	1	6	A S
-0.	-7.07107E-01	0.	0.	0.	0.	8	7	3	A S
-0.	-0.	-0.	-0.	-0.	1.00000E 00	9	1	6	A S
-0.	-0.	0.	0.	0.	0.	9	7	3	A S

A(STAR)*(D*F*D + D(C)*F(C)*D(C))

1.5899325E-02	-0.	0.	-0.	0.	-0.	1	1	3	A*F
-9.2925628E-03	6.7514420E-03	-4.9037212E-11	0.	-0.	0.	1	4	3	A*F
1.5899325E-02	-0.	0.	-0.	0.	-0.	1	7	3	A*F
-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	0.	-3.4674545E-11	0.	2	1	3	A*F
1.2284555E-02	0.	0.	-0.	0.	-0.	2	4	3	A*F
-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	0.	3.4674545E-11	0.	2	7	3	A*F
1.1272529E-02	-0.	0.	-0.	0.	-0.	3	1	3	A*F

-0.	-0.	-0.	0.	-4.9037212E-11	0.	3	4	3	A*F
-1.1272529E-02	-0.	0.	-0.	0.	-0.	3	7	3	A*F
0.	-0.	1.0130902E-02	-0.	0.	-0.	4	1	3	A*F
-4.9037212E-11	-0.	-6.0645191E-03	4.4061310E-03	-0.	0.	4	4	3	A*F
0.	-0.	1.0130902E-02	-0.	0.	-0.	4	7	3	A*F
0.	0.	0.	0.	1.2444300E-02	0.	5	1	3	A*F
-4.9037212E-11	0.	-3.3855975E-03	-4.6598751E-03	-0.	-0.	5	4	3	A*F
0.	0.	0.	0.	-1.2444300E-02	0.	5	7	3	A*F
-3.4674545E-11	0.	-4.2882626E-03	-3.1156052E-03	-2.3939790E-03	3.2950294E-03	6	1	3	A*F
0.	0.	8.8204002E-03	-0.	0.	-0.	6	4	3	A*F
-3.4674545E-11	0.	-4.2882626E-03	-3.1156052E-03	2.3939790E-03	-3.2950294E-03	6	7	3	A*F
0.	-0.	0.	-0.	1.0130902E-02	-0.	7	1	3	A*F
-0.	-0.	-0.	0.	-6.0645191E-03	4.4061310E-03	7	4	3	A*F
0.	-0.	0.	-0.	1.0130902E-02	-0.	7	7	3	A*F
0.	-0.	1.2444300E-02	-0.	0.	-0.	8	1	3	A*F
-0.	-0.	-0.	0.	-3.3855975E-03	-4.6598751E-03	8	4	3	A*F
0.	-0.	-1.2444300E-02	-0.	0.	-0.	8	7	3	A*F
-3.4674545E-11	-0.	-2.3939790E-03	3.2950294E-03	-4.2882626E-03	-3.1156052E-03	9	1	3	A*F
0.	-0.	0.	0.	8.8204002E-03	0.	9	4	3	A*F
3.4674545E-11	-0.	2.3939790E-03	-3.2950294E-03	-4.2882626E-03	-3.1156052E-03	9	7	3	A*F
M									
2.2485041E-02	-0.	-9.2925628E-03	6.7514420E-03	0.	-0.	1	1	3	M
0.	-0.	0.	0.	-4.9037212E-11	0.	1	4	3	M
0.	-0.	0.	-0.	0.	-0.	1	7	3	M
-9.2925628E-03	-6.7514420E-03	1.2284555E-02	-0.	-0.	0.	2	1	3	M
-4.9037212E-11	0.	-4.9037212E-11	-0.	0.	-0.	2	4	3	M
-0.	0.	-0.	0.	0.	0.	2	7	3	M
0.	-0.	0.	0.	1.5941763E-02	-0.	3	1	3	M
0.	-0.	0.	0.	0.	0.	3	4	3	M
0.	-0.	0.	-0.	-4.9037212E-11	-0.	3	7	3	M
0.	-0.	-4.9037212E-11	0.	0.	-0.	4	1	3	M
1.4327258E-02	-0.	0.	0.	-6.0645191E-03	4.4061310E-03	4	4	3	M
0.	-0.	0.	-0.	0.	-0.	4	7	3	M
0.	0.	-4.9037212E-11	-0.	0.	0.	5	1	3	M
0.	0.	1.7598897E-02	-0.	-3.3855975E-03	-4.6598751E-03	5	4	3	M
0.	0.	0.	0.	0.	0.	5	7	3	M
-4.9037212E-11	-0.	0.	0.	-0.	-0.	6	1	3	M
-6.0645191E-03	-4.4061310E-03	-3.3855975E-03	4.6598751E-03	8.8204002E-03	0.	6	4	3	M
-0.	-0.	-0.	-0.	0.	-0.	6	7	3	M
0.	-0.	0.	0.	0.	-0.	7	1	3	M
0.	-0.	0.	0.	0.	0.	7	4	3	M
1.4327258E-02	-0.	0.	-0.	-6.0645191E-03	4.4061310E-03	7	7	3	M
0.	-0.	0.	0.	0.	-0.	8	1	3	M
0.	-0.	0.	0.	0.	0.	8	4	3	M
0.	-0.	1.7598897E-02	-0.	-3.3855975E-03	-4.6598751E-03	8	7	3	M
-0.	-0.	0.	0.	-4.9037212E-11	-0.	9	1	3	M
-0.	-0.	-0.	0.	0.	0.	9	4	3	M
-6.0645191E-03	-4.4061310E-03	-3.3855975E-03	4.6598751E-03	8.8204002E-03	-0.	9	7	3	M
M(HERMITIAN)									
2.2485041E-02	0.	-9.2925628E-03	6.7514420E-03	0.	-0.	1	1	3	M
0.	-0.	0.	-0.	-4.9037212E-11	-0.	1	4	3	M
0.	-0.	0.	-0.	-0.	-0.	1	7	3	M
-9.2925628E-03	-6.7514420E-03	1.2284555E-02	0.	0.	-0.	2	1	3	M
-4.9037212E-11	-0.	-4.9037212E-11	-0.	0.	-0.	2	4	3	M
0.	-0.	0.	-0.	0.	-0.	2	7	3	M
0.	0.	0.	0.	1.5941763E-02	0.	3	1	3	M
0.	-0.	0.	-0.	-0.	-0.	3	4	3	M

0.	-0.	0.	-0.	-4.9037212E-11	-0.	3	7	3	..
0.	0.	-4.9037212E-11	0.	0.	0.	4	1	3	M
1.4327258E-02	0.	0.	-0.	-6.0645191E-03	-4.4061310E-03	4	4	3	M
0.	-0.	0.	-0.	-0.	-0.	4	7	3	M
0.	0.	-4.9037212E-11	0.	0.	0.	5	1	3	M
0.	0.	1.7598897E-02	0.	-3.3855975E-03	-4.6598751E-03	5	4	3	M
0.	-0.	0.	-0.	-0.	-0.	5	7	3	M
-4.9037212E-11	0.	0.	0.	-0.	0.	6	1	3	M
-6.0645191E-03	-4.4061310E-03	-3.3855975E-03	4.6598751E-03	8.8204002E-03	-0.	6	4	3	M
0.	-0.	0.	-0.	0.	-0.	6	7	3	M
0.	0.	0.	0.	0.	0.	7	1	3	M
0.	0.	0.	0.	0.	0.	7	4	3	M
1.4327258E-02	0.	0.	-0.	-6.0645191E-03	4.4061310E-03	7	7	3	M
0.	0.	0.	0.	0.	0.	8	1	3	M
0.	0.	0.	0.	0.	0.	8	4	3	M
0.	0.	1.7598897E-02	0.	-3.3855975E-03	-4.6598751E-03	8	7	3	M
-0.	0.	0.	0.	-4.9037212E-11	0.	9	1	3	M
-0.	0.	-0.	0.	0.	0.	9	4	3	M
-6.0645191E-03	-4.4061310E-03	-3.3855975E-03	4.6598751E-03	8.8204002E-03	0.	9	7	3	M
2.24850E-02	-9.29256E-03	0.	0.	0.	1	1	6	HTR	
0.	0.	0.	0.	-6.75144E-03	0.	1	7	6	HTR
0.	0.	0.	0.	0.	0.	1	13	6	HTR
-9.29256E-03	1.22846E-02	0.	0.	0.	0.	2	1	6	HTR
0.	0.	0.	6.75144E-03	0.	0.	2	7	6	HTR
0.	0.	0.	0.	0.	0.	2	13	6	HTR
0.	0.	1.59418E-02	0.	0.	0.	3	1	6	HTR
0.	0.	0.	0.	0.	0.	3	7	6	HTR
0.	0.	0.	0.	0.	0.	3	13	6	HTR
0.	0.	0.	1.43273E-02	0.	-6.06452E-03	4	1	6	HTR
0.	0.	0.	0.	0.	0.	4	7	6	HTR
0.	0.	-4.40613E-03	0.	0.	0.	4	13	6	HTR
0.	0.	0.	0.	1.75989E-02	-3.38560E-03	5	1	6	HTR
0.	0.	0.	0.	0.	0.	5	7	6	HTR
0.	0.	4.65988E-03	0.	0.	0.	5	13	6	HTR
0.	0.	0.	-6.06452E-03	-3.38560E-03	8.82040E-03	6	1	6	HTR
0.	0.	0.	0.	0.	0.	6	7	6	HTR
4.40613E-03	-4.65988E-03	0.	0.	0.	0.	6	13	6	HTR
0.	0.	0.	0.	0.	0.	7	1	6	HTR
1.43273E-02	0.	-6.06452E-03	0.	0.	0.	7	7	6	HTR
0.	0.	0.	0.	0.	-4.40613E-03	7	13	6	HTR
0.	0.	0.	0.	0.	0.	8	1	6	HTR
0.	1.75989E-02	-3.38560E-03	0.	0.	0.	8	7	6	HTR
0.	0.	0.	0.	0.	4.65988E-03	8	13	6	HTR
0.	0.	0.	0.	0.	0.	9	1	6	HTR
-6.06452E-03	-3.38560E-03	8.82040E-03	0.	0.	0.	9	7	6	HTR
0.	0.	0.	4.40613E-03	-4.65988E-03	0.	9	13	6	HTR
0.	6.75144E-03	0.	0.	0.	0.	10	1	6	HTR
0.	0.	0.	2.24850E-02	-9.29256E-03	0.	10	7	6	HTR
0.	0.	0.	0.	0.	0.	10	13	6	HTR
-6.75144E-03	0.	0.	0.	0.	0.	11	1	6	HTR
0.	0.	0.	-9.29256E-03	1.22846E-02	0.	11	7	6	HTR
0.	0.	0.	0.	0.	0.	11	13	6	HTR
0.	0.	0.	0.	0.	0.	12	1	6	HTR
0.	0.	0.	0.	0.	1.59418E-02	12	7	6	HTR
0.	0.	0.	0.	0.	0.	12	13	6	HTR
0.	0.	0.	0.	0.	4.40613E-03	13	1	6	HTR
0.	0.	0.	0.	0.	0.	13	7	6	HTR
1.43273E-02	0.	-6.06452E-03	0.	0.	0.	13	13	6	HTR
0.	0.	0.	0.	0.	-4.65988E-03	14	1	6	HTR

0.	0.	0.	0.	0.	0.	14	7	6	HTR
0.	1.75989E-02	-3.38560E-03	0.	0.	0.	14	13	6	HTR
0.	0.	0.	-4.40613E-03	4.65988E-03	0.	15	1	6	HTR
0.	0.	0.	0.	0.	0.	15	7	6	HTR
-6.06452E-03	-3.38560E-03	8.82040E-03	0.	0.	0.	15	13	6	HTR
0.	0.	0.	0.	0.	0.	16	1	6	HTR
0.	0.	4.40613E-03	0.	0.	0.	16	7	6	HTR
0.	0.	0.	1.43273E-02	0.	-6.06452E-03	16	13	6	HTR
0.	0.	0.	0.	0.	0.	17	1	6	HTR
0.	0.	-4.65988E-03	0.	0.	0.	17	7	6	HTR
0.	0.	0.	0.	1.75989E-02	-3.38560E-03	17	13	6	HTR
0.	0.	0.	0.	0.	0.	18	1	6	HTR
-4.40613E-03	4.65988E-03	0.	0.	0.	0.	18	7	6	HTR
0.	0.	0.	-6.06452E-03	-3.38560E-03	8.82040E-03	18	13	6	HTR

	RAW EIGENVALUES	WAVE NUMBERS	ELECTRON VOLTS	CPS*E12
1	2.9954E-02	2.2552E 02	2.7960E-02	6.7657E 00
2	2.9952E-02	2.2552E 02	2.7959E-02	6.7655E 00
3	2.3038E-02	1.9778E 02	2.4521E-02	5.9335E 00
4	2.2489E-02	1.9541E 02	2.4227E-02	5.8624E 00
5	2.2489E-02	1.9541E 02	2.4227E-02	5.8624E 00
6	2.2488E-02	1.9541E 02	2.4226E-02	5.8623E 00
7	1.6169E-02	1.6569E 02	2.0542E-02	4.9707E 00
8	1.6168E-02	1.6569E 02	2.0542E-02	4.9706E 00
9	1.6168E-02	1.6569E 02	2.0542E-02	4.9706E 00
10	1.6162E-02	1.6566E 02	2.0538E-02	4.9697E 00
11	1.6080E-02	1.6524E 02	2.0486E-02	4.9571E 00
12	4.8237E-03	9.0501E 01	1.1220E-02	2.7150E 00
13	4.8171E-03	9.0440E 01	1.1212E-02	2.7132E 00
14	2.3038E-03	6.2545E 01	7.7541E-03	1.8763E 00
15	2.0896E-03	5.9565E 01	7.3847E-03	1.7870E 00
16	2.0896E-03	5.9565E 01	7.3847E-03	1.7870E 00
17	2.0896E-03	5.9565E 01	7.3847E-03	1.7870E 00
18	1.8771E-03	5.6455E 01	6.9992E-03	1.6937E 00

TRACE = 2.5441E-01

SUM OF EIGENVALUES = 2.5125E-01

TRACE-SUM = 1.3161E-02

F = (0.000000, 0.200000, 0.200000)

EIGENVECTORS IN PSEUDO-POLAR FORM

8.3834536E-01	-0.	-5.4513948E-01	3.6000002E 01	0.	0.	1	1	3	PPE
0.	0.	0.	0.	0.	0.	1	4	3	PPE
0.	0.	0.	0.	0.	0.	1	7	3	PPE
8.3839695E-01	-0.	-5.4506012E-01	3.6000002E 01	0.	0.	2	1	3	PPE
0.	0.	0.	0.	0.	0.	2	4	3	PPE
0.	0.	0.	0.	0.	0.	2	7	3	PPE
0.	0.	0.	0.	0.	0.	3	1	3	PPE
2.7341799E-02	-0.	6.0144889E-02	9.8000582E 01	-3.1681636E-02	3.6000261E 01	3	4	3	PPE
-5.2242826E-01	9.0525535E 01	6.4790279E-01	5.8105383E 00	5.4947421E-01	1.2885473E 02	3	7	3	PPE
0.	0.	0.	0.	0.	0.	4	1	3	PPE
3.6754401E-02	-0.	4.7031321E-02	8.9990053E 01	-3.9999054E-02	3.5995695E 01	4	4	3	PPE
-5.0962640E-01	1.0209693E 02	6.5350023E-01	1.2386228E 01	5.5490551E-01	1.3809225E 02	4	7	3	PPE
0.	0.	0.	0.	0.	0.	5	1	3	PPE
4.3151280E-01	-0.	5.5323590E-01	8.9999979E 01	-4.6978372E-01	3.5999989E 01	5	4	3	PPE
2.7371535E-01	5.4912672E 00	3.5110109E-01	9.5483665E 01	-2.9805668E-01	4.1487955E 01	5	7	3	PPE
0.	0.	0.	0.	0.	0.	6	1	3	PPE
3.5502369E-02	0.	4.7337699E-02	8.9989883E 01	-3.9340836E-02	3.5995524E 01	6	4	3	PPE
-5.1024508E-01	9.3026096E 01	6.5336105E-01	3.3909359E 00	5.5507422E-01	1.2918555E 02	6	7	3	PPE
0.	0.	0.	0.	0.	0.	7	1	3	PPE
5.9738531E-01	0.	-5.9036034E-01	9.0000000E 01	-1.4667500E-01	3.6000002E 01	7	4	3	PPE
3.6616040E-01	1.5509501E 02	3.6135035E-01	6.5094901E 01	8.9903304E-02	1.1094953E 01	7	7	3	PPE
0.	0.	0.	0.	0.	0.	8	1	3	PPE
5.8000027E-01	0.	-5.7317559E-01	9.0000000E 01	-1.4240778E-01	3.6000002E 01	8	4	3	PPE
3.9312041E-01	1.5896766E 02	3.8849581E-01	6.8967815E 01	9.6522620E-02	1.4967564E 01	8	7	3	PPE
0.	0.	0.	0.	0.	0.	9	1	3	PPE
2.3637958E-01	0.	-2.3359759E-01	8.9999985E 01	-5.8038797E-02	3.6000036E 01	9	4	3	PPE
-6.5959848E-01	1.0195687E 02	-6.5133534E-01	1.1956877E 01	1.6195280E-01	1.3795685E 02	9	7	3	PPE
0.	0.	0.	0.	0.	0.	10	1	3	PPE
5.9790011E-01	0.	-5.9033040E-01	9.0000000E 01	-1.4681360E-01	3.6000000E 01	10	4	3	PPE
3.6533606E-01	1.5496331E 02	3.6105974E-01	6.4965862E 01	8.9698865E-02	1.0962350E 01	10	7	3	PPE
0.	0.	0.	0.	0.	0.	11	1	3	PPE
5.9805770E-01	0.	-5.9051539E-01	9.0000000E 01	-1.4700033E-01	3.6000000E 01	11	4	3	PPE
3.6528309E-01	1.5496196E 02	3.6130069E-01	6.4996994E 01	3.9662350E-02	1.0950628E 01	11	7	3	PPE
5.4492656E-01	0.	3.3848375E-01	3.6000000E 01	0.	0.	12	1	3	PPE
0.	0.	0.	0.	0.	0.	12	4	3	PPE
0.	0.	0.	0.	0.	0.	12	7	3	PPE
5.4505816E-01	0.	8.3839820E-01	3.6000000E 01	0.	0.	13	1	3	PPE
0.	0.	0.	0.	0.	0.	13	4	3	PPE
0.	0.	0.	0.	0.	0.	13	7	3	PPE
0.	0.	0.	0.	0.	0.	14	1	3	PPE
3.9174838E-01	2.3841858E-05	2.3551192E-01	9.0000022E 01	6.3305151E-01	3.6000023E 01	14	4	3	PPE
3.0733877E-01	1.1926522E 02	-1.9423029E-01	2.8911791E 01	5.0798014E-01	1.5445780E 02	14	7	3	PPE
0.	0.	0.	0.	0.	0.	15	1	3	PPE
1.2636328E-01	-0.	7.6511317E-02	8.9999982E 01	2.0616732E-01	3.5999992E 01	15	4	3	PPE
4.8165067E-01	9.5799017E 00	2.9207519E-01	9.9572891E 01	7.8636959E-01	4.5576833E 01	15	7	3	PPE
0.	0.	0.	0.	0.	0.	16	1	3	PPE
2.8539625E-01	-0.	1.7294123E-01	8.9999659E 01	4.6580824E-01	3.5999849E 01	16	4	3	PPE
-4.0806115E-01	9.0268211E 01	2.4748696E-01	2.2090149E-01	-6.6625763E-01	1.2624744E 02	16	7	3	PPE
0.	0.	0.	0.	0.	0.	17	1	3	PPE
4.9780971E-01	1.8000000E 02	-3.0207438E-01	9.0000000E 01	-8.1298061E-01	3.5999998E 01	17	4	3	PPE
0.	0.	0.	0.	0.	0.	17	7	3	PPE
0.	0.	0.	0.	0.	0.	18	1	3	PPE
3.8935318E-01	2.0980835E-05	2.3247232E-01	9.0000019E 01	6.3564810E-01	3.6000021E 01	18	4	3	PPE
3.0560577E-01	1.1864199E 02	-1.9157404E-01	2.7642933E 01	5.0988058E-01	1.5486656E 02	18	7	3	PPE

ILTAPE= 0 IFTAPE= 0 IVTAPE= 0 IATAPE= 0

KLTAPE= 0 KFTAPE= 0 KVTAPE= 0 KATAPE= 0

NUMBER OF COLUMNS IN D,N2= 9

NUMBER OF ROWS IN D,N3= 9

NUMBER OF ROWS IN A,N5= 9

NUMBER OF D MATRICES WITH POSITIVE SUBSCRIPTS,NUMAT 7

F = (0.000000, 0.200000, 0.200000)

CELL VOLUME OF DIRECT SPACE = 77.05800

ATOM MASSES AND POSITIONS

I	M(I)	L1(I)	L2(I)	L3(I)
1	2.43100E 01	2.50000E-01	2.50000E-01	2.50000E-01
2	1.18700E 02	0.	0.	0.
3	2.43100E 01	2.50000E-01	2.50000E-01	7.50000E-01

FRACTIONAL CHARGE ON ATOMS

1	-4.80000E-01
2	1.04000E 00
3	-4.80000E-01

	RAW EIGENVALUES	WAVE NUMBERS	ELECTRON VOLTS	CPS*E12
1	2.9696E-02	2.2455E 02	2.7839E-02	6.7366E 00
2	2.9695E-02	2.2455E 02	2.7838E-02	6.7364E 00
3	2.3014E-02	1.9768E 02	2.4508E-02	5.9303E 00
4	2.2509E-02	1.9550E 02	2.4238E-02	5.8650E 00
5	2.2509E-02	1.9550E 02	2.4238E-02	5.8650E 00
6	2.2509E-02	1.9550E 02	2.4238E-02	5.8650E 00
7	1.6249E-02	1.6610E 02	2.0593E-02	4.9831E 00
8	1.6249E-02	1.6610E 02	2.0593E-02	4.9830E 00
9	1.6249E-02	1.6610E 02	2.0593E-02	4.9830E 00
10	1.6245E-02	1.6608E 02	2.0590E-02	4.9824E 00
11	1.6206E-02	1.6588E 02	2.0565E-02	4.9764E 00
12	4.7935E-03	9.0217E 01	1.1185E-02	2.7065E 00
13	4.7935E-03	9.0217E 01	1.1185E-02	2.7065E 00
14	4.7934E-03	9.0217E 01	1.1185E-02	2.7065E 00
15	2.0861E-03	5.9516E 01	7.3786E-03	1.7855E 00
16	2.0861E-03	5.9516E 01	7.3786E-03	1.7855E 00
17	2.0861E-03	5.9516E 01	7.3786E-03	1.7855E 00
18	1.8730E-03	5.6394E 01	6.9916E-03	1.6918E 00

TRACE = 2.6441E-01
SUM OF EIGENVALUES = 2.5364E-01
TRACE-SUM = 1.0768E-02

F = (0.000000, 0.200000, 0.200000)

EIGENVECTORS IN PSEUDO-POLAR FORM

8.3261681E-01	-0.	-5.5384947E-01	3.6000002E 01	0.	0.	1	1	3	PPE
0.	0.	0.	0.	0.	0.	1	4	3	PPE
0.	0.	0.	0.	0.	0.	1	7	3	PPE
8.3267551E-01	-0.	-5.5376121E-01	3.6000002E 01	0.	0.	2	1	3	PPE
0.	0.	0.	0.	0.	0.	2	4	3	PPE
0.	0.	0.	0.	0.	0.	2	7	3	PPE
0.	0.	0.	0.	0.	0.	3	1	3	PPE
8.9522933E-02	-0.	1.1090117E-01	9.0000265E 01	-9.6459364E-02	3.6000137E 01	3	4	3	PPE
-5.2036095E-01	9.0249555E 01	6.4083513E-01	4.1526022E 00	5.3752849E-01	1.2799819E 02	3	7	3	PPE
0.	0.	0.	0.	0.	0.	4	1	3	PPE
5.2271171E-01	0.	6.4658190E-01	8.9999998E 01	-5.5561160E-01	3.6000004E 01	4	4	3	PPE
0.	0.	0.	0.	0.	0.	4	7	3	PPE
0.	0.	0.	0.	0.	0.	5	1	3	PPE
9.0632101E-02	0.	1.1206945E-01	9.0000038E 01	-9.6321430E-02	3.6000025E 01	5	4	3	PPE
-5.1490433E-01	9.9223679E 01	6.3668523E-01	9.1999397E 00	5.4722371E-01	1.3521338E 02	5	7	3	PPE
0.	0.	0.	0.	0.	0.	6	1	3	PPE
3.1447377E-01	-0.	3.9148473E-01	9.0000431E 01	-3.3519350E-01	3.6000187E 01	6	4	3	PPE
4.1662297E-01	7.3920307E 00	5.1551142E-01	9.7724693E 01	-4.4290451E-01	4.3536264E 01	6	7	3	PPE
0.	0.	0.	0.	0.	0.	7	1	3	PPE
5.2341151E-01	-0.	-5.2576996E-01	8.9999992E 01	-1.1923096E-01	3.6000031E 01	7	4	3	PPE
-4.5963011E-01	9.1148495E 01	-4.6170094E-01	1.1485043E 00	1.0470200E-01	1.2714851E 02	7	7	3	PPE
0.	0.	0.	0.	0.	0.	8	1	3	PPE
3.1386511E-03	-0.	-3.1547896E-03	8.9941338E 01	-7.1413580E-04	3.6108878E 01	8	4	3	PPE
6.9657271E-01	1.2277531E 02	6.9970531E-01	3.2775158E 01	-1.5867742E-01	1.5877553E 02	8	7	3	PPE
0.	0.	0.	0.	0.	0.	9	1	3	PPE
6.9657759E-01	-0.	-6.9971486E-01	9.0000034E 01	-1.5867797E-01	3.5999832E 01	9	4	3	PPE
0.	0.	0.	0.	0.	0.	9	7	3	PPE
0.	0.	0.	0.	0.	0.	10	1	3	PPE
4.5823590E-01	-0.	-4.6027524E-01	9.0000007E 01	-1.0439346E-01	3.5999970E 01	10	4	3	PPE
5.2464417E-01	9.0877256E 01	5.2700418E-01	8.7486935E-01	-1.1951332E-01	1.2688084E 02	10	7	3	PPE
0.	0.	0.	0.	0.	0.	11	1	3	PPE
4.5823259E-01	-0.	-4.6027953E-01	9.0000007E 01	-1.0438878E-01	3.5999970E 01	11	4	3	PPE
5.2464346E-01	9.0876374E 01	5.2700517E-01	8.7228584E-01	-1.1951246E-01	1.2687936E 02	11	7	3	PPE
5.5375990E-01	0.	8.3267635E-01	3.6000000E 01	0.	0.	12	1	3	PPE
0.	0.	0.	0.	0.	0.	12	4	3	PPE
0.	0.	0.	0.	0.	0.	12	7	3	PPE
5.5376036E-01	-0.	8.3267605E-01	3.6000004E 01	0.	0.	13	1	3	PPE
0.	0.	0.	0.	0.	0.	13	4	3	PPE
0.	0.	0.	0.	0.	0.	13	7	3	PPE
0.	0.	0.	0.	0.	0.	14	1	3	PPE
9.4810089E-02	-0.	6.8909094E-02	8.9999940E 01	1.0312729E-01	3.5999995E 01	14	4	3	PPE
4.5934806E-01	1.7973688E 02	-2.6855528E-01	8.9539974E 01	-8.3216865E-01	3.6743206E 01	14	7	3	PPE
0.	0.	0.	0.	0.	0.	15	1	3	PPE
4.9130097E-01	-0.	3.0415323E-01	9.0000002E 01	8.1615812E-01	3.6000000E 01	15	4	3	PPE
0.	0.	0.	0.	0.	0.	15	7	3	PPE
0.	0.	0.	0.	0.	0.	16	1	3	PPE
4.5077011E-02	-0.	2.7895557E-02	9.0000267E 01	7.4871417E-02	3.5999972E 01	16	4	3	PPE
4.8929516E-01	7.0924252E 01	3.0280451E-01	1.6089994E 02	8.1270152E-01	1.0691370E 02	16	7	3	PPE
0.	0.	0.	0.	0.	0.	17	1	3	PPE
7.5217145E-02	0.	4.6311992E-02	9.0000490E 01	1.2465851E-01	3.6000212E 01	17	4	3	PPE
4.8560228E-01	1.7976745E 02	-3.0051089E-01	8.9818989E 01	-8.0656143E-01	3.5789786E 01	17	7	3	PPE
0.	0.	0.	0.	0.	0.	18	1	3	PPE
7.4343012E-02	-0.	4.3639775E-02	8.9999939E 01	1.2521611E-01	3.5999972E 01	18	4	3	PPE
-4.8738621E-01	3.1780625E-01	-3.0267255E-01	9.0590384E 01	-8.0481891E-01	3.6409426E 01	18	7	3	PPE

COLUMN 1 OF JACOBIAN MATRICES

I	RAW PARTIALS	ELECTRON VOLTS
1	-1.3146E-02	-6.1488E-03
2	-1.3157E-02	-6.1539E-03
3	-1.2588E-03	-6.7008E-04
4	1.0305E-03	5.5492E-04
5	1.0305E-03	5.5492E-04
6	1.0735E-03	5.7811E-04
7	4.0902E-03	2.5950E-03
8	4.1189E-03	2.6133E-03
9	4.1189E-03	2.6133E-03
10	4.2142E-03	2.6742E-03
11	6.4098E-03	4.0751E-03
12	-1.5410E-03	-1.7950E-03
13	-1.2074E-03	-1.4069E-03
14	1.2702E-01	1.7504E-01
15	-1.7688E-04	-3.1269E-04
16	-1.7688E-04	-3.1269E-04
17	-1.7688E-04	-3.1269E-04
18	-2.0827E-04	-3.8850E-04

I 'E= 0 IFTAPE= 0 IVTAPE= 0 IATAPE= 1
 KLTAPE= 0 KFTAPE= 0 KVTAPE= 0 KATAPE= 1
 NUMBER OF COLUMNS IN D,N2= 9
 NUMBER OF ROWS IN D,N3= 9
 NUMBER OF ROWS IN A,N5= 2
 NUMBER OF D MATRICES WITH POSITIVE SUBSCRIPTS,NUMAT = 7

F = (0.000000, 0.200000, 0.200000)											
8.4048068E-02	0.	0.	0.	0.	0.	1	1	3	F*D		
-2.4894745E-02	1.8087091E-02	-1.7096326E-10	0.	-1.7096326E-10	0.	1	4	3	F*D		
0.	0.	0.	0.	0.	0.	1	7	3	F*D		
0.	0.	8.4048068E-02	0.	0.	0.	2	1	3	F*D		
-1.7096326E-10	0.	-2.4894745E-02	1.8087091E-02	-1.6667305E-02	-2.2940577E-02	2	4	3	F*D		
0.	0.	0.	0.	0.	0.	2	7	3	F*D		
0.	0.	0.	0.	8.4048068E-02	0.	3	1	3	F*D		
-1.7096326E-10	0.	-1.6667305E-02	-2.2940577E-02	-2.4894745E-02	1.8087091E-02	3	4	3	F*D		
0.	0.	0.	0.	0.	0.	3	7	3	F*D		
-5.5010174E-02	-3.9967231E-02	-3.7777926E-10	-0.	-3.7777926E-10	-0.	4	1	3	F*D		
1.1450024E-01	-0.	0.	-0.	0.	-0.	4	4	3	F*D		
-5.5010174E-02	-3.9967231E-02	-3.7777926E-10	-0.	3.7777926E-10	-0.	4	7	3	F*D		
-3.7777926E-10	-0.	-5.5010174E-02	-3.9967231E-02	-3.6829914E-02	5.0692029E-02	5	1	3	F*D		
0.	-0.	1.0576830E-01	-0.	0.	-0.	5	4	3	F*D		
-3.7777926E-10	-0.	-5.5010174E-02	-3.9967231E-02	3.6829914E-02	-5.0692029E-02	5	7	3	F*D		
-3.7777926E-10	-0.	-3.6829914E-02	5.0692029E-02	-5.5010174E-02	-3.9967231E-02	6	1	3	F*D		
0.	-0.	0.	-0.	1.0576830E-01	-0.	6	4	3	F*D		
3.7777926E-10	-0.	3.6829914E-02	-5.0692029E-02	-5.5010174E-02	-3.9967231E-02	6	7	3	F*D		
0.	-0.	0.	-0.	0.	-0.	7	1	3	F*D		
-2.4894745E-02	1.8087091E-02	-1.7096326E-10	-0.	1.7096326E-10	-0.	7	4	3	F*D		
8.4048068E-02	-0.	0.	-0.	0.	-0.	7	7	3	F*D		
0.	-0.	0.	-0.	0.	-0.	8	1	3	F*D		
-1.7096326E-10	-0.	-2.4894745E-02	1.8087091E-02	1.6667305E-02	2.2940577E-02	8	4	3	F*D		
0.	-0.	8.4048068E-02	-0.	0.	-0.	8	7	3	F*D		
0.	-0.	0.	-0.	0.	-0.	9	1	3	F*D		
1.7096326E-10	-0.	1.6667305E-02	2.2940577E-02	-2.4894745E-02	1.8087091E-02	9	4	3	F*D		
0.	-0.	0.	-0.	8.4048068E-02	-0.	9	7	3	F*D		
1.7046520E-02	-0.	0.	-0.	0.	-0.	1	1	3	DFD		
-5.0491198E-03	3.6684003E-03	-3.4674545E-11	-0.	-3.4674545E-11	0.	1	4	3	DFD		
0.	-0.	0.	-0.	0.	-0.	1	7	3	DFD		
0.	-0.	1.7046520E-02	-0.	0.	-0.	2	1	3	DFD		
-3.4674545E-11	-0.	-5.0491198E-03	3.6684003E-03	-3.3804410E-03	-4.6527779E-03	2	4	3	DFD		
0.	-0.	0.	-0.	0.	-0.	2	7	3	DFD		
0.	-0.	0.	-0.	1.7046520E-02	-0.	3	1	3	DFD		
-3.4674545E-11	-0.	-3.3804410E-03	-4.6527779E-03	-5.0491198E-03	3.6684003E-03	3	4	3	DFD		
0.	-0.	0.	-0.	0.	-0.	3	7	3	DFD		
-5.0491198E-03	-3.6684003E-03	-3.4674545E-11	-0.	-3.4674545E-11	-0.	4	1	3	DFD		
1.0509427E-02	-0.	0.	-0.	0.	0.	4	4	3	DFD		
-5.0491198E-03	-3.6684003E-03	-3.4674545E-11	-0.	3.4674545E-11	-0.	4	7	3	DFD		
-3.4674545E-11	-0.	-5.0491198E-03	-3.6684003E-03	-3.3804410E-03	4.6527779E-03	5	1	3	DFD		
0.	-0.	9.7079642E-03	-0.	0.	0.	5	4	3	DFD		
-3.4674545E-11	-0.	-5.0491198E-03	-3.6684003E-03	3.3804410E-03	-4.6527779E-03	5	7	3	DFD		
-3.4674545E-11	-0.	-3.3804410E-03	4.6527779E-03	-5.0491198E-03	-3.6684003E-03	6	1	3	DFD		
0.	-0.	0.	-0.	0.	0.	6	4	3	DFD		
3.4674545E-11	-0.	3.3804410E-03	-4.6527779E-03	-5.0491198E-03	-3.6684003E-03	6	7	3	DFD		
0.	-0.	0.	-0.	0.	-0.	7	1	3	DFD		

-5.0491198E-03	3.6684003E-03	-3.4674545E-11	-0.	3.4674545E-11	0.	7	4	3	DFD
1.7046520E-02	-0.	0.	-0.	0.	-0.	7	7	3	DFD
0.	-0.	0.	-0.	0.	-0.	8	1	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	3.6684003E-03	3.3804410E-03	4.6527779E-03	8	4	3	DFD
0.	-0.	1.7046520E-02	-0.	0.	-0.	8	7	3	DFD
0.	-0.	0.	-0.	0.	-0.	9	1	3	DFD
3.4674545E-11	-0.	3.3804410E-03	4.6527779E-03	-5.0491198E-03	3.6684003E-03	9	4	3	DFD
0.	-0.	0.	-0.	1.7046520E-02	-0.	9	7	3	DFD
2.307/V*D(C)*Z*CCC*Z*D(C)									
2.1668827E-03	-0.	-0.	-0.	-0.	-0.	1	1	3	DCD
-1.8809424E-03	0.	0.	0.	0.	0.	1	4	3	DCD
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	1	7	3	DCD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	2	1	3	DCD
0.	0.	9.4047122E-04	0.	0.	-1.6782696E-03	2	4	3	DCD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	2	7	3	DCD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	3	1	3	DCD
0.	0.	0.	-1.6782696E-03	9.4047122E-04	0.	3	4	3	DCD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	DCD
-1.8809424E-03	0.	0.	0.	0.	0.	4	1	3	DCD
1.7751279E-03	-0.	-0.	-0.	-0.	-0.	4	4	3	DCD
-1.8809424E-03	0.	0.	0.	0.	0.	4	7	3	DCD
0.	0.	9.4047122E-04	0.	0.	1.6782696E-03	5	1	3	DCD
-0.	-0.	-8.8756394E-04	-0.	-0.	-0.	5	4	3	DCD
0.	0.	9.4047122E-04	0.	0.	-1.6782696E-03	5	7	3	DCD
0.	0.	0.	1.6782696E-03	9.4047122E-04	0.	6	1	3	DCD
-0.	-0.	-0.	-0.	-8.8756394E-04	-0.	6	4	3	DCD
0.	0.	0.	-1.6782696E-03	9.4047122E-04	0.	6	7	3	DCD
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	7	1	3	DCD
-1.8809424E-03	0.	0.	0.	0.	0.	7	4	3	DCD
2.1668827E-03	-0.	-0.	-0.	-0.	-0.	7	7	3	DCD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	8	1	3	DCD
0.	0.	9.4047122E-04	0.	0.	1.6782696E-03	8	4	3	DCD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	8	7	3	DCD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	9	1	3	DCD
0.	0.	0.	1.6782696E-03	9.4047122E-04	0.	9	4	3	DCD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	9	7	3	DCD
D(C)*F(C)*D(C)									
2.1668827E-03	0.	-0.	-0.	-0.	-0.	1	1	3	DMD
-1.5217144E-03	1.1055902E-03	0.	-0.	0.	-0.	1	4	3	DMD
3.2716388E-03	0.	-0.	-0.	-0.	-0.	1	7	3	DMD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	2	1	3	DMD
0.	-0.	7.6085719E-04	-5.5279510E-04	9.8646208E-04	1.3577486E-03	2	4	3	DMD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	2	7	3	DMD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	3	1	3	DMD
0.	-0.	9.8646208E-04	1.3577486E-03	7.6085719E-04	-5.5279510E-04	3	4	3	DMD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	DMD
-1.5217144E-03	-1.1055902E-03	0.	0.	0.	0.	4	1	3	DMD
1.7751279E-03	0.	-0.	-0.	-0.	-0.	4	4	3	DMD
-1.5217144E-03	-1.1055902E-03	0.	0.	0.	0.	4	7	3	DMD
0.	0.	7.6085719E-04	5.5279510E-04	9.8646208E-04	-1.3577486E-03	5	1	3	DMD
-0.	-0.	-8.8756394E-04	-0.	-0.	-0.	5	4	3	DMD
0.	0.	7.6085719E-04	5.5279510E-04	-9.8646208E-04	1.3577486E-03	5	7	3	DMD
0.	0.	9.8646208E-04	-1.3577486E-03	7.6085719E-04	5.5279510E-04	6	1	3	DMD
-0.	-0.	-0.	-0.	-8.8756394E-04	-0.	6	4	3	DMD
0.	0.	-9.8646208E-04	1.3577486E-03	7.6085719E-04	5.5279510E-04	6	7	3	DMD
3.2716388E-03	-0.	-0.	0.	-0.	0.	7	1	3	DMD
-1.5217144E-03	1.1055902E-03	0.	-0.	0.	-0.	7	4	3	DMD

0.68827E-03	0.	-0.	-0.	-0.	-0.	7	7	3	)
0.	0.	-1.6358194E-03	0.	-0.	0.	8	1	3	DMD
0.	-0.	7.6085719E-04	-5.5279510E-04	-9.8646208E-04	-1.3577486E-03	8	4	3	DMD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	8	7	3	DMD
-0.	0.	-0.	0.	-1.6358194E-03	0.	9	1	3	DMD
0.	-0.	-9.8646208E-04	-1.3577486E-03	7.6085719E-04	-5.5279510E-04	9	4	3	DMD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	9	7	3	DMD

D(TRANSPDSE)*F*D + D(C)*F(C)*D(C)									
1.9213402E-02	-0.	-0.	-0.	-0.	-0.	1	1	3	FFM
-6.5708342E-03	4.7739905E-03	-3.4674545E-11	-0.	-0.	-3.4674545E-11	1	4	3	FFM
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	1	7	3	FFM
-0.	-0.	1.5963078E-02	-0.	-0.	-0.	2	1	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	3.1156052E-03	-2.3939790E-03	-3.2950294E-03	2	4	3	FFM
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	2	7	3	FFM
-0.	-0.	-0.	-0.	1.5963078E-02	-0.	3	1	3	FFM
-3.4674545E-11	-0.	-2.3939790E-03	-3.2950294E-03	-4.2882626E-03	3.1156052E-03	3	4	3	FFM
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	FFM
-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	-0.	-0.	-3.4674545E-11	4	1	3	FFM
1.2284555E-02	-0.	-0.	-0.	-0.	0.	4	4	3	FFM
-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	-0.	-0.	3.4674545E-11	4	7	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	-3.1156052E-03	-2.3939790E-03	3.2950294E-03	5	1	3	FFM
-0.	-0.	8.8204002E-03	-0.	-0.	0.	5	4	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	-3.1156052E-03	-2.3939790E-03	-3.2950294E-03	5	7	3	FFM
-3.4674545E-11	-0.	-2.3939790E-03	3.2950294E-03	-4.2882626E-03	-3.1156052E-03	6	1	3	FFM
-0.	-0.	-0.	-0.	8.8204002E-03	0.	6	4	3	FFM
3.4674545E-11	-0.	2.3939790E-03	-3.2950294E-03	-4.2882626E-03	-3.1156052E-03	6	7	3	FFM
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	7	1	3	FFM
-6.5708342E-03	4.7739905E-03	-3.4674545E-11	-0.	-0.	3.4674545E-11	7	4	3	FFM
1.9213402E-02	-0.	-0.	-0.	-0.	-0.	7	7	3	FFM
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	8	1	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	3.1156052E-03	2.3939790E-03	3.2950294E-03	8	4	3	FFM
-0.	-0.	1.5963078E-02	-0.	-0.	-0.	8	7	3	FFM
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	9	1	3	FFM
3.4674545E-11	-0.	2.3939790E-03	3.2950294E-03	-4.2882626E-03	3.1156052E-03	9	4	3	FFM
-0.	-0.	-0.	-0.	1.5963078E-02	-0.	9	7	3	FFM

A									
1.00000E 00	-0.	-0.	-0.	-0.	-0.	1	1	6	A
1.00000E 00	-0.	-0.	0.	0.	0.	1	7	3	A
-0.	-0.	-0.	1.00000E 00	-0.	-0.	2	1	6	A
-0.	-0.	0.	0.	0.	0.	2	7	3	A

NORMALIZED A									
7.07107E-01	-0.	-0.	-0.	-0.	-0.	1	1	6	A N
7.07107E-01	-0.	-0.	0.	0.	0.	1	7	3	A N
-0.	-0.	-0.	1.00000E 00	-0.	-0.	2	1	6	A N
-0.	-0.	0.	0.	0.	0.	2	7	3	A N

A(STAR)									
7.07107E-01	-0.	-0.	0.	-0.	-0.	1	1	6	A S
7.07107E-01	-0.	0.	0.	0.	0.	1	7	3	A S
-0.	-0.	-0.	1.00000E 00	-0.	-0.	2	1	6	A S
-0.	-0.	0.	0.	0.	0.	2	7	3	A S

A(STAR)*(D*F*D + D(C)*F(C)*D(C))									
1.5899325E-02	-0.	0.	-0.	0.	-0.	1	1	3	A*F
-9.2925628E-03	6.7514420E-03	-4.9037212E-11	0.	-0.	0.	1	4	3	A*F
1.5899325E-02	-0.	0.	-0.	0.	-0.	1	7	3	A*F

-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	-0.	-3.4674545E-11	-0.	2	1	3	A*F
1.2284555E-02	-0.	0.	0.	0.	0.	2	4	3	A*F
-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	-0.	3.4674545E-11	-0.	2	7	3	A*F
M									
2.2485041E-02	-0.	-9.2925628E-03	6.7514420E-03	-0.	-0.	1	1	2	M
-9.2925628E-03	-6.7514420E-03	1.2284555E-02	-0.	-0.	-0.	2	1	2	M
M(HERMITIAN)									
2.2485041E-02	0.	-9.2925628E-03	6.7514420E-03	-0.	-0.	1	1	2	M
-9.2925628E-03	-6.7514420E-03	1.2284555E-02	0.	-0.	-0.	2	1	2	M
2.24850E-02	-9.29256E-03	0.	-6.75144E-03	-0.	-0.	1	1	4	HTR
-9.29256E-03	1.22846E-02	6.75144E-03	0.	-0.	-0.	2	1	4	HTR
0.	6.75144E-03	2.24850E-02	-9.29256E-03	-1.31400E-01	-1.03600E-01	3	1	4	HTR
-6.75144E-03	0.	-9.29256E-03	1.22846E-02	-0.	-0.	4	1	4	HTR

	RAW EIGENVALUES	WAVE NUMBERS	ELECTRON VOLTS	CPS*E12
1	2.9952E-02	2.2552E 02	2.7959E-02	6.7655E 00
2	2.9952E-02	2.2552E 02	2.7959E-02	6.7655E 00
3	4.8172E-03	9.0440E 01	1.1212E-02	2.7132E 00
4	4.8172E-03	9.0440E 01	1.1212E-02	2.7132E 00

TRACE = 6.9539E-02
 SUM OF EIGENVALUES = 6.9539E-02
 TRACE-SUM = -9.2201E-08

F = (0.000000, 0.200000, 0.200000)

EIGENVECTORS IN PSEUDO-POLAR FORM

8.3839733E-01	-0.	-5.4505952E-01	3.6000002E 01	0.	-0.	1	1	2	PPE
8.3839895E-01	0.	-5.4505701E-01	3.5999994E 01	-3.4674545E-11	-0.	2	1	2	PPE
5.4505792E-01	0.	8.3839837E-01	3.6000001E 01	2.0281870E-01	0.	3	1	2	PPE
5.4505893E-01	-0.	8.3839770E-01	3.6000004E 01	0.	0.	4	1	2	PPE

.....PE= 0 IFTAPE= 0 IVTAPE= 0 IATAPE= 1

KLTAPE= 1 KFTAPE= 1 KVTAPE= 0 KATAPE= 1

NUMBER OF COLUMNS IN D,N2= 9

NUMBER OF ROWS IN D,N3= 9

NUMBER OF ROWS IN A,N5= 1

NUMBER OF D MATRICES WITH POSITIVE SUBSCRIPTS,NUMAT 7

F = (0.000000, 0.200000, 0.200000)

8.4048068E-02	0.	0.	0.	0.	0.	1	1	3	F*D
-2.4894745E-02	1.8087091E-02	-1.7096326E-10	0.	-1.7096326E-10	0.	1	4	3	F*D
0.	0.	0.	0.	0.	0.	1	7	3	F*D
0.	0.	8.4048068E-02	0.	0.	0.	2	1	3	F*D
-1.7096326E-10	0.	-2.4894745E-02	1.8087091E-02	-1.6667305E-02	-2.2940577E-02	2	4	3	F*D
0.	0.	0.	0.	0.	0.	2	7	3	F*D
0.	0.	0.	0.	8.4048068E-02	0.	3	1	3	F*D
-1.7096326E-10	0.	-1.6667305E-02	-2.2940577E-02	-2.4894745E-02	1.8087091E-02	3	4	3	F*D
0.	0.	0.	0.	0.	0.	3	7	3	F*D
-5.5010174E-02	-3.9967231E-02	-3.7777926E-10	-0.	-3.7777926E-10	-0.	4	1	3	F*D
1.1450024E-01	-0.	0.	-0.	0.	-0.	4	4	3	F*D
-5.5010174E-02	-3.9967231E-02	-3.7777926E-10	-0.	3.7777926E-10	-0.	4	7	3	F*D
-3.7777926E-10	-0.	-5.5010174E-02	-3.9967231E-02	-3.6829914E-02	5.0692029E-02	5	1	3	F*D
0.	-0.	1.0576830E-01	-0.	0.	-0.	5	4	3	F*D
-3.7777926E-10	-0.	-5.5010174E-02	-3.9967231E-02	3.6829914E-02	-5.0692029E-02	5	7	3	F*D
-3.7777926E-10	-0.	-3.6829914E-02	5.0692029E-02	-5.5010174E-02	-3.9967231E-02	6	1	3	F*D
0.	-0.	0.	-0.	1.0576830E-01	-0.	6	4	3	F*D
3.7777926E-10	-0.	3.6829914E-02	-5.0692029E-02	-5.5010174E-02	-3.9967231E-02	6	7	3	F*D
0.	-0.	0.	-0.	0.	-0.	7	1	3	F*D
-2.4894745E-02	1.8087091E-02	-1.7096326E-10	-0.	1.7096326E-10	-0.	7	4	3	F*D
8.4048068E-02	-0.	0.	-0.	0.	-0.	7	7	3	F*D
0.	-0.	0.	-0.	0.	-0.	8	1	3	F*D
-1.7096326E-10	-0.	-2.4894745E-02	1.8087091E-02	1.6667305E-02	2.2940577E-02	8	4	3	F*D
0.	-0.	8.4048068E-02	-0.	0.	-0.	8	7	3	F*D
0.	-0.	0.	-0.	0.	-0.	9	1	3	F*D
1.7096326E-10	-0.	1.6667305E-02	2.2940577E-02	-2.4894745E-02	1.8087091E-02	9	4	3	F*D
0.	-0.	0.	-0.	8.4048068E-02	-0.	9	7	3	F*D
1.7046520E-02	-0.	0.	-0.	0.	-0.	1	1	3	DFD
-5.0491198E-03	3.6684003E-03	-3.4674545E-11	-0.	-3.4674545E-11	0.	1	4	3	DFD
0.	-0.	0.	-0.	0.	-0.	1	7	3	DFD
0.	-0.	1.7046520E-02	-0.	0.	-0.	2	1	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	3.6684003E-03	-3.3804410E-03	-4.6527779E-03	2	4	3	DFD
0.	-0.	0.	-0.	0.	-0.	2	7	3	DFD
0.	-0.	0.	-0.	1.7046520E-02	-0.	3	1	3	DFD
-3.4674545E-11	-0.	-3.3804410E-03	-4.6527779E-03	-5.0491198E-03	3.6684003E-03	3	4	3	DFD
0.	-0.	0.	-0.	0.	-0.	3	7	3	DFD
-5.0491198E-03	-3.6684003E-03	-3.4674545E-11	-0.	-3.4674545E-11	-0.	4	1	3	DFD
1.0509427E-02	-0.	0.	-0.	0.	0.	4	4	3	DFD
-5.0491198E-03	-3.6684003E-03	-3.4674545E-11	-0.	3.4674545E-11	-0.	4	7	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	-3.6684003E-03	-3.3804410E-03	4.6527779E-03	5	1	3	DFD
0.	-0.	9.7079642E-03	-0.	0.	0.	5	4	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	-3.6684003E-03	3.3804410E-03	-4.6527779E-03	5	7	3	DFD
-3.4674545E-11	-0.	-3.3804410E-03	4.6527779E-03	-5.0491198E-03	-3.6684003E-03	6	1	3	DFD
0.	-0.	0.	-0.	9.7079642E-03	0.	6	4	3	DFD
3.4674545E-11	-0.	3.3804410E-03	-4.6527779E-03	-5.0491198E-03	-3.6684003E-03	6	7	3	DFD
0.	-0.	0.	-0.	0.	-0.	7	1	3	DFD

-5.0491198E-03	3.6684003E-03	-3.4674545E-11	-0.	3.4674545E-11	0.	7	4	3	DFD
1.7046520E-02	-0.	0.	-0.	0.	-0.	7	7	3	DFD
0.	-0.	0.	-0.	0.	-0.	8	1	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	3.6684003E-03	3.3804410E-03	4.6527779E-03	8	4	3	DFD
0.	-0.	1.7046520E-02	-0.	0.	-0.	8	7	3	DFD
0.	-0.	0.	-0.	0.	-0.	9	1	3	DFD
3.4674545E-11	-0.	3.3804410E-03	4.6527779E-03	-5.0491198E-03	3.6684003E-03	9	4	3	DFD
0.	-0.	0.	-0.	1.7046520E-02	-0.	9	7	3	DFD
2.307/V*D(C)*Z*CCC*Z*D(C)									
2.1668827E-03	-0.	-0.	-0.	-0.	-0.	1	1	3	DCD
-1.8809424E-03	0.	0.	0.	0.	0.	1	4	3	DCD
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	1	7	3	DCD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	2	1	3	DCD
0.	0.	9.4047122E-04	0.	0.	-1.6782696E-03	2	4	3	DCD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	2	7	3	DCD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	3	1	3	DCD
0.	0.	0.	-1.6782696E-03	9.4047122E-04	0.	3	4	3	DCD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	DCD
-1.8809424E-03	0.	0.	0.	0.	0.	4	1	3	DCD
1.7751279E-03	-0.	-0.	-0.	-0.	-0.	4	4	3	DCD
-1.6809424E-03	0.	0.	0.	0.	0.	4	7	3	DCD
0.	0.	9.4047122E-04	0.	0.	1.6782696E-03	5	1	3	DCD
-0.	-0.	-8.8756394E-04	-0.	-0.	-0.	5	4	3	DCD
0.	0.	9.4047122E-04	0.	0.	-1.6782696E-03	5	7	3	DCD
0.	0.	0.	1.6782696E-03	9.4047122E-04	0.	6	1	3	DCD
-0.	-0.	-0.	-0.	-8.8756394E-04	-0.	6	4	3	DCD
0.	0.	0.	-1.6782696E-03	9.4047122E-04	0.	6	7	3	DCD
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	7	1	3	DCD
-1.8809424E-03	0.	0.	0.	0.	0.	7	4	3	DCD
2.1668827E-03	-0.	-0.	-0.	-0.	-0.	7	7	3	DCD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	8	1	3	DCD
0.	0.	9.4047122E-04	0.	0.	1.6782696E-03	8	4	3	DCD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	8	7	3	DCD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	9	1	3	DCD
0.	0.	0.	1.6782696E-03	9.4047122E-04	0.	9	4	3	DCD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	9	7	3	DCD
D(C)*F(C)*D(C)									
2.1668827E-03	0.	-0.	-0.	-0.	-0.	1	1	3	DMD
-1.5217144E-03	1.1055902E-03	0.	-0.	0.	-0.	1	4	3	DMD
3.2716388E-03	0.	-0.	-0.	-0.	-0.	1	7	3	DMD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	2	1	3	DMD
0.	-0.	7.6085719E-04	-5.5279510E-04	9.8646208E-04	1.3577486E-03	2	4	3	DMD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	2	7	3	DMD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	3	1	3	DMD
0.	-0.	9.8646208E-04	1.3577486E-03	7.6085719E-04	-5.5279510E-04	3	4	3	DMD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	DMD
-1.5217144E-03	-1.1055902E-03	0.	0.	0.	0.	4	1	3	DMD
1.7751279E-03	0.	-0.	-0.	-0.	-0.	4	4	3	DMD
-1.5217144E-03	-1.1055902E-03	0.	0.	0.	0.	4	7	3	DMD
0.	0.	7.6085719E-04	5.5279510E-04	9.8646208E-04	-1.3577486E-03	5	1	3	DMD
-0.	-0.	-8.8756394E-04	-0.	-0.	-0.	5	4	3	DMD
0.	0.	7.6085719E-04	5.5279510E-04	-9.8646208E-04	1.3577486E-03	5	7	3	DMD
0.	0.	9.8646208E-04	-1.3577486E-03	7.6085719E-04	5.5279510E-04	6	1	3	DMD
-0.	-0.	-0.	-0.	-8.8756394E-04	-0.	6	4	3	DMD
0.	0.	-9.8646208E-04	1.3577486E-03	7.6085719E-04	5.5279510E-04	6	7	3	DMD
3.2716388E-03	-0.	-0.	0.	-0.	0.	7	1	3	DMD
-1.5217144E-03	1.1055902E-03	0.	-0.	0.	-0.	7	4	3	DMD

2.1068827E-03	0.	-0.	-0.	-0.	-0.	7	7	3	DMO
-0.	0.	-1.6358194E-03	0.	-0.	0.	8	1	3	DMO
0.	-0.	7.6085719E-04	-5.5279510E-04	-9.8646208E-04	-1.3577486E-03	8	4	3	DMO
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	8	7	3	DMO
-0.	0.	-0.	0.	-1.6358194E-03	0.	9	1	3	DMO
0.	-0.	-9.8646208E-04	-1.3577486E-03	7.6085719E-04	-5.5279510E-04	9	4	3	DMO
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	9	7	3	DMO

D(TRANPOSE)*F*D + D(C)*F(C)*D(C)									
1.9213402E-02	-0.	-0.	-0.	-0.	-0.	1	1	3	FFM
-6.5708342E-03	4.7739905E-03	-3.4674545E-11	-0.	-0.	-3.4674545E-11	1	4	3	FFM
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	1	7	3	FFM
-0.	-0.	1.5963078E-02	-0.	-0.	-0.	2	1	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	3.1156052E-03	-2.3939790E-03	-3.2950294E-03	2	4	3	FFM
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	2	7	3	FFM
-0.	-0.	-0.	-0.	1.5963078E-02	-0.	3	1	3	FFM
-3.4674545E-11	-0.	-2.3939790E-03	-3.2950294E-03	-4.2882626E-03	3.1156052E-03	3	4	3	FFM
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	FFM
-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	-0.	-0.	-3.4674545E-11	4	1	3	FFM
1.2284555E-02	-0.	-0.	-0.	-0.	0.	4	4	3	FFM
-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	-0.	-0.	3.4674545E-11	4	7	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	-3.1156052E-03	-2.3939790E-03	3.2950294E-03	5	1	3	FFM
-0.	-0.	8.8204002E-03	-0.	-0.	0.	5	4	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	-3.1156052E-03	2.3939790E-03	-3.2950294E-03	5	7	3	FFM
-3.4674545E-11	-0.	-2.3939790E-03	3.2950294E-03	-4.2882626E-03	-3.1156052E-03	6	1	3	FFM
-0.	-0.	-0.	-0.	8.8204002E-03	0.	6	4	3	FFM
3.4674545E-11	-0.	2.3939790E-03	-3.2950294E-03	-4.2882626E-03	-3.1156052E-03	6	7	3	FFM
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	7	1	3	FFM
-6.5708342E-03	4.7739905E-03	-3.4674545E-11	-0.	-0.	3.4674545E-11	7	4	3	FFM
1.9213402E-02	-0.	-0.	-0.	-0.	-0.	7	7	3	FFM
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	8	1	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	3.1156052E-03	2.3939790E-03	3.2950294E-03	8	4	3	FFM
-0.	-0.	1.5963078E-02	-0.	-0.	-0.	8	7	3	FFM
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	9	1	3	FFM
3.4674545E-11	-0.	2.3939790E-03	3.2950294E-03	-4.2882626E-03	3.1156052E-03	9	4	3	FFM
-0.	-0.	-0.	-0.	1.5963078E-02	-0.	9	7	3	FFM

A	1.00000E 00	-0.	-0.	-0.	-0.	-0.	1	1	6	A
	-1.00000E 00	-0.	-0.	0.	0.	0.	1	7	3	A

NORMALIZED A										
	7.07107E-01	-0.	-0.	-0.	-0.	-0.	1	1	6	A N
	-7.07107E-01	-0.	-0.	0.	0.	0.	1	7	3	A N

A(STAR)										
	7.07107E-01	-0.	-0.	-0.	-0.	-0.	1	1	6	A S
	-7.07107E-01	-0.	-0.	0.	0.	0.	1	7	3	A S

A(STAR)*(D*F*D + D(C)*F(C)*D(C))										
	1.1272529E-02	0.	0.	0.	0.	0.	1	1	3	A*F
	-0.	0.	-0.	-0.	-0.	-4.9037212E-11	1	4	3	A*F
	-1.1272529E-02	0.	0.	0.	0.	0.	1	7	3	A*F

M										
	1.5941763E-02	-0.	-0.	-0.	-0.	-0.	1	1	1	M

M(HERMITIAN)										
	1.5941763E-02	0.	-0.	-0.	-0.	-0.	1	1	1	M

1.59418E-02	0.	-0.	-0.	-0.	-0.	1	1	2	HTR
0.	1.59418E-02	-0.	-1.31400E-01	-1.03600E-01	-1.31400E-01	2	1	2	HTR

	RAW EIGENVALUES	WAVE NUMBERS	ELECTRON VOLTS	CPS*E12
1	1.5942E-02	1.6453E 02	2.0397E-02	4.9358E 00
2	1.5942E-02	1.6453E 02	2.0397E-02	4.9358E 00

TRACE = 3.1384E-02
SUM OF EIGENVALUES = 3.1884E-02
TRACE-SUM = -3.3528E-08

F = (0.000000, 0.200000, 0.200000)

EIGENVECTORS IN PSEUDO-POLAR FORM

1.0000000E 00	-0.	0.	0.	0.	0.	1	1	1	PPE
1.0000000E 00	0.	2.0281870E-01	0.	0.	0.	2	1	1	PPE

II E= 0 IFTAPE= 0 IVTAPE= 0 IATAPE= 1

<LTAPE= 1 KFTAPE= 1 KVTAPE= 1 KATAPE= 1

NUMBER OF COLUMNS IN D,N2= 9

NUMBER OF ROWS IN D,N3= 9

NUMBER OF ROWS IN A,N5= 3

NUMBER OF D MATRICES WITH POSITIVE SUBSCRIPTS,NUMAT 7

F = (0.000000, 0.200000, 0.200000)

8.4048068E-02	0.	0.	0.	0.	0.	1	1	3	F*D
-2.4694745E-02	1.8087091E-02	-1.7096326E-10	0.	-1.7096326E-10	0.	1	4	3	F*D
0.	0.	0.	0.	0.	0.	1	7	3	F*D
0.	0.	8.4048068E-02	0.	0.	0.	2	1	3	F*D
-1.7096326E-10	0.	-2.4894745E-02	1.8087091E-02	-1.6667305E-02	-2.2940577E-02	2	4	3	F*D
0.	0.	0.	0.	0.	0.	2	7	3	F*D
0.	0.	0.	0.	8.4048068E-02	0.	3	1	3	F*D
-1.7096326E-10	0.	-1.6667305E-02	-2.2940577E-02	-2.4894745E-02	1.8087091E-02	3	4	3	F*D
0.	0.	0.	0.	0.	0.	3	7	3	F*D
-5.5010174E-02	-3.9967231E-02	-3.7777926E-10	-0.	-3.7777926E-10	-0.	4	1	3	F*D
1.1450024E-01	0.	0.	-0.	0.	-0.	4	4	3	F*D
-5.5010174E-02	-3.9967231E-02	-3.7777926E-10	-0.	3.7777926E-10	-0.	4	7	3	F*D
-3.7777926E-10	-0.	-5.5010174E-02	-3.9967231E-02	-3.6829914E-02	5.0692029E-02	5	1	3	F*D
0.	-0.	1.0576830E-01	-0.	0.	-0.	5	4	3	F*D
-3.7777926E-10	-0.	-5.5010174E-02	-3.9967231E-02	3.6829914E-02	-5.0692029E-02	5	7	3	F*D
-3.7777926E-10	-0.	-3.6829914E-02	5.0692029E-02	-5.5010174E-02	-3.9967231E-02	6	1	3	F*D
0.	-0.	0.	-0.	1.0576830E-01	-0.	6	4	3	F*D
3.7777926E-10	-0.	3.6829914E-02	-5.0692029E-02	-5.5010174E-02	-3.9967231E-02	6	7	3	F*D
0.	-0.	0.	-0.	0.	-0.	7	1	3	F*D
-2.4894745E-02	1.8087091E-02	-1.7096326E-10	-0.	1.7096326E-10	-0.	7	4	3	F*D
8.4048068E-02	-0.	0.	-0.	0.	-0.	7	7	3	F*D
0.	-0.	0.	-0.	0.	-0.	8	1	3	F*D
-1.7096326E-10	-0.	-2.4894745E-02	1.8087091E-02	1.6667305E-02	2.2940577E-02	8	4	3	F*D
0.	-0.	8.4048068E-02	-0.	0.	-0.	8	7	3	F*D
0.	-0.	0.	-0.	0.	-0.	9	1	3	F*D
1.7096326E-10	-0.	1.6667305E-02	2.2940577E-02	-2.4894745E-02	1.8087091E-02	9	4	3	F*D
0.	-0.	0.	-0.	8.4048068E-02	-0.	9	7	3	F*D
1.7046520E-02	-0.	0.	-0.	0.	-0.	1	1	3	DFD
-5.0491198E-03	3.6684003E-03	-3.4674545E-11	-0.	-3.4674545E-11	0.	1	4	3	DFD
0.	-0.	0.	-0.	0.	-0.	1	7	3	DFD
0.	-0.	1.7046520E-02	-0.	0.	-0.	2	1	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	3.6684003E-03	-3.3804410E-03	-4.6527779E-03	2	4	3	DFD
0.	-0.	0.	-0.	0.	-0.	2	7	3	DFD
0.	-0.	0.	-0.	1.7046520E-02	-0.	3	1	3	DFD
-3.4674545E-11	-0.	-3.3804410E-03	-4.6527779E-03	-5.0491198E-03	3.6684003E-03	3	4	3	DFD
0.	-0.	0.	-0.	0.	-0.	3	7	3	DFD
-5.0491198E-03	-3.6684003E-03	-3.4674545E-11	-0.	-3.4674545E-11	-0.	4	1	3	DFD
1.0509427E-02	-0.	0.	-0.	0.	0.	4	4	3	DFD
-5.0491198E-03	-3.6684003E-03	-3.4674545E-11	-0.	3.4674545E-11	-0.	4	7	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	-3.6684003E-03	-3.3804410E-03	4.6527779E-03	5	1	3	DFD
0.	-0.	9.7079642E-03	-0.	0.	0.	5	4	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	-3.6684003E-03	3.3804410E-03	-4.6527779E-03	5	7	3	DFD
-3.4674545E-11	-0.	-3.3804410E-03	4.6527779E-03	-5.0491198E-03	-3.6684003E-03	6	1	3	DFD
0.	-0.	0.	-0.	9.7079642E-03	0.	6	4	3	DFD
3.4674545E-11	-0.	3.3804410E-03	-4.6527779E-03	-5.0491198E-03	-3.6684003E-03	6	7	3	DFD
0.	-0.	0.	-0.	0.	-0.	7	1	3	DFD

-5.0491198E-03	3.6684003E-03	-3.4674545E-11	-0.	3.4674545E-11	0.	7	4	3	DFD
1.7046520E-02	-0.	0.	-0.	0.	-0.	7	7	3	DFD
0.	-0.	0.	-0.	0.	-0.	8	1	3	DFD
-3.4674545E-11	-0.	-5.0491198E-03	3.6684003E-03	3.3804410E-03	4.6527779E-03	8	4	3	DFD
0.	-0.	1.7046520E-02	-0.	0.	-0.	8	7	3	DFD
0.	-0.	0.	-0.	0.	-0.	9	1	3	DFD
3.4674545E-11	-0.	3.3804410E-03	4.6527779E-03	-5.0491198E-03	3.6684003E-03	9	4	3	DFD
0.	-0.	0.	-0.	1.7046520E-02	-0.	9	7	3	DFD
2.307/V*D(C)*Z*CCC*Z*D(C)									
2.1668827E-03	-0.	-0.	-0.	-0.	-0.	1	1	3	DCD
-1.3809424E-03	0.	0.	0.	0.	0.	1	4	3	DCD
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	1	7	3	DCD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	2	1	3	DCD
0.	0.	9.4047122E-04	0.	0.	-1.6782696E-03	2	4	3	UCD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	2	7	3	DCD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	3	1	3	DCD
0.	0.	0.	-1.6782696E-03	9.4047122E-04	0.	3	4	3	DCD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	UCD
-1.3809424E-03	0.	0.	0.	0.	0.	4	1	3	DCD
1.7751279E-03	-0.	-0.	-0.	-0.	-0.	4	4	3	DCD
-1.3809424E-03	0.	0.	0.	0.	0.	4	7	3	DCD
0.	0.	9.4047122E-04	0.	0.	1.6782696E-03	5	1	3	DCD
-0.	-0.	-8.8756394E-04	-0.	-0.	-0.	5	4	3	DCD
0.	0.	9.4047122E-04	0.	0.	-1.6782696E-03	5	7	3	DCD
0.	0.	0.	1.6782696E-03	9.4047122E-04	0.	6	1	3	DCD
-0.	-0.	-0.	-0.	-8.8756394E-04	-0.	6	4	3	DCD
0.	0.	0.	-1.6782696E-03	9.4047122E-04	0.	6	7	3	DCD
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	7	1	3	DCD
-1.3809424E-03	0.	0.	0.	0.	0.	7	4	3	DCD
2.1668827E-03	-0.	-0.	-0.	-0.	-0.	7	7	3	DCD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	8	1	3	DCD
0.	0.	9.4047122E-04	0.	0.	1.6782696E-03	8	4	3	DCD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	8	7	3	DCD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	9	1	3	DCD
0.	0.	0.	1.6782696E-03	9.4047122E-04	0.	9	4	3	DCD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	9	7	3	DCD
D(C)*F(C)*D(C)									
2.1668827E-03	0.	-0.	-0.	-0.	-0.	1	1	3	DMD
-1.5217144E-03	1.1055902E-03	0.	-0.	0.	-0.	1	4	3	DMD
3.2716388E-03	0.	-0.	-0.	-0.	-0.	1	7	3	DMD
-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	2	1	3	DMD
0.	-0.	7.6085719E-04	-5.5279510E-04	9.8646208E-04	1.3577486E-03	2	4	3	DMD
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	2	7	3	DMD
-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	3	1	3	DMD
0.	-0.	9.8646208E-04	1.3577486E-03	7.6085719E-04	-5.5279510E-04	3	4	3	DMD
-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	DMD
-1.5217144E-03	-1.1055902E-03	0.	0.	0.	0.	4	1	3	DMD
1.7751279E-03	0.	-0.	-0.	-0.	-0.	4	4	3	DMD
-1.5217144E-03	-1.1055902E-03	0.	0.	0.	0.	4	7	3	DMD
0.	0.	7.6085719E-04	5.5279510E-04	9.8646208E-04	-1.3577486E-03	5	1	3	DMD
-0.	-0.	-8.8756394E-04	-0.	-0.	-0.	5	4	3	DMD
0.	0.	7.6085719E-04	5.5279510E-04	-9.8646208E-04	1.3577486E-03	5	7	3	DMD
0.	0.	9.8646208E-04	-1.3577486E-03	7.6085719E-04	5.5279510E-04	6	1	3	DMD
-0.	-0.	-0.	-0.	-8.8756394E-04	-0.	6	4	3	DMD
0.	0.	-9.8646208E-04	1.3577486E-03	7.6085719E-04	5.5279510E-04	6	7	3	DMD
1.6388E-03	-0.	-0.	0.	-0.	0.	7	1	3	DMD
-1.17144E-03	1.1055902E-03	0.	-0.	0.	-0.	7	4	3	DMD

2	.8827E-03	0.	-0.	-0.	-0.	-0.	7	7	3	
-0.		0.	-1.6358194E-03	0.	-0.	0.	3	1	3	DMO
0.	-0.	-0.	7.6085719E-04	-5.5279510E-04	-9.8646208E-04	-1.3577486E-03	3	4	3	DMO
-0.	-0.	-0.	-1.0834413E-03	-0.	-0.	-0.	3	7	3	DMO
-0.	0.	-0.	0.	0.	-1.6358194E-03	0.	3	1	3	DMO
0.	-0.	-0.	-9.8646208E-04	-1.3577486E-03	7.6085719E-04	-5.5279510E-04	3	4	3	DMO
-0.	-0.	-0.	-0.	-0.	-1.0834413E-03	-0.	3	7	3	DMO

D(TRANPOSE)*F*D + D(C)*F(C)*D(C)

1.9213402E-02	-0.	-0.	-0.	-0.	-0.	-0.	1	1	3	FFM
-6.5708342E-03	4.7739905E-03	-3.4674545E-11	-0.	-0.	-3.4674545E-11	0.	1	4	3	FFM
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	-0.	1	7	3	FFM
-0.	-0.	1.5963078E-02	-0.	-0.	-0.	-0.	2	1	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	3.1156052E-03	-2.3939790E-03	-3.2950294E-03	-3.2950294E-03	2	4	3	FFM
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	-0.	2	7	3	FFM
-0.	-0.	-0.	-0.	-0.	1.5963078E-02	-0.	3	1	3	FFM
-3.4674545E-11	-0.	-2.3939790E-03	-3.2950294E-03	-4.2882626E-03	3.1156052E-03	-0.	3	4	3	FFM
-0.	-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	3	7	3	FFM
-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	-0.	-0.	-3.4674545E-11	-0.	4	1	3	FFM
1.2284555E-02	-0.	-0.	-0.	-0.	-0.	0.	4	4	3	FFM
-6.5708342E-03	-4.7739905E-03	-3.4674545E-11	-0.	-0.	3.4674545E-11	-0.	4	7	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	-3.1156052E-03	-2.3939790E-03	3.2950294E-03	-3.2950294E-03	5	1	3	FFM
-0.	-0.	8.8204002E-03	-0.	-0.	0.	0.	5	4	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	-3.1156052E-03	2.3939790E-03	-3.2950294E-03	-3.2950294E-03	5	7	3	FFM
-3.4674545E-11	-0.	-2.3939790E-03	3.2950294E-03	-4.2882626E-03	-3.1156052E-03	-3.1156052E-03	6	1	3	FFM
-0.	-0.	-0.	-0.	8.8204002E-03	0.	0.	6	4	3	FFM
3.4674545E-11	-0.	2.3939790E-03	-3.2950294E-03	-4.2882626E-03	-3.1156052E-03	-3.1156052E-03	6	7	3	FFM
3.2716388E-03	-0.	-0.	-0.	-0.	-0.	-0.	7	1	3	FFM
-6.5708342E-03	4.7739905E-03	-3.4674545E-11	-0.	-0.	3.4674545E-11	0.	7	4	3	FFM
1.9213402E-02	-0.	-0.	-0.	-0.	-0.	-0.	7	7	3	FFM
-0.	-0.	-1.6358194E-03	-0.	-0.	-0.	-0.	8	1	3	FFM
-3.4674545E-11	-0.	-4.2882626E-03	3.1156052E-03	2.3939790E-03	3.2950294E-03	-3.2950294E-03	8	4	3	FFM
-0.	-0.	1.5963078E-02	-0.	-0.	-0.	-0.	8	7	3	FFM
-0.	-0.	-0.	-0.	-0.	-1.6358194E-03	-0.	9	1	3	FFM
3.4674545E-11	-0.	2.3939790E-03	3.2950294E-03	-4.2882626E-03	3.1156052E-03	-3.1156052E-03	9	4	3	FFM
-0.	-0.	-0.	-0.	1.5963078E-02	-0.	-0.	9	7	3	FFM

A							1	1	6	A
-0.	1.00000E 00	-0.	-0.	-0.	-0.	0.	1	7	3	A
-0.	1.00000E 00	-0.	0.	0.	0.	0.	2	1	6	A
-0.	-0.	1.00000E 00	-0.	-0.	-0.	0.	2	7	3	A
-0.	-0.	-1.00000E 00	0.	0.	0.	0.	2	7	3	A
-0.	-0.	-0.	-0.	1.00000E 00	-0.	-0.	3	1	6	A
-0.	-0.	0.	0.	0.	0.	0.	3	7	3	A

NORMALIZED A

-0.	7.07107E-01	-0.	-0.	-0.	-0.	1	1	6	A	N
-0.	7.07107E-01	-0.	0.	0.	0.	1	7	3	A	N
-0.	-0.	7.07107E-01	-0.	-0.	-0.	2	1	6	A	N
-0.	-0.	-7.07107E-01	0.	0.	0.	2	7	3	A	N
-0.	-0.	-0.	-0.	1.00000E 00	-0.	3	1	6	A	N
-0.	-0.	0.	0.	0.	0.	3	7	3	A	N

A(STAR)

-0.	7.07107E-01	-0.	-0.	0.	-0.	1	1	6	A	S
-0.	7.07107E-01	0.	0.	0.	0.	1	7	3	A	S
-0.	-0.	7.07107E-01	-0.	0.	-0.	2	1	6	A	S
-0.	-0.	-7.07107E-01	0.	0.	0.	2	7	3	A	S
-0.	-0.	-0.	-0.	1.00000E 00	-0.	3	1	6	A	S

-0.	-0.	0.	0.	0.	0.	0.	3	7	3	A	S	
A(STAR)*(D*F*D + D(C)*F(C)*D(C))												
0.	-0.	1.0130902E-02	-0.	0.	-0.		1	1	3	A	F	
-4.9037212E-11	-0.	-6.0645191E-03	4.4061310E-03	-0.	0.		1	4	3	A	F	
0.	-0.	1.0130902E-02	-0.	0.	-0.		1	7	3	A	F	
0.	0.	0.	0.	1.2444300E-02	0.		2	1	3	A	F	
-4.9037212E-11	0.	-3.3855975E-03	-4.6598751E-03	-0.	-0.		2	4	3	A	F	
0.	0.	0.	0.	-1.2444300E-02	0.		2	7	3	A	F	
-3.4674545E-11	-0.	-4.2882626E-03	-3.1156052E-03	-2.3939790E-03	3.2950294E-03		3	1	3	A	F	
0.	-0.	8.8204002E-03	0.	0.	0.		3	4	3	A	F	
-3.4674545E-11	-0.	-4.2882626E-03	-3.1156052E-03	2.3939790E-03	-3.2950294E-03		3	7	3	A	F	
M												
1.4327258E-02	-0.	0.	0.	-6.0645191E-03	4.4061310E-03		1	1	3	M		
0.	0.	1.7598897E-02	-0.	-3.3855975E-03	-4.6598751E-03		2	1	3	M		
-6.0645191E-03	-4.4061310E-03	-3.3855975E-03	4.6598751E-03	8.8204002E-03	-0.		3	1	3	M		
M(HERMITIAN)												
1.4327258E-02	0.	0.	-0.	-6.0645191E-03	4.4061310E-03		1	1	3	M		
0.	0.	1.7598897E-02	0.	-3.3855975E-03	-4.6598751E-03		2	1	3	M		
-6.0645191E-03	-4.4061310E-03	-3.3855975E-03	4.6598751E-03	8.8204002E-03	0.		3	1	3	M		
1.43273E-02	0.	-6.06452E-03	0.	0.	-4.40613E-03	1	1	6	HTR			
0.	1.75989E-02	-3.38560E-03	0.	0.	4.65983E-03	2	1	6	HTR			
-6.06452E-03	-3.38560E-03	8.82040E-03	4.40613E-03	-4.65988E-03	0.	3	1	6	HTR			
0.	0.	4.40613E-03	1.43273E-02	0.	-6.06452E-03	4	1	6	HTR			
0.	0.	-4.65988E-03	0.	1.75989E-02	-3.38560E-03	5	1	6	HTR			
-4.40613E-03	4.65988E-03	0.	-6.06452E-03	-3.38560E-03	8.82040E-03	6	1	6	HTR			

	RAW EIGENVALUES	WAVE NUMBERS	ELECTRON VOLTS	CPS*E12
1	2.2489E-02	1.9541E 02	2.4227E-02	5.8624E 00
2	2.2489E-02	1.9541E 02	2.4227E-02	5.8624E 00
3	1.6168E-02	1.6569E 02	2.0542E-02	4.9706E 00
4	1.6168E-02	1.6569E 02	2.0542E-02	4.9706E 00
5	2.0896E-03	5.9565E 01	7.3847E-03	1.7870E 00
6	2.0896E-03	5.9565E 01	7.3847E-03	1.7870E 00

TRACE = 8.1493E-02
 SUM OF EIGENVALUES = 8.1493E-02
 TRACE-SUM = -1.2573E-07

F = (0.000000, 0.200000, 0.200000)

EIGENVECTORS IN PSEUDO-POLAR FORM

5.1096321E-01	-0.	6.5528131E-01	9.0000003E 01	-5.5634791E-01	3.6000002E 01	1	1	3	PPE
5.1094930E-01	-0.	6.5529417E-01	9.0000029E 01	-5.5634540E-01	3.6000014E 01	2	1	3	PPE
7.0067523E-01	0.	-6.9242828E-01	9.0000004E 01	-1.7203843E-01	3.6000000E 01	3	1	3	PPE
7.0067594E-01	-0.	-6.9242723E-01	9.0000004E 01	-1.7203997E-01	3.5999998E 01	4	1	3	PPE
4.9796664E-01	-0.	3.0190888E-01	9.0000003E 01	8.1294540E-01	3.5999999E 01	5	1	3	PPE
4.9794659E-01	0.	3.0193565E-01	8.9999981E 01	8.1294758E-01	3.5999994E 01	6	1	3	PPE

END-OF-DATA ENCOUNTERED ON SYSTEM INPUT FILE.