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WMIN, A Computer Program to Model Molecules and Crystals in Terms of Potential Energy Functions

William R. Busing

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WMIN, A COMPUTER PROGRAM TO MODEL MOLECULES AND CRYSTALS IN TERMS OF POTENTIAL ENERGY FUNCTIONS

William R. Busing

Date Published: April 1981

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ABSTRACT

This report describes the computer program WMIN which can be used to manipulate static and dynamic models of crystals or isolated molecules and to calculate their energies from interatomic potential functions. It is applicable to a wide variety of substances ranging from ionic crystals to large organic molecules.

The report includes a description of the program, instructions for data input, a program listing, and the output from test problems. The program is available from the author on request.

1. INTRODUCTION

This report describes the computer program WMIN which is capable of manipulating static and dynamic models of crystals or isolated molecules and calculating their energies from interatomic potential functions. The program may be used for a wide variety of substances ranging from ionic crystals to large organic molecules.

The models under consideration may be built up of rigid molecules which may rotate or translate, molecules composed of rigid segments but with internal rotation about certain bonds, or individual atoms with positions which can change independently. These units may be used to describe either crystals or isolated molecules, and the model may be constrained to conform to any desired crystal or molecular symmetry. The parameters which describe the structure include the crystal lattice parameters and the translations and orientations of the rigid units.

The energy calculated for the model may include the following contributions: (1) Coulomb energy, (2) van der Waals attraction, (3) interatomic repulsion, (4) a quadratic potential associated with a covalent bond, (5) a quadratic potential associated with an intra-molecular bond angle, (6) an energy associated with torsional strain about a covalent bond, and (7) any additional energy terms specified by user subroutines.

One application of the program is to minimize the energy by adjusting the structural parameters, and three different techniques are available for this purpose. These are Newton's method which requires second derivatives of the energy with respect to the parameters, the method of steepest descents which requires first derivatives, and a search technique which requires no derivatives.

The program can also calculate the vibrational frequencies and normal coordinates for any structure at an energy minimum. In this way it is possible to study the internal modes of an isolated molecule, the lattice modes of rigid molecules in a crystal, or the interaction of lattice modes and internal modes of flexible molecules in a crystal.

Another scheme of operation may be used to adjust parameters of the potential functions using the method of least squares. Observations for

this calculation may include known structural parameters and experimental lattice energies, and it is possible to use information from several substances to adjust potential parameters common to them. These observations may be appropriately weighted.

In all of these calculations where first and second derivatives are needed, they are obtained numerically. This greatly simplifies the application of constraints and increases the flexibility of the program.

This report includes a preliminary description of the program, detailed descriptions of various procedures, instructions for data input, a program listing, and the output from test problems. Some information on WMIN was presented earlier (Busing, 1972), and examples of published research using the program are listed in Section 11.2. The program is available from the author on request.

2. OVERALL DESCRIPTION

2.1 General

This section is intended as a brief overall description of the program. Later sections will deal with various aspects in more detail. We will begin by describing some of the program variables making use of their symbolic names where applicable. A glossary of these symbols is included in the listing of the program, Section 9.2.

Of central importance is the energy W of the molecule or crystal and this is always calculated by the function subprogram WCALC. This energy W is a function of parameters which can be divided into two categories: the energy parameters, which are coefficients in the expressions for the potential energy of the model, and the structural parameters, which define the geometrical positions of the atoms in the molecule or crystal. The principal purpose of the program WMIN is to manipulate either the energy parameters or the structural parameters for one or more substances in a way which depends on the MODE of the calculation. Any parameters to be adjusted in this way must appear in the overall parameter list P. This array is made up of the common parameters PC, which are usually the energy parameters of the model; the lattice parameters A for each substance; rotations SXR, SYR, and SZR and translations TR for each rigid group (or individual atom) in each substance; and extra parameters PX for each substance.

For mode 0 (i.e., MODE = 0) the program WMIN performs a least-squares adjustment of certain parameters (usually the energy parameters) using certain other parameters (usually the structural parameters) as observations. The matrix equation solved is

$$\tilde{\underset{\sim}{B}}\ \underset{\sim}{w}\ \underset{\sim}{B}\ \underset{\sim}{\Delta q} = -\tilde{\underset{\sim}{B}}\ \underset{\sim}{w}\ \underset{\sim}{d} \qquad (1)$$

where $d_i = \partial W/\partial p_i$, the first derivative of the energy with respect to a structural parameter p_i, and $B_{ij} = \partial^2 W/\partial p_i \partial q_j$, the second derivative of the energy with respect to a structural parameter p_i and an energy parameter q_j. The equation is solved for Δq_j, the changes in the energy parameters which will tend to minimize the values of the first derivatives d_i, using an appropriate weight matrix $\underset{\sim}{w}$.

Program WMIN computes all of the required first and second derivatives numerically by modifying one or two parameters in the overall list P and entering subprogram WCALC to calculate the modified energy. This procedure will be discussed in detail in Section 6.5.

Both the observations p_i and the variables q_j are represented in the overall parameter list P. In one to one correspondence with this array are two integer arrays KP and KQ, the observation selection integers and the variable selection integers, respectively. These arrays are set up from the input data to the program, and non-zero values of KP or KQ specify observations or variables, respectively.

For modes 1, 2, 3, or 4 the program minimizes the energy by adjusting only the structural parameters. For this purpose the program ignores the input values of KQ and substitutes those of KP so that the structural parameters specified by KP serve as both observations and variables.

For mode 1 the energy is minimized by Newton's method solving the matrix equation

$$\underset{\sim}{B}\ \underset{\sim}{\Delta p} = -\underset{\sim}{d} \tag{2}$$

where $\underset{\sim}{d}$ and $\underset{\sim}{B}$ are made up of the first and second derivatives as before. In this mode, however, $\underset{\sim}{B}$ is a symmetric matrix because the structural parameters which define the observations are also the parameters to be varied.

For mode 2 the program minimizes the energy by the method of steepest descents which requires only the first derivatives to be calculated, and in mode 3 the program uses a search technique which requires no derivatives. For mode 4 the program minimizes the energy as for mode 1 and then solves the dynamical eigenvalue problem for the vibrational frequencies and normal coordinates. In mode -1 the program steps through values of any three specified parameters in the array P, enters WCALC, and prints the resulting energy for each combination of parameter values.

Although parameter list P is the only array which can be varied directly by WMIN, several other arrays are important to the energy

calculation. Array XYZ contains the fractional coordinates of the NA atoms in the basic asymmetric unit of a crystal or isolated molecule. These coordinates which are read as input are not in general used as variables of the program. Instead, the variables are the rotations SXR, SYR, and SZR or translations TR of the rigid bodies away from these basic positions. The coordinates of the NA atoms after rotation and translation are stored in XYZR. A list of the NAC atoms in a unit cell is generated from the coordinates of NA atoms and the NS symmetry transformations giving the proper weight to atoms in crystallographic special positions. The coordinates of these NAC atoms are generated from the basic asymmetric unit on each entry to WCALC and stored in arrays XC, YC, and ZC. It is these coordinate arrays, which include the effects of rigid body rotation and translation, that are used directly in the energy calculation.

Other arrays of importance are those which describe the properties of NKA chemical kinds of atoms. These include the atomic masses AMASS and the following energy parameters: Q, the Coulomb charges on the atoms; PL, the van der Waals coefficients; AR, the repulsion radii; and BR, the softness parameters for repulsion. The roles of these parameters in the potential energy expression will be discussed in detail in another section. Although the parameters Q, PL, AR, and BR cannot be varied directly by program WMIN, it is the purpose of the common parameter array PC to permit the indirect adjustment of these and various other parameters. The link between these energy parameters and the array PC is subroutine CNSTRN prepared by the user. This routine may set the values of Q, PL, AR, and BR in terms of the values of the common parameters PC, and in this way CNSTRN serves to define the meaning of the parameters PC. In general the common parameters PC have no effect on the energy calculation except as defined by subroutine CNSTRN and two other routines to be mentioned below. Parameters PC are called <u>common</u> because one set of values may apply to more than one substance in a single calculation. The extra parameters PX play this same role as parameters defined by the user except that a separate array PX is associated with each substance. Subroutine CNSTRN can also be used to specify any desired relationship between atomic coordinates or rigid body translations and rotations.

2.2 MAIN Program

Execution begins in a MAIN program (in the Fortran sense of the word MAIN). This routine, which does not appear in the flowcharts of Figs. 2.1 to 2.5, has the principal purpose of assigning space to 133 arrays at run time. Storage is allocated on the basis of 16 input integers, LIM, which set upper limits on various dimensions. MAIN passes these arrays to the rest of the program as subroutine arguments. This procedure is described in detail in Section 7.1.

2.3 Basic Subroutine WMIN

We will describe briefly the flow of the program for a typical calculation referring to the flow charts of Figs. 2.1 to 2.5. Numbers of the boxes in these charts correspond to statement numbers in the source program.

There are two main paths which the calculation takes depending on whether several substances are to be treated together or separately. If common parameters PC are to be varied by the program (NVC $\neq$ 0; this can only occur in mode 0) then information about each substance is written on auxiliary storage (disk or tape). This information is then read back and the contribution of each substance is added to the least-squares matrix of normal equations. If no common parameters are to be varied (NVC = 0; this must be the case except in mode 0) then each substance is treated separately and no auxiliary storage is used.

The basic subroutine WMIN (Fig. 2.1) begins in Box 500 by reading control information, including the MODE and common parameters PC. NVC, the number of variable common parameters, is determined and used throughout WMIN to control whether calculations for various substances are to be combined or not. We will first trace the flow for NVC = 0 so that substances are treated separately and no auxiliary storage is used.

The substance identifier ISB is read in Box 595 and a zero value signals the program (Box 597) that no further substances will be included. When NVC = 0 this terminates the job. Subroutine WPRE is called from Box 620 to read input and make preliminary calculations for the one substance. This subroutine (Fig. 2.2) stores parameters in the overall list P and sets the observation and variable selection integers

KP and KQ. Subroutines SETA and CNSTRN are also called from WPRE. Upon return from WPRE the MODE is tested (Box 630) and for mode -1 the mapping procedure (Box 1710) is initiated. Otherwise the program prints the overall parameter list P (Box 635) and initializes a cycle of parameter adjustment (Box 745).

In Box 800 the program makes the first energy calculation of the cycle by entering function subprogram WCALC. Because this energy calculation is a major part of the program we will discuss it in some detail in Section 2.4. At this point we will merely note that on this first entry WCALC prints various contributions to the energy and lists the shortest interatomic distances. If intramolecular energy is to be calculated for flexible molecules then WCALC calls GCWX which computes and prints bond distances, bond angles, and conformation angles and their contributions to the energy. Finally WCALC prints WC, WV, WR, WX, and WT the Coulomb, van der Waals, repulsion, and intramolecular energy contributions, and the total energy, respectively. Upon return from WCALC the total energy is also stored as the variable W.

In Box 815 the program tests the MODE and branches to the minimum energy search (Box 2035) for mode 3. Otherwise WMIN enters a series of loops in Box 820 to generate numerically the first and second derivatives of the energy with respect to parameters specified by the observation and variable selection integers KP and KQ. For each derivative one or two parameters P are modified and WCALC is entered to calculate the modified energy. On these entries, however, WCALC follows a much faster procedure than on the first entry and produces no printed output. Again this will be described in more detail in Section 2.4.

If the experimental energy WOBS is to serve as an observation in a least-squares adjustment of parameters, then its contributions to the least-squares matrix AN and vector VN are computed in Box 1010. This can only occur in mode 0.

In Box 1030 the MODE is again tested and in mode 2 the program branches to minimize the energy by the method of steepest descents (Box 1850). For mode 0, 1, or 4 the program proceeds to Box 1085 where the derivatives are printed. The vector DYC is the negative of DW, the first derivatives of the energy with respect to structural parameters (i.e.,

the vector $\tilde{d}$ of Eqs. 1 and 2), and it is these first derivatives which the program will attempt to reduce to zero. The matrix BTR ($\tilde{B}$ of Eqs. 1 and 2) contains the second derivatives so that BTR and DYC together define the observational equations. These arrays are used to set up the matrix AN and the vector VN either for Newton's method or for the method of least squares. In the latter case the weight matrix WMAT may or may not be included depending on the control input.

In Box 1200 these linear equations are solved for the changes in the variable parameters. For this purpose the matrix AN is inverted using the method of principal component analysis. That is, the eigenvalues EVAL and eigenvectors EVEC of AN are determined and used to generate its inverse. Eigenvalues which are smaller than ARE times the largest one correspond to poorly determined linear combinations of variables, and these are omitted from this calculation. The overall result is to avoid the problem of singular or ill-conditioned matrices and to reveal to the user the sets of redundant parameters which cause them. Finally the revised parameters are calculated and printed, and the program returns to Boxes 745, 800, and 820 for another cycle of refinement.

On the final cycle (cycle number NC + 1) the program does not make any parameter adjustment. Instead it branches at Box 1007 to Box 1505 where only the first derivatives of the energy are printed. In mode 4 the program calls subroutine WDYN (Box 1540) to calculate vibrational frequencies and normal coordinates. This routine will be described in detail in Sections 2.5 and 6.10. Finally in Box 1550 the program generates revised atom coordinates and punches cards for any parameters which have been varied. These cards may be used for input to further calculations.

In Box 1605 two copies of a summary of the calculation are printed. One of these is diverted to a separate output stream so that it may be readily saved as an abstract of the calculation. The program then returns to Box 595 to read input for another substance or terminate the job.

When NVC $\neq$ 0 indicating that parameters PC which may be common to more than one substance are to be varied (and this can only occur in

mode 0) then WMIN follows a somewhat different path as indicated in Fig. 2.1. Initial input to the job is read in Box 500 as before, and auxiliary disk or tape storage is initialized or rewound in Box 590. The substance name STITLE and a non-zero identifying integer ISB are read in Box 595 and WPRE is called from Box 620 to read input and initialize the calculation for one substance. In Box 625 all the necessary information for one substance is written as a record on the auxiliary storage and the program returns to Box 595 to read input for the next substance.

When the input for all substances has been read and stored a zero value of ISB terminates this loop, and in Box 610 an end-of-file is written on the auxiliary storage. In Box 635 the program prints the overall parameter list P which includes the common parameters PC and the parameters A, SXR, SYR, SZR, TR, and PX for each substance. A cycle of refinement is initialized in Box 745, the auxiliary storage is rewound (Box 775) and information for the first substance is read from this storage in Box 780. The program now proceeds through Boxes 800, 820, 1010, and 1085 as before adding the contributions of one substance to the least-squares matrix and vector AN and VN.

Information for the next substance is read (Box 780) and the process is repeated until the end-of-file is encountered on the auxiliary storage. At this point the AN and VN include contributions from all the substances and the program proceeds in Box 1200 to obtain the revised parameters as before.

Further cycles are performed in the same way until the final cycle when any revised parameters for each substance are punched on cards (Box 1550). When the end-of-file is encountered on this final cycle the revised common parameters are punched (Box 1600), one pair of summaries are printed for the calculation, and the job is terminated.

2.4 Function WCALC

The function subprogram WCALC which calculates the energy for a substance is shown schematically in Fig. 2.3. On the first entry to this routine (from Box 800 of the main program) the calculation in WCALC follows a path which is considerably different from that taken on

subsequent entries. This division of flow is controlled by a switch ISW which is set to one before the first entry and to zero thereafter. The principal purpose of this division is to increase the speed of execution of the later calculations which make use of information stored on the first entry. Because WCALC is entered repeatedly in the course of calculating numerical first and second derivatives, this procedure often saves a factor of ten or more in computing time.

Another important purpose of this division is to insure that the energy calculated on subsequent entries includes contributions from exactly the same terms as that from the first entry. This is necessary for the accurate calculation of numerical derivatives. WCALC also prints certain output on the first entry but not on subsequent passes.

Several other indicators including the argument IBY and the switch IBK may cause certain sections of the program to be bypassed in subsequent entries to WCALC, but on this first entry both of these indicators are zero so that no by-passing occurs.

In Boxes 500-555 WCALC picks up parameters from the overall list P, calls subroutine SETA to establish symmetry constraints on the lattice parameters, and calculates quantities based on these parameters. Then after calling the user routine CNSTRN (Box 560) the program uses the rigid body rotations and translations to establish the basic atom coordinates XYZR and those of all atoms in the cell, XC, YC, and ZC (Boxes 605-665).

The Ewald constant CK controls whether reciprocal lattice sums for the Coulomb or van der Waals energy terms are to be calculated in Boxes 686, 700-775, and 800-870. If CK = 0 these summations are bypassed. Otherwise these sums are made over NQ shells in reciprocal space with radii specified by QLIM so that their values accumulated to each limit can be examined for convergence. Each set of indices HX, HY, HZ of a reciprocal lattice point is tested in Box 750 against the limits of the shell and then checked by the user's subroutine REJECT which can be programmed to eliminate space group absences thus speeding up the calculation. The indices of acceptable lattice points are saved in arrays HXT, HYT, and HZT (Box 775) for use in subsequent entries to WCALC.

In Box 800 the structure factors are computed and terms are added to Coulomb and van der Waals sums with modification factors based on the

Ewald constant CK to increase the rate of convergence. Sums over the unit cell are also computed in Box 895 as a part of the reciprocal lattice calculation.

Next in Boxes 940-1305 subroutine WCALC computes various sums over the interatomic vectors of the direct lattice. This summation is made in two parts. First, if a reciprocal lattice summation has been made ($CK \neq 0$) it is necessary to subtract out the effects of all vectors (with no limitation on their lengths) between bonded atoms or atoms in the same rigid body (Box 955). These contributions are not wanted in the total energy, but there is no simple way to omit them from the reciprocal lattice sums.

Next, the contributions of vectors not between bonded atoms or atoms in the same rigid body are computed including the appropriate modification factors if the Ewald constant CK is not zero. These vectors are divided into NR shells depending upon their lengths and the specified limits RLIM so that the results accumulated to each limit can be examined for convergence. The specifications for each vector used in either part of the direct lattice sum are stored (Boxes 955 and 1215) during this first entry to WCALC for use on subsequent entries. After completing these loops a specified number of the shortest interatomic distances and their contributions to the energy are printed (Box 1305).

Next, in Box 1365 subroutine CWX is entered to compute any extra energy WX such as the internal energy of polarization which has been programmed by the user. Then the general extra energy subroutine GCWX is entered to add contributions which depend on bond distances, bond angles, and conformation angles in a way specified by the NCT input cards which set up the connection tables IACT, ICT, IDZ, IAZ, and ITBR. This subroutine which is diagrammed in the flow chart of Fig. 2.4 also has two paths of flow controlled by the switch ISW. On the first entry subroutine GCWX generates all distances, angles, and conformation angles, and calculates the contribution of each to WX. This information is printed and stored for use by the subroutine on subsequent entries.

Upon return from GCWX function subroutine WCALC prints WC, WV, WR, WX, and WT, the Coulomb, van der Waals, repulsion, and internal energies, and the total energy, respectively. The value of the function WCALC is set to WT and the subprogram returns to WMIN.

Later entries to WCALC from Box 820 (Fig. 2.1) for the calculation of numerical derivatives, from Box 1710 for energy mapping, from Box 1850 for the method of steepest descents, or from Box 2035 for the minimum energy search are made with the switch ISW = 0 so that the subprogram makes use of quantities stored on the first entry. After making initial calculations and setting up the atomic coordinates (Boxes 500-665, Fig. 2.3) the subroutine makes a rapid reciprocal lattice summation (Boxes 780-885) using the indices of the reciprocal lattice points which were stored on the first entry. The unit cell sums are made (Box 895) and the direct lattice sums are accumulated (Box 1390) for the list of vectors stored earlier.

Subroutines CWX and GCWX are called (Box 1500) to calculate extra energy WX. The latter routine (Fig. 2.4) loops over distances, angles, and conformation angles which were stored on the first entry. Finally WCALC returns to WMIN with the total energy as WT and also as the value of the function WCALC.

Several indicators are used by WCALC to speed up the calculation of the energy on all entries after the first one of each cycle, that is for switch ISW = 0. These will be mentioned briefly here and described in more detail in Section 7.2.

The indicator IBY which serves as an argument of WCALC has a value of 0 to 7 established by function subroutine IBYPAS. This indicator operates to bypass the entire reciprocal lattice summation, direct lattice summation, or extra energy calculation when the results of these will be unchanged from the previous entry. IBY causes this bypassing only in mode 0 and if derivatives with respect to common parameters PC are being calculated.

WCALC also sets another indicator ICCAX to zero if there has been no change in common parameters PC, lattice parameters A, or extra parameters PX since the previous entry. The array ICC serves as a set of similar indicators for the coordinates of each atom in the cell. If ICCAX = 0 and the indicators ICC are zero for all the atoms involved in a particular direct lattice vector in WCALC or in a bond, angle, or conformation angle in GCWX, then the corresponding energy term will be the same as it was on the previous entry and it is simply picked up from

storage and added to the sum. Otherwise the program recalculates the term for the sum and also saves it for use on the next entry.

2.5 Subroutine WDYN

In mode 4 the program proceeds to minimize the energy by Newton's method just as it does for mode 1. On the final cycle of refinement, however, the matrix of second derivatives BTR is saved and in Box 1540 (Fig. 2.1) the main program calls subroutine WDYN to calculate and print the vibrational frequencies and normal coordinates for the potential energy model of the substance. The flow diagram for this subprogram is shown schematically in Fig. 2.5.

In Box 500 WDYN obtains DXQ, DYQ, and DZQ, the derivatives of Cartesian coordinates of the atoms with respect to the rigid-body rotations and translations which serve as the NVD dynamic variables. These derivatives are obtained numerically by incrementing one variable parameter P(I) at a time and entering WCALC to obtain the corresponding set of Cartesian atomic coordinates. For this purpose a switch IBK is set non-zero to indicate that WCALC need only compute the atom coordinates and can then return without calculating the energy (Box 662, Fig. 2.3).

In Box 535 (Fig. 2.5) WDYN uses these derivatives and the atomic masses AMASS to set up the matrix AKE with elements which are the second derivatives of the kinetic energy with respect to the velocities expressed in terms of the dynamic variables.

If lattice parameters served as variables in the energy minimization procedure, then the corresponding rows and columns are removed from matrix BTR (Box 555) since these parameters cannot serve as dynamic variables. Matrices BTR and AKE are then printed.

In Box 605 subroutines are called which solve the general matrix eigenvalue problem

$$\underset{\sim}{B}\,\underset{\sim}{U} = \underset{\sim}{K}\,\underset{\sim}{U}\,\underset{\sim}{\Lambda} \tag{3}$$

where $\underset{\sim}{B}$ and $\underset{\sim}{K}$ are matrices BTR and AKE, respectively, which correspond to the $\underset{\sim}{F}$ and $\underset{\sim}{G}^{-1}$ matrices in the usual spectroscopic notation. The subroutines solve for $\underset{\sim}{\Lambda}$, the diagonal eigenvalue matrix which is stored as

the vector EVAL, and $\underset{\sim}{U}$, the eigenvectors which are stored in array BTR. The frequencies in wave numbers are stored in FREQ (Box 645), and the eigenvalues and eigenvectors are printed (Box 655).

Next WDYN starts a loop over the NVD normal modes of vibration. For each such mode (Box 667) it uses EVEC and DXQ, DYQ, and DZQ to generate the displacements XYZD of each atom referred to a Cartesian system. (This system is taken as that defined by the input data for the first rigid body.) The frequency and atomic displacements for one normal mode are then printed.

In Box 676 the program performs a series of loops to generate for each symmetry operation a quantity CHAR which is the group-theoretical character of a non-degenerate mode and which is related to that character for a degenerate one. These quantities are printed and the program repeats the calculation for the next normal mode. When all NVD modes have been analyzed subroutine WDYN returns to WMIN.

ORNL-DWG. 73-12821A

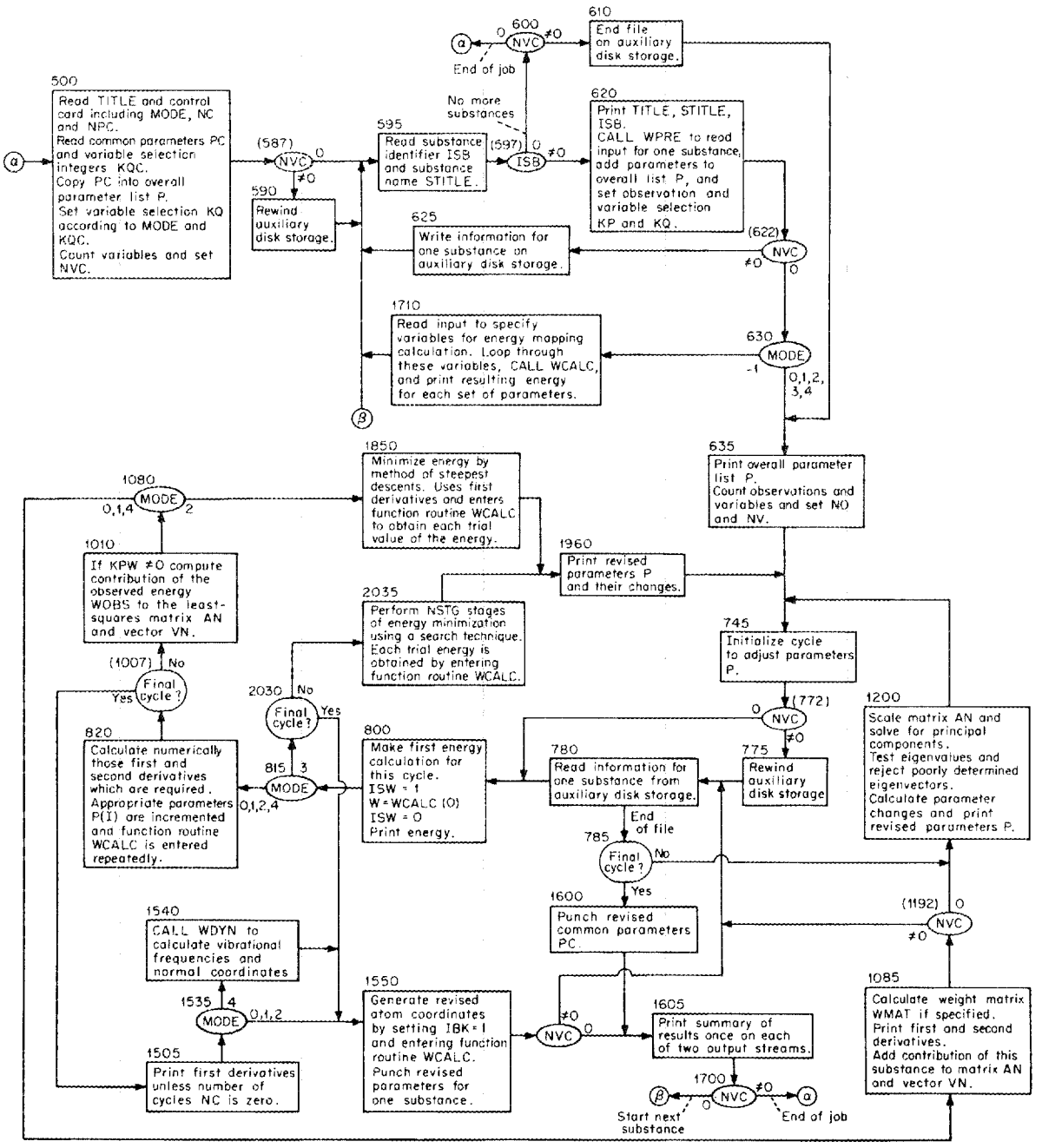


Figure 2.1. Basic subroutine WMIN, which adjusts selected parameters by various procedures depending on the mode specified.

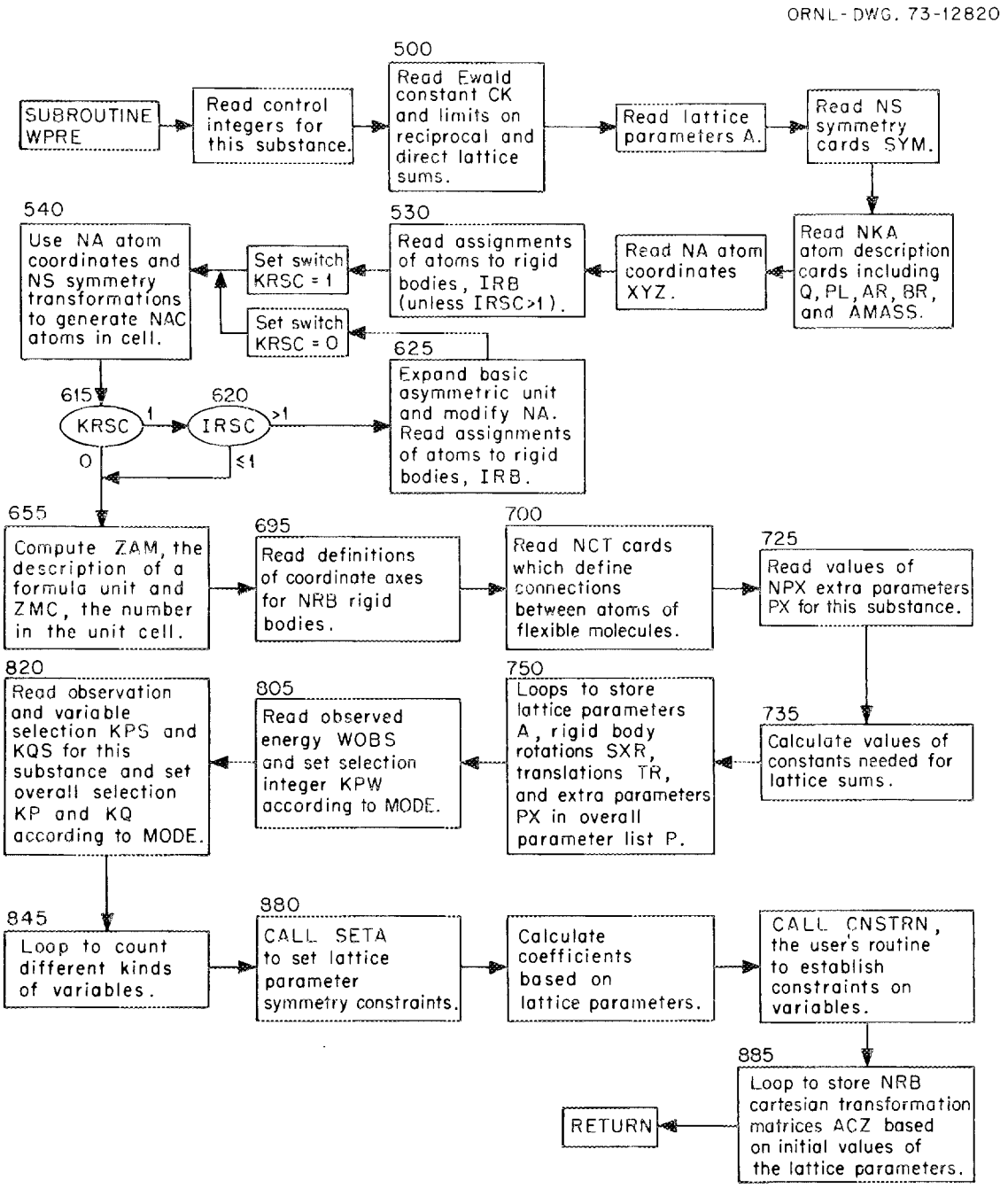


Figure 2.2. Subroutine WPRE, which reads the input and makes preliminary calculations for one substance.

ORNL-DWG. 73-12817A

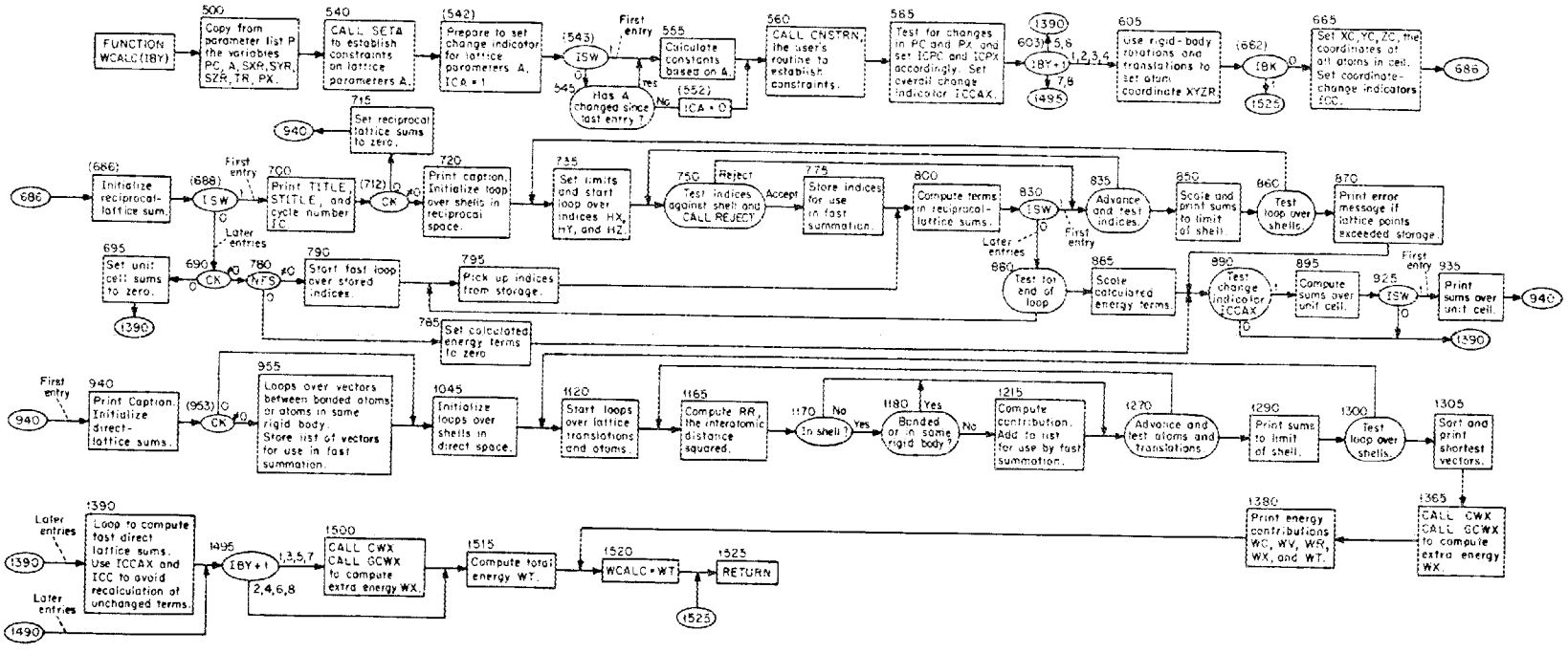


Figure 2.3. Function subroutine WCALC, which calculates the energy for one substance from a given set of structural and energy parameters.

ORNL-DWG. 73-12819A

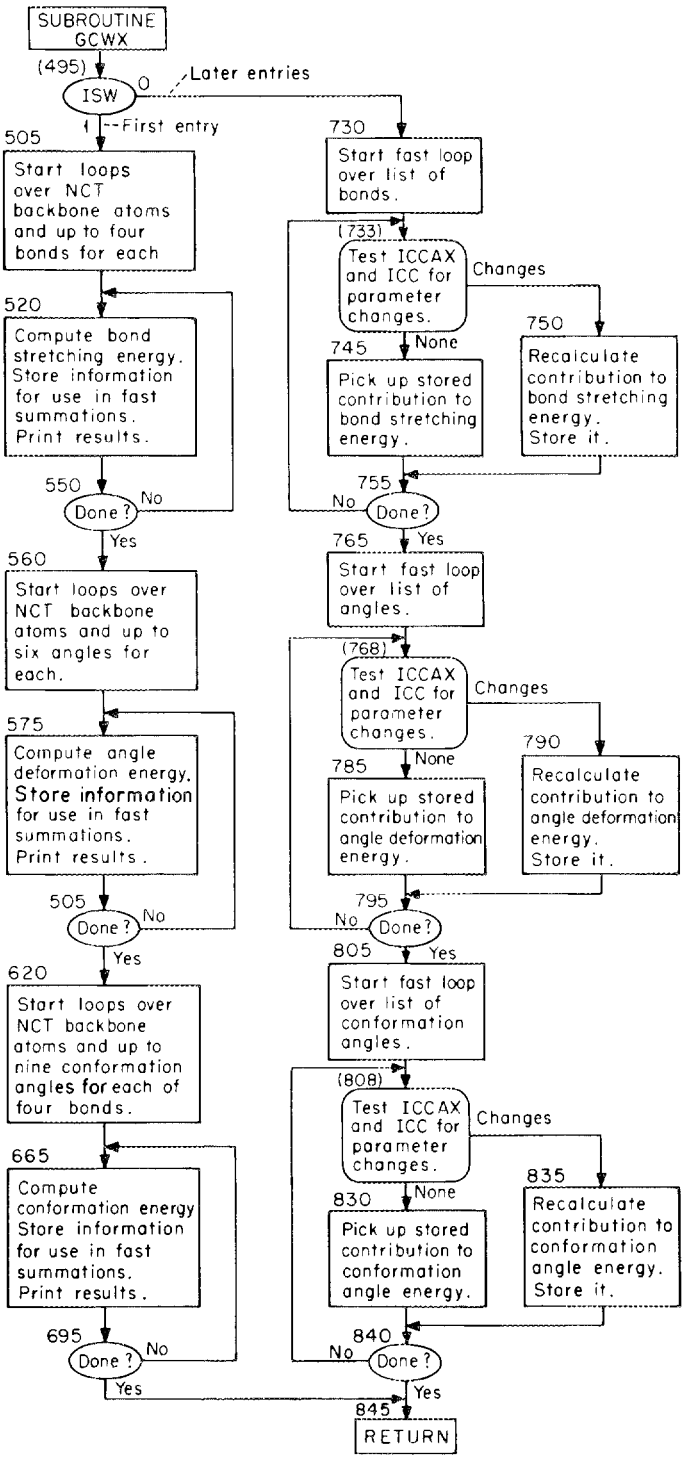


Figure 2.4. Subroutine GCWX, which makes a general calculation of the internal energy of a molecule.

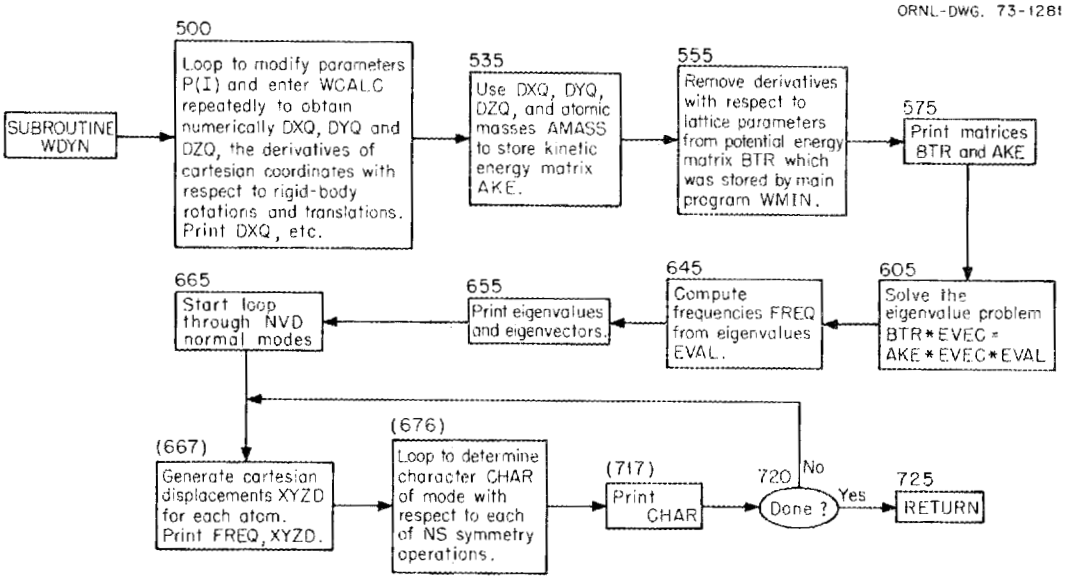


Figure 2.5. Subroutine WDYN, which calculates the vibrational frequencies and normal modes for a substance.

3. THE STRUCTURAL MODEL

3.1 Introduction

The structural model which is manipulated by WMIN may consist of rigid molecules which rotate or translate, molecules made up of rigid segments, or individual atoms with positions which can vary independently. These units are used to describe either crystals or isolated molecules, and the model may be constrained to any desired crystal or molecular symmetry. In this section we will describe how the program sets up these models. Examples of some of the possibilities available to the user are presented in Section 5.

3.2 Generating the Complete Unit Cell

All structures are set up initially by subroutine WPRE in terms of the crystallographic unit cell parameters, fractional atom coordinates, and symmetry operations. The six unit cell or lattice parameters, a, b, c, cos α, cos β, and cos γ, are input to the array A, and these define the axes to which the atom coordinates are referred. Fractional coordinates for each of NA atoms in the basic asymmetric unit are read to array XYZ, and NS symmetry cards defining operations which will generate all the atoms of the unit cell are input to array SYM. The symmetry cards must include the identity operation x,y,z, usually as the first entry. Some other restrictions on the sequence of the symmetry cards will be mentioned below; these are especially important if the structure is described as centrosymmetric with ICENT = 1.

Each of the NA input atoms is defined as a chemical kind by specifying an integer stored in array IKA. This input may include some extra pseudo-atoms or points which do not contribute to the energy, but which are used as described below to define rigid-body coordinate systems. For these extra atoms IKA is set to zero. Each atom in the asymmetric unit is assigned to one of NRB rigid bodies by specifying an integer stored in array IRB. This will be discussed in more detail below.

An isolated molecule may be described in a Cartesian Ångstrom coordinate system by setting the lattice parameters A at 1,1,1,0,0,0,

using only one symmetry card for x,y,z, and reading the atom coordinates expressed in Ångstrom units.

Subroutine WPRE uses the NA input atoms and the NS symmetry cards to generate NAC atoms in the unit cell. Information about each such atom is stored in several arrays which are printed for the user's inspection. In this output the arrays JAC and ISC consist respectively of the sequence number of the atom in the input list and the number of the symmetry card used to generate atom I in the cell. The arrays XC, YC, and ZC contain the fractional coordinates of the generated atoms. Later these coordinates will define the atom positions from which the energy is computed, and XC, YC, and ZC will be recomputed each time the model is adjusted by moving a rigid body or an individual atom. In WPRE, however, these generated coordinates are stored only so that newly generated coordinates can be compared with them (modulo 1.0) to avoid placing two atoms in the same position. (This comparison is only made for two atoms with the same IKA. Occasionally the user may wish to put an extra atom at the same position as another atom, and this is permitted. A core-shell model for an atom could also be generated with the two components at the same location provided that they have different values of IKA.) The comparison enables the program to recognize atoms on special crystallographic positions such as inversion centers, rotation axes, or mirror planes. The array SMC stores a count of the number of times each position is generated. This information is used later to establish the expression for the formula unit and the multiplicity of each atom's contribution to the energy.

A multiplier used in the structure factor calculation is stored in FMC. This is different from 1.0 only for certain atoms in special positions and only when the structure is treated as centrosymmetric.

In this initial calculation subroutine WPRE also stores an integer in IRBC which assigns each atom of the unit cell to one of the NRB*NS rigid bodies in the cell.

3.3 Relaxing Symmetry Constraints

Subroutine WPRE includes a feature which permits the user to expand the asymmetric unit to include atoms generated by the first several

symmetry cards. This procedure is invoked by setting control integer IRSC to the number of symmetry operations to be used for this expansion. When IRSC is greater than one the program generates a new list of atoms from the beginning of the unit cell arrays described above. The value of NA is increased, and this list is used as though it was the input list to regenerate the atoms in the unit cell. This time, however, the second symmetry card (and perhaps others) generates atoms which duplicate those from the first. Thus some of the symmetry cards are ignored, and the atoms generated are in the same or equivalent positions as those previously found.

There are two reasons that the user may wish to call on this procedure. The first is related to the fact that WMIN requires that any collection of atoms which is treated as a rigid body must be contained entirely in one asymmetric unit. A problem arises for crystalline benzene (C_6H_6), for example, where there are three unique C atoms and three unique H atoms each related to another atom of the molecule by a center of inversion. If all twelve atoms are to be included in the same rigid body then they must all be in the atom list. This can be accomplished (as illustrated in Example 5.2.1 and Test Problems 2A and 2B) by making the second symmetry card correspond to the center of inversion -x, -y, -z and setting IRSC at 2. Since this symmetry card is thereafter effectively bypassed, it is necessary to treat the structure as noncentrosymmetric with ICENT = 2.

The second reason for using this feature is that ordinarily WMIN constrains the structure to maintain the symmetry specified by the symmetry cards. This applies not only to the energy minimization in modes 1, 2, or 3, but also to the vibrations calculated in mode 4. If it is desired that these symmetry constraints be relaxed then the size of the asymmetric unit must be increased and the specified symmetry operations bypassed. This is illustrated for the isolated ethane molecule, C_2H_6, in Example 5.3.3 and Test Problem 3B. Six symmetry cards are needed to generate the eight atoms of the molecule from the two input atoms. By setting IRSC = 6 the asymmetric unit is expanded to eight atoms and only the first symmetry card is effective, so there are no constraints on the vibrations allowed in mode 4. (This example and the test problem also

illustrate that it is permissible to add redundant symmetry cards which facilitate the identification of the characters of the vibrations in mode 4.)

3.4 Rigid Bodies as Structural Variables

Each atom of the basic asymmetric unit (as read or as generated) is assigned to one of NRB rigid bodies by specifying an integer stored in array IRB. It is the rotations and translations of these rigid bodies which are used as the structural variables in WMIN, not the atomic coordinates themselves. For each rigid body the user specifies an atom (or extra atom) which is to serve as its origin. The user also establishes a Cartesian coordinate system for each rigid body which is defined either in terms of the crystal axes or in terms of three atoms (or extra atoms) of the structure.

If defined in terms of the crystal axes, the right-handed system has its x-axis parallel to the a-axis and its y-axis in the a,b plane. Thus if the crystal axes are orthogonal, the Cartesian axes parallel them. When defined in terms of three atoms u, v, and w, the x-axis parallels the direction u to v, and the y-axis lies in the three-atom plane on the side of w.

The translation of a rigid body is defined by the vector TR which specifies the displacements of the origin measured in Ångstron units along the three directions of its Cartesian axes. The rotation of a rigid body is defined by SXR, SYR, and SZR, rotations measured in radians about each of its three Cartesian axes. The way in which the program performs these variations will now be described.

When subroutine WCALC is entered values of TR, SXR, SYR, and SZR, which define the rigid body translations and rotations, have been set. The program uses this information to convert the input coordinates XYZ of the asymmetric unit to adjusted coordinates XYZR in a way which is described by the following pseudo-Fortran matrix equation:

```
XYZR(-,I) = XYZR(-,IZJ) + CA * {TR(-,J)
            + RM * ACZ(-,J) * [XYZ(-,I) - XYZ(-,IZJ)]} .
```

XYZ(-,IZJ) is the vector of input coordinates for the origin atom of rigid body J. This is subtracted from XYZ(-,I), the input coordinates

of atom I. Matrix ACZ(-,J) converts the coordinates to the Cartesian system of rigid body J. RM is an orthogonal rotation matrix derived from SXR(J), SYR(J), and SZR(J), the rotations for rigid body J. After these Cartesian coordinates are rotated, the specified translation TR(-,J) is added. Then the Cartesian coordinates are converted back to the crystal system by matrix CA which is specific for rigid body J. Finally the coordinates of the origin atom, XYZR(-,IZJ), are added to produce the transformed atom coordinates XYZR(-,I).

In order to keep the geometry of a rigid body unchanged even though the lattice parameters are adjusted, subroutine WPRE sets up the matrices ACZ(-,J) for each rigid body on a basis of the input unit cell parameters. The matrix CA, on the other hand, is based on the current values of these parameters.

Before beginning this transformation the program copies array XYZ to array XYZR. Then it steps through the rigid bodies 1,2,...NRB in sequence transforming all the atoms of one before starting on the atoms of the next. Note the effect which this sequence has on the origin-defining atoms. XYZ(-,IZJ) is an atom in its input position, but XYZR(-,IZJ) may either be in its input position or it may have been generated by a previous rigid body transformation. Similarly matrices ACZ are defined for Cartesian axes based on input atom positions, but matrix CA is for axes based on atoms which may belong to a previously transformed rigid body. Thus when the origin and axes of rigid body 2 are defined in terms of atoms of rigid body 1, then rigid body 2 "rides" on rigid body 1 and undergoes the translations and rotations of both. These considerations make it easy to set up models for segmented or flexible molecules. Some examples of these will be given in Section 5.

Note also that atoms assigned an IRB of zero do not belong to any rigid body. They may contribute to the energy, but they remain in positions defined by their fixed fractional coordinates.

After subroutine WCALC has finished storing the transformed coordinates XYZR for the asymmetric unit, it loops through the NAC atoms of the unit cell and recalculates XC, YC, and ZC from XYZR and SYM using the atom and symmetry operation specified by JAC and ISC. Thus even after a rigid body rotation or translation the overall structure maintains

the desired symmetry. It is the coordinates XC, YC, and ZC which are used for the energy calculation.

At the beginning of a calculation the translations and rotations, TR, SXR, SYR, and SZR, are usually read as zero. In this case the initial values of XYZR are the same as XYZ. During the course of a job which minimizes the energy the translations and rotations may become non-zero and the lattice parameters may also change. At the end of each job the program punches the revised lattice parameters. It also punches atom coordinate cards, but these transmit coordinates XYZR rather than XYZ, and, together with the new lattice parameters, describe the revised structure. If further adjustments are to be made these cards can be used as input, and TR, SXR, SYR, and SZR can again be assumed to start at zero.

4. CALCULATION OF THE ENERGY

4.1 Introduction

The terms in the energy calculated by subroutine WCALC can be divided into non-bonded interactions and interactions between bonded atoms. Non-bonded interactions include the Coulomb energy, van der Waals attraction, and repulsion terms. These may arise from intermolecular interactions in crystals and intramolecular terms for flexible groups either in crystals or in isolated molecules.

Bonded interactions include terms for bond stretching, bond angle deformation, and changes in conformation angles. These contributions apply to flexible molecules, either isolated or in a crystal, but they would not generally be included in a model of a crystal composed of rigid molecules.

The program permits considerable flexibility in the form of the potential by allowing the user to prepare subroutines which define the repulsion terms, the conformation energy, and any other desired contribution to the total energy. This flexibility is permitted primarily because any derivatives of the energy which are required are obtained numerically. For the same reason it should not be difficult for a programmer to make drastic changes in the way the energy is calculated if these appear desirable.

We will begin by discussing the mathematical methods used to calculate the Coulomb and van der Waals energies for crystal lattices. Then we will describe how these methods are implemented by the program. Finally the calculation of the bonded interactions will be described in detail.

4.2 Lattice Sums for Coulomb and van der Waals Energy

We consider a crystal to be an infinite periodic array of atoms and define its lattice energy as the negative of the work required to separate these atoms infinitely far apart. The Coulomb energy per formula unit is then

$$W_c \equiv \frac{1}{2Z} \sum_{i}^{\substack{\text{one}\\\text{cell}}} \sum_{j \neq i}^{\substack{\text{all}\\\text{cells}}} q_i q_j r_{ij}^{-1} \tag{1}$$

where q_i and q_j are point charges, r_{ij} is the distance between them, and Z is the number of formula units per cell. The factor 1/2 is needed because, considering a sum over the entire crystal, each distance is included twice.

The van der Waals energy per formula unit is given by a similar expression

$$W_v \equiv \frac{-1}{2Z} \sum_{i}^{\substack{\text{one}\\\text{cell}}} \sum_{j \neq i}^{\substack{\text{all}\\\text{cells}}} p_i p_j r_{ij}^{-6} \tag{2}$$

where p_i and p_j are suitable coefficients for atoms i and j.

4.2.1 <u>The Ewald-Bertaut-Williams Method</u>

It is well known that the summation of equation (1) for the Coulomb energy of a crystal converges very slowly unless special procedures are adopted. The method which is used in this program was pioneered by Ewald (1921) and amplified by Bertaut (1952). Recently Williams (1971) has shown that similar methods can be applied to the calculation of the van der Waals energy, Eq. (2), in order to improve its convergence. A paper by Nijboer and DeWette (1957) also contains much useful background information on these methods.

For calculations involving isolated molecules the method reduces to the usual straightforward summation over the interatomic distances, and the reader who is not interested in crystals may omit this section. Section 4.2.2 on avoiding duplicate terms in the direct lattice sum may be important, however.

Williams shows that expressions (1) and (2) can be rewritten as follows:

$$W_c = \frac{1}{2Z} \sum_{i}^{\substack{\text{one}\\\text{cell}}} \sum_{j \neq i}^{\substack{\text{all}\\\text{cells}}} q_i q_j r_{ij}^{-1} \, [\mathrm{erfc}(a)]$$

$$+ \frac{1}{2\pi V Z} \sum_{\underset{\sim}{h} \neq \underset{\sim}{0}}^{\substack{\text{reciprocal}\\\text{lattice}}} |F_c(\underset{\sim}{h})|^2 Q(\underset{\sim}{h})^{-2} [\exp(-b^2)]$$

$$- \frac{K}{Z} \sum_{i}^{\substack{\text{one}\\\text{cell}}} q_i^2 \, , \tag{3}$$

and

$$W_v = \frac{-1}{2Z} \sum_{i}^{\substack{\text{one}\\\text{cell}}} \sum_{j \neq i}^{\substack{\text{all}\\\text{cells}}} p_i p_j r_{ij}^{-6} [(1 + a^2 + a^4/2)\exp(-a^2)]$$

$$- \frac{\pi^{9/2}}{3VZ} \sum_{\underset{\sim}{h} \neq \underset{\sim}{0}}^{\substack{\text{reciprocal}\\\text{lattice}}} |F_v(\underset{\sim}{h})|^2 Q(\underset{\sim}{h})^3 [\sqrt{\pi}\ \mathrm{erfc}(b) +$$

$$+ \left(\frac{1}{2b^3} - \frac{1}{b}\right)\exp(-b^2)] + \frac{\pi^3 K^6}{12Z} \sum_{i}^{\substack{\text{one}\\\text{cell}}} p_i^2 - \frac{\pi^3 K^3}{6VZ} \left(\sum_{i}^{\substack{\text{one}\\\text{cell}}} p_i \right)^2 \tag{4}$$

where

$$a^2 = \pi K^2 r_{ij}^2 \tag{5}$$

and

$$b^2 = \pi Q(\underset{\sim}{h})^2 / K^2 . \tag{6}$$

The first summations in expressions (3) and (4) will be called the direct lattice sums and these are simply sums over the interatomic vectors. Convergence of these direct lattice sums is accelerated by multiplying each term by a modification function in brackets [ ] which has a value decreasing from unity to zero as the distance r_{ij} (and thus the argument a) increases. The function erfc(a) in Eq. (3) is the error function complement.

The amount that is lost from each direct lattice sum because of the modification function is compensated for exactly by the reciprocal lattice sum which makes up the remaining part of Eqs. (3) and (4). This summation is made over reciprocal lattice points analogous to reflections with indices $h = \{h,k,\ell\}$ in x-ray diffraction experiments. The quantities $|F_c(\underset{\sim}{h})|$ and $|F_v(\underset{\sim}{h})|$ are analogous to the structure factor magnitudes for reflection $\underset{\sim}{h}$ but with the charge q_i or the coefficient p_i replacing the atomic scattering factor in the usual x-ray expressions. Thus

$$F_c(\underset{\sim}{h}) = \sum_{i}^{\substack{\text{one}\\\text{cell}}} q_i \exp(2\pi i \underset{\sim}{h}\cdot\underset{\sim}{x}_i) \tag{7}$$

$$F_v(\underset{\sim}{h}) = \sum_{i}^{\substack{\text{one}\\\text{cell}}} p_i \exp(2\pi i \underset{\sim}{h}\cdot\underset{\sim}{x}_i) \tag{8}$$

where $\underset{\sim}{x}_i$ is a vector of coordinates for atom i. The quantity $Q(\underset{\sim}{h}) = |\underset{\sim}{h}|$ is the length of the reciprocal lattice vector and V is the volume of a unit cell. Convergence of these reciprocal lattice sums is accelerated by multiplying each term by the modification function (in brackets) which decreases from unity to zero as $Q(\underset{\sim}{h})$ (and therefore the argument b) increases.

Also included in expressions (3) and (4) are summations of q_i^2, p_i^2, and p_i over one unit cell. These sums are in effect the contributions of the $\underset{\sim}{h} = \underset{\sim}{0}$ terms to the reciprocal lattice sums.

The value of W_c or W_v obtained from expressions (3) or (4) is independent of the quantity K which is known as the Ewald constant. This constant K does determine what parts of the results will be obtained from the direct and reciprocal lattice sums, because it enters into a and b, the arguments for the modification functions. For K = 0 only the direct lattice sum contributes, because its modification function is unity and that of the reciprocal lattice sum is identically zero. For larger values of K the reciprocal lattice sum becomes increasingly important.

4.2.2 Avoiding the Duplication of Terms

In computing the Coulomb and van der Waals energies, W_c and W_v, it is desirable to avoid recalculation of terms which are identical because of symmetry. We will now show that expressions (3) and (4) can be reduced to the following equations from which duplicate terms have been largely eliminated:

$$W_c = \sum_{i}^{\substack{\text{asym}\\ \text{unit}}} \sum_{\substack{j\neq i\\ k(j)\geq i}}^{\substack{\text{all}\\ \text{cells}}} g_{ij} n_i q_i q_j r_{ij}^{-1} [\mathrm{erfc}(a)]$$

$$+ \frac{1}{2\pi VZ} \sum_{\substack{\underset{\sim}{h}\neq \underset{\sim}{0}}}^{\substack{1,2,\text{or } 4\\ \text{octants}}} c(\underset{\sim}{h}) |F_c(\underset{\sim}{h})|^2 Q(\underset{\sim}{h})^{-2} [\exp(-b^2)]$$

$$- K \sum_{i}^{\substack{\text{asym}\\ \text{unit}}} n_i q_i^2 \ , \qquad (9)$$

$$W_v = -\sum_{i}^{\substack{\text{asym}\\ \text{unit}}} \sum_{\substack{j\neq i\\ k(j)\geq i}}^{\substack{\text{all}\\ \text{cells}}} g_{ij} n_i p_i p_j r_{ij}^{-6} [(1 + a^2 + a^4/2)\exp(-a^2)]$$

$$- \frac{\pi^{9/2}}{3VZ} \sum_{\substack{\text{1,2,or 4 octants} \\ \underset{\sim}{h} \neq \underset{\sim}{0}}} c(\underset{\sim}{h}) |F_v(\underset{\sim}{h})|^2 Q(\underset{\sim}{h})^3 [\sqrt{\pi}\, \mathrm{erfc}(b)$$

$$+ \left(\frac{1}{2b^3} - \frac{1}{b}\right) \exp(-b^2)] + \frac{\pi^3 K^6}{12} \sum_{i}^{\text{asym unit}} n_i p_i^{\,2}$$

$$- \frac{\pi^3 K^3 Z}{6V} \left(\sum_{i}^{\text{asym unit}} n_i p_i \right)^2 . \qquad (10)$$

For the direct lattice terms the summation over i for one cell has been replaced by a summation over one of the asymmetric units in the cell. This change is compensated for by multiplying each term by n_i, the number of times atom i appears in the formula unit. The reason for this is that $n_i = sm_i/Z$ where s is the number of asymmetric units in the cell. The atom multiplier m_i would be unity unless atom i is shared by more than one asymmetric unit in which case it would be the appropriate fraction.

These considerations have also been applied to the unit cell sums to obtain the final terms in Eqs. (9) and (10).

The number of terms in the direct lattice sum has been still further reduced by modifying the range of the sum over j. The index i numbers the atoms in the basic asymmetric unit, and each atom j is symmetrically equivalent to some atom i. Let k(j) be the value of i for that equivalent atom so that k(j) defines the crystallographic kind of atom j. For every interatomic vector r_{ij} there is another symmetry related vector $r_{i'j'}$ with i' = k(j) which would duplicate the contribution of r_{ij} to the sum provided that $i \neq k(j)$. We have therefore included in the sum over j only those terms for which $k(j) \geq i$ and doubled the final value of the result. If i = k(j) then the vector $r_{i'j'}$ is identical to the vector r_{ij} so that no duplication would have occurred. This is

compensated for by the multiplicity factor g_{ij} which is one if $k(j) > i$, and one half for $k(j) = i$.

The reciprocal lattice sums need not be made over the entire lattice. Because $Q(\underset{\sim}{h}) = Q(-\underset{\sim}{h})$ and $|F(\underset{\sim}{h})| = |F(-\underset{\sim}{h})|$ (Friedel's Law) it is never necessary to sum over more than one hemisphere of reciprocal space. The multiplicity factor $c(\underset{\sim}{h})$ then has the value of two for all lattice points except those shared by the two hemispheres; for these its value is one.

The range of the reciprocal lattice sum can often be further reduced depending on the Laue group of the crystal. For monoclinic crystals, for example, only one quadrant of reciprocal space is needed, and for orthorhombic or cubic systems one octant of space suffices. In these cases the quantity $c(\underset{\sim}{h})$ takes on values of 2, 4, or 8 depending on how the point $\underset{\sim}{h}$ is situated with respect to the boundaries of the volume included.

The usual crystallographic procedures are applied to the calculation of the structure factor magnitudes $|F_c(\underset{\sim}{h})|$ and $|F_v(\underset{\sim}{h})|$. For non-centrosymmetric crystals

$$|F_c(\underset{\sim}{h})|^2 = A_c^{\,2} + B_c^{\,2} \tag{11}$$

where

$$A_c = \sum_{i}^{\text{one cell}} q_i \cos 2\pi(hx_i + ky_i + \ell z_i) \tag{12}$$

$$B_c = \sum_{i}^{\text{one cell}} q_i \sin 2\pi(hx_i + ky_i + \ell z_i) \ . \tag{13}$$

Here x_i, y_i, and z_i are the fractional coordinates of the atoms referred to the crystallographic axes, and h, k, and ℓ are the Miller indices which define the vector $\underset{\sim}{h}$. For crystals with a symmetry center at the origin the calculation can be simplifed to

$$|F_c(\underset{\sim}{h})|^2 = (2A_c)^2 \tag{14}$$

where

$$A_c = \sum_{i}^{\text{half cell}} q_i m_i \cos 2\pi(hx_i + ky_i + \ell z_i) \ . \tag{15}$$

Here the summation is made only over one atom of each centrosymmetrically related pair. The multiplier m_i is one except for atoms in special positions (such as the origin) which participate in both centrosymmetrically related halves of the cell. For these atoms m_i is one half. In WMIN it is sometimes necessary to treat a centrosymmetric crystal as non-centrosymmetric. This increases the calculation time but produces the correct result.

$|F_v(\underset{\sim}{h})|^2$ is calculated in an analogous way by substituting p_i for q_i in Eqs. (11) to (15).

4.2.3 Elimination of Certain Non-bonded Terms

It is usually desirable for non-bonded Coulomb, van der Waals, and repulsion terms to be omitted for atom pairs within the same rigid body or for certain atom pairs in a flexible molecule. When only the direct lattice sum is being made, as is the case for an isolated molecule or for the calculation of the repulsion, the particular terms can simply be left out of the summation. This is not the case, however, for Coulomb or van der Waals terms when the Ewald-Bertaut-Williams method is being used because there is no simple way of omitting specific interactions from the reciprocal lattice sum. Instead it is necessary to compute these terms and subtract them from the final result. The direct lattice terms for such a pair in Eqs. (9) and (10) then become

$$t_c(r_{ij}) = g_{ij} n_i q_i q_j r_{ij}^{-1}[\mathrm{erfc}(a) - 1] \tag{16}$$

and

$$t_v(r_{ij}) = - g_{ij} n_i p_i p_j r_{ij}^{-6}[(1 + a^2 + a^4/2)\exp(-a^2) - 1] \tag{17}$$

Note, however, that although the direct lattice sums in Eqs. (9) and (10) often need not be made out to more than a few Ångstrom units, all terms to be eliminated must be computed regardless of the length of vector r_{ij}.

Occasionally it will be desirable to use a model in which two atoms are located in the same position. This situation may occur in a core-shell model of a polarizable atom, for example. The Coulomb or van der Waals term for such a pair of coincident atoms would be undefined, so that we are only interested in the case when the interaction term is to be eliminated. The quantities needed are the values of $t_c(r_{ij})$ and $t_v(r_{ij})$, expressions (16) and (17), for $r_{ij} = 0$, and these are given by

$$t_c(0) = -2Kg_{ij}n_iq_iq_j \tag{18}$$

and

$$t_v(0) = g_{ij}n_ip_ip_j(\pi^3K^6/6) \ . \tag{19}$$

4.2.4 Implementation of the Lattice Sum Calculations

Equations (9) to (19) are used to calculate the Coulomb and van der Waals contributions to the energy of non-bonded interaction for the structural model. Table 4.1 relates the mathematical symbols of the previous section to the Fortran symbols in the program and lists the statement numbers after which each quantity is evaluated. These statement numbers correspond approximately to the box numbers in the flow charts of Figs. 2.2 and 2.3. A description of the program sequence has been given in Section 2.4.

Table 4.1. Symbols used in implementing the calculation of Coulomb and van der Waals energy.

Program symbol	Algebraic symbol	Equation	Evaluated in WPRE at statement number:
CK	K	5,6	495
FMC(J)	m_i	15	570,580
ZMC	Z	9,10	680
ZAM(I)	n_i	9,10,16,17,18,19	680
FM	1 or 2	11 or 14	735
SQTPIK	$\sqrt{\pi}\ K$	5	735
SQTPDK	$\sqrt{\pi}/K$	6	740

Table 4.1. (Continued)

Program symbol	Algebraic symbol	Equation	Evaluated in WPRE at statement number:
PIDKSQ	π/K^2	6	740
RTPIZ	$1/2\pi Z$ (kcal/mole)**	9	745
PINHZ	$-\pi^{9/2}/3Z$	10	745
PICKZ	$-\pi^3K^3Z/6$	10	745
PICK	$\pi^3K^6/12$	10	745
CKKCAL	-K (kcal/mole)	9	745
			Evaluated in WCALC at statement number:
VA	V	9,10	555
RTPIZV	$1/2\pi VZ$ (kcal/mole)	9	555
PINHZV	$-\pi^{9/2}/3VZ$	10	555
PICKZV	$-\pi^3K^3Z/6V$	10	555
HX	$\underset{\sim}{h} = \begin{pmatrix} h \\ k \\ \ell \end{pmatrix}$	9,10,11,12,13,	735,795,845
HY		14,15	740,795,840
HZ			745,795,835
QQ	$Q(\underset{\sim}{h})^2$	9,10	750,795
HM	$c(\underset{\sim}{h})$	9,10	765,795
ARG	$2\pi(hx_i + ky_i + \ell z_i)$	12,13,15	802
QJA	q_i	12,13,15	802
PLJA	p_i	12*,13*,15*	802
AF	A_c	11,12,15	802
AFV	A_v	11*,12*,15*	802
BF	B_c	11,13	805
BFV	B_v	11*,13*	805
YYM	b^2	9,10	810
EXPYYM	$\exp(-b^2)$	9,10	810
FSQ	$\lvert F_c(\underset{\sim}{h})\rvert^2$	9,11,14	815
SF	$\sum_{h\neq 0}$	9	815
FSQV	$\lvert F_v(\underset{\sim}{h})\rvert^2$	10,11*,14*	825
QH	Q	10	825

Table 4.1. (Continued)

Program symbol	Algebraic symbol	Equation	Evaluated in WCALC at statement number:
YM	b	10	825
SFV	$\sum_{h\neq 0}$	10	825
CSF	$(\tilde{1}/2\pi\tilde{V}\tilde{Z})\sum_{h\neq 0}$ (kcal/mole)	9	850,885
VSF	$-(\pi^{9/2}/3\tilde{V}\tilde{Z})\sum_{h\neq 0}$	10	850,885
SQ	$\sum_i n_i q_i^2$	9	897
SPP	$\sum_i n_i p_i^2$	10	897
SPL	$\sum_i n_i p_i$	10	897
SQK	$-K\sum_i n_i q_i^2$ (kcal/mole)	9	905
SPPK	$(\pi^3 K^6/12)\sum_i n_i p_i^2$	10	915
SPLK	$-(\pi^3 K^3/6V)(\sum_i n_i p_i)^2$	10	915
I	i	16,17,18,19	955
		9,10	1150,1395
IA	i	16,17,18,19	955
		9,10	1150,1415
GMI	n_i	16,17,18,19	957
		9,10	1152
J	j	16,17,18,19	958
		9,10	1152,1395
JA	j	16,17,18,19	958
	$k(j)$	9,10	1152,1415
GM	$g_{ij}n_i$	16,17,18,19	960,965
		9,10	1155,1160,1415

Table 4.1. (Continued)

Program symbol	Algebraic symbol	Equation	Evaluated in WCALC at statement number:
R	r_{ij}	16,17	995
		9,10	1175,1415
VTM	$t_v(0)$	19	997,1462
	$t_v(r_{ij})$	17	1005,1470
	$-g_{ij}n_ip_ip_jr_{ij}^{-6}\cdot[(1+a^2+a^4/2)\exp(-a^2)]$	10	1240,1450,1470
SVDW	$-\sum_i\sum_{j\neq 1}$	10	997,1005,1240,1410, 1450,1462,1470
CTM	$t_c(0)$	18	999,1464
	$t_c(r_{ij})$	16	1015,1480
	$g_{ij}n_iq_iq_jr_{ij}^{-1}[\mathrm{erfc}(a)]$	9	1250,1458,1480
SG	$\sum_i\sum_{j\neq i}$	9	999,1015,1250,1410, 1458,1464,1480
SGK	$\sum_i\sum_{j\neq i}$ (kcal/mole)	9	1290,1490
XM	a	16	1000,1465
		9	1175
XXM	a^2	17	1005,1470
		10	1240,1470
VDW	$-p_ip_jr_{ij}^{-6}$	17	1005,1470
		10	1240,1470
CMB	$q_iq_jr_{ij}^{-1}$	16	1015,1480
		9	1250,1480
WC	W_c	9	1365,1490
WV	W_v	10	1365,1490

*An asterisk on the equation number means that the quantity is used for the analogous calculation of the van der Waals energy.

**Quantities labeled (kcal/mole) have been multiplied by 332.17 to convert from e^2 Å^{-1}.

4.3 Non-bonded Repulsion Terms

The repulsion energy WR is accumulated in the same loops as the direct-lattice sums SG and SVDW described above. Each term is given the same weighting factor GMI as the corresponding Coulomb or van der Waals term. Just as in the above sums, terms are omitted for interatomic contacts within the same rigid body or for bonded contacts defined by the molecular connection table. If IGEM = 1 then terms are also omitted for contacts between two atoms bonded to the same atom.

Because WR is accumulated only as a direct-lattice sum, it is important to set the summation limit RLIM large enough to achieve the desired convergence. Convergence can be verified by examining WR calculated for two or more shells in direct space.

Repulsion (or attraction) terms from three sources may be included or omitted, depending on the control integer IREP. Built into the program is a standard repulsion term of the form suggested by Gilbert (1968):

$$V(r_{ij}) = (b_i + b_j) \exp[(a_i + a_j - r_{ij})/(b_i + b_j)] \qquad (20)$$

where the a_i is a radius and b_i is a softness parameter corresponding to AR(I) and BR(I) in the potential parameter input. The units are kcal/mole and Ångstroms.

Additional terms for each non-bonded contact may be computed by user's function subprograms REPL and GPOT. REPL permits the calculation of a term which is any desired function of the distance R. Such an expression could also include special forms of attractive terms if they are needed. The potential parameters AR and BR may be redefined for use by this routine, or common parameters PC or extra parameters PX may be used to specify the potential. The use of REPL is illustrated in Test Problems 2A and 2B, Sections 9.4 and 10.2.

GPOT serves a similar purpose, but more arguments are available to it, so that more complicated functions can be programmed. For example, GPOT permits the introduction of a potential which depends on the angles subtended by atoms adjacent to the non-bonded contact.

4.4 Molecular Conformation Energy

For structural models which include flexible or segmented molecules it is usually necessary to include an extra energy WX which depends on the bond distances, bond angles, and torsion angles defining the molecular conformation. A general calculation of WX is performed by subroutine GCWX which generates all of these distances, angles, and conformation angles from a connection table provided as input. Section 5 and also Test Problems 2A, 3A, and 3B give illustrative examples.

NCT cards are included in this connection table, one for each backbone atom, that is one for each atom which is bonded to more than one other atom. (Thus for a hydrocarbon molecule the carbon atoms are the backbone atoms.) On card J is IACT(J), the atom number of a backbone atom; and ICT(1,J), ICT(2,J), ICT(3,J), ICT(4,J), the numbers of up to four atoms bonded to it. If fewer than four atoms are bonded to that backbone atom, then the last values of ICT are left blank.

The atom numbers used are the sequence numbers of the atoms in the arrays XC, YC, and ZC which describe the complete unit cell. (See Section 3.2.) Often these are just the input atom numbers, but if a molecule has crystallographic symmetry then it may be important to include more than the asymmetric unit in the connection table. Example 5.2.5 illustrates this situation.

For each backbone atom up to four bond distances can be generated, but the program examines the connection table to avoid duplicating bonds. The program also generates up to six angles with each backbone atom as the vertex. Finally, for each bond to another backbone atom the program generates up to nine conformation angles. In general these calculated distances and angles are printed as output, and it may be useful to include a connection table for a molecule even if no conformation energy is to be calculated. The connection table should not be used to obtain distances or angles between non-bonded atoms, however, as such use would cause the corresponding non-bonded energy terms to be omitted.

If the structural model constrains bond distances and angles to be fixed then it is not necessary to include terms which depend on these distances and angles in the energy calculation. But any distance, angle, or torsion angle which is allowed to vary probably requires a corresponding

term in WX. Subroutine GCWX computes such terms using coefficients stored as common parameters PC and selected by the input integer arrays IDZ, IAZ, and ITBR associated with the connection table.

The energy of a bond distance d is calculated as

$$W(d) = \tfrac{1}{2} k_d (d - d_0)^2 \tag{21}$$

where k_d is a force constant and d_0 is an equilibrium distance. The parameters d_0 and k_d are taken as common parameters PC(IDZJI) and PC(IDZJI + 1), respectively, where IDZJI is specified for each bond in array IDZ. The units of d_0 are Ångstroms and those of k_d are kcal mole^{-1} Å^{-2}. The input in PC(IDZJI + 1) is made smaller by a factor of 0.01 to keep it in a reasonable range.

The energy of a bond angle α is calculated similarly as

$$W(\alpha) = \tfrac{1}{2} k_\alpha (\alpha - \alpha_0)^2 \tag{22}$$

where k_α is a force constant and α_0 is an equilibrium angle. Again the parameters α_0 and k_α are taken as PC(IAZNJ) and PC(IAZNJ + 1), respectively, where IAZNJ is specified for each angle in array IAZ. The units of α_0 are degrees and those of k_α are kcal mole^{-1} degree^{-2}.

A contribution to the conformation energy WX may be made for each of up to nine torsion angles about a bond between two backbone atoms. One integer ITKJ stored in array ITBR controls the calculation of the energy terms for all nine of these angles. If ITKJ is set at a negative value the program calls the user's subroutine WCNF which may be programmed to calculate the energy contribution, WCF $\equiv W(\phi)$, in any desired way. An example of a subroutine which calculates

$$W(\phi) = \tfrac{1}{2} E_\phi \, (1 + \cos 3\phi) \tag{23}$$

is used in Test Problems 3A and 3B for the molecules ethane and propane. In this case the programmer elected to store the barrier height E_ϕ as one of the common parameters PC. In setting this barrier height the user must take into account the fact that a contribution WCF (in kcal/mole) will be made for each of the nine torsion angles about a bond.

An alternative form for the energy associated with a torsion angle is built into the program. This form is the wrap-around Gaussian

$$W(\phi) = a \sum_{n=-\infty}^{\infty} \exp[-(\phi - 2\pi n)^2/2b^2] \ . \tag{24}$$

Here a and b are height and width parameters of a Gaussian function of the torsion angle ϕ. To avoid discontinuities, ϕ is considered to cover many revolutions and the contribution from each is summed. This function has a maximum at $\phi = 0$ and a minimum at $\phi = \pi$. For large values of b it approaches the form of the function cos ϕ. Subroutine GCWX implements this function by taking parameters a and b from PC(ITKJ) and PC(ITKJ + 1), respectively. A term is calculated for each of the torsion angles about a bond.

4.5 Additional Energy Terms

Any other terms which may be desired can be included in the extra energy WX by means of subroutine CWX programmed by the user. One example of such a term might be the internal energy of an induced dipole

$$W_i = \mu^2/2\alpha \tag{25}$$

where μ is the dipole moment and α is the polarizability. The dipole moment can also be expressed as the product of a charge q and a separation ℓ so that

$$W_i = \ell^2 q^2/2\alpha \ . \tag{26}$$

In a core-shell model of an atom one might assume fixed charges with a variable geometry. Subroutine DST could be used to obtain the separation ℓ, and WX would be calculated according to Eq. (26).

Alternatively, in a polarizable molecule it might be reasonable to hold the geometry fixed and let the charges vary. These charges could be defined by one or more extra parameters PX which would be used by subroutine CNSTRN to set Q for the various kinds of atoms. Subroutine CWX would calculate WX either from the PX values or from the Q's.

Another use of CWX would be to simulate the effect of applying a high hydrostatic pressure to the crystal by adding a negative term proportional to $p\Delta V$. In this case WX would be proportional to the (negative) change in unit cell volume:

$$WX = CONST * PRES * (VA - VAZ)/ZMC \ . \qquad (27)$$

Here VA is the unit cell volume in $Å^3$ (from COMMON/AB/), VAZ is the cell volume at zero pressure, ZMC is the number of formula units per cell (from COMMON/DUBL/), PRES is the pressure in kilobars, and CONST = 1.43929×10^{-2} to convert WX to kcal/mole.

Other examples of extra energy terms would include any forms of conformational energy not calculated by GCWX. A term for the out-of-plane bend of a bond to a benzene ring could be computed for example.

In programming subroutine CWX the user may call on any of the available subroutines such as DST, ANG, or CONF for computing a distance, angle, or torsion angle, respectively. Also available are subroutines VEC, NORM, and AVV for manipulating vectors defined by atom positions. Other 3-by-3 matrix and vector routines include DIFV, SUMV, MM, MV, and VMV. The operation of these subroutines is described in the program listing.

4.6 Size of the Formula Unit

The Coulomb, van der Waals, and repulsion energy terms, calculated as described above, are expressed in kcal/mole for one formula unit. For some purposes the size of this formula unit is unimportant since it merely establishes the scale of the calculated non-bonded interaction energy. However, when molecular conformation energy or other extra energy terms are to be included it is necessary to choose the formula unit in a consistent way.

Subroutine WPRE (Box 655) establishes the size of this formula unit in one of two ways depending on the input integer IZAM. If IZAM = 0 then the program examines the list of atoms generated for the unit cell and chooses the formula unit as the smallest fraction of this cell which contains an integral number of each crystallographic kind of atom. Alternatively the user may control the size of the formula unit by setting

IZAM at the number of times the first input atom is to be included. In either case the program prints ZMC, the number of formula units in the cell, and ZAM(I), the number of atoms of each kind I in this formula.

Example 5.2.5 describes the situation for solid binaphthyl which has a crystallographic twofold axis relating the two naphthyl groups. With IZAM = 0 the program would generate the formula $C_{10}H_7$, but by setting IZAM = 2 the user can cause the program to generate the correct formula $C_{20}H_{14}$. Conformational energy terms would be included for each of the two naphthyl groups, but a term based on the bond distance in the naphthy-naphthyl link, for example, would be included only once.

5. ILLUSTRATIVE EXAMPLES

5.1 Introduction

In this section we tabulate in schematic form some of the input required for several specific problems. The substances used as examples include both molecular and ionic crystals as well as isolated molecules. The structural models represent rigid, segmented, and flexible molecules. Some of these examples correspond directly with the Test Problems included in Sections 9 and 10.

The information listed for these examples pertains mostly to the establishment of the structural models and the selection of the internal energy terms. It is important to realize that the program allows considerable flexibility in the way the models are set up. We have tried to include notes explaining which choices are mandatory and which are optional.

For matters pertaining to crystal symmetry the user will find it useful to refer to the International Tables for X-ray Crystallography (1952).

5.2 Molecular Crystals

Example 5.2.1

Substance: Benzene, C_6H_6

Treatment: Rigid molecule

Phase: Crystal

Reference to structure: Bacon, Curry, and Wilson (1964).

See also: Test Problems 2A and 2B

Unit cell: Orthorhombic, variables: a, b, c

Symmetry: Pbca (No. 61), NS = 8

Sequence of cards:

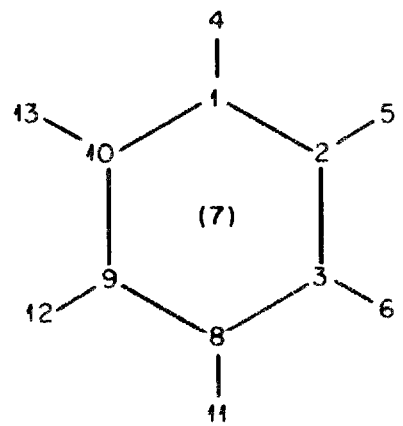
x	y	z
-x	-y	-z
½+x	½-y	-z
½-x	½+y	z
-x	½+y	½-z
x	½-y	½+z
½-x	-y	½+z
½+x	y	½-z

The molecule with 12 atoms has a center of inversion at the origin, and it is generated from six input atoms by the first two symmetry cards.

Because of this sequence the structure must be treated as noncentrosymmetric in the reciprocal lattice sums.

Reciprocal lattice symmetry: ICENT = 2, HXNEG = 0, HYNEG = 0, HZNEG = 0. REJECT terms with HX = 0 and HY ≠ 2n or HY = 0 and HZ ≠ 2n or HZ = 0 and HX ≠ 2n, because they will be zero. See subroutine REJECT included in the Test Problems.

Atom numbers: NA = 7, IRSC = 2, generates NA = 13



Extra atom 7 is used as the origin about which the molecule can rotate.

Formula unit: C_6H_6, IZAM = 0

Rigid bodies: NRB = 1, IRBA = 0

Rigid body	Atoms included	Origin IZ	Axes IU	IV	IW	Variables: Rotations x	y	z	Translations x	y	z
1	1 - 13	7	0			1	1	1	0	0	0

The Cartesian axes parallel the crystal axes. Because the molecule is located at a center of symmetry no translation is permitted.

Connection table: NCT = 6

IACT	ICT			
1	2	4	10	0
2	1	3	5	0
3	2	6	8	0
8	3	9	11	0
9	8	10	12	0
10	1	9	13	0

This table is optional but may be included to calculate distances and angles. See Test Problem 2A.

Example 5.2.2

Substance: Benzene, C_6H_6

Treatment: Flexible molecule

Phase: Crystal

Reference: Bacon, Curry and Wilson (1964).

Unit cell: Orthorhombic, variables: a, b, c

Symmetry: Pbca (No. 61), NS = 8

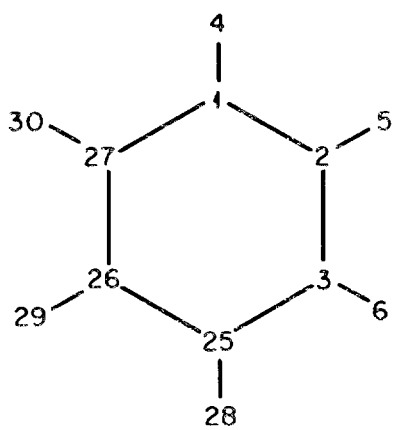
Sequence of cards:

x	y	z
½+x	½-y	-z
-x	½+y	½-z
½-x	-y	½+x
-x	-y	-z
½-x	½+y	z
x	½-y	½+z
½+x	y	½-z

This sequence allows the structure to be treated as centrosymmetric in the reciprocal lattice sums.

Reciprocal lattice symmetry: Same as Example 5.2.1 except that ICENT = 1.

Atom numbers: NA = 6



Since the molecule is not treated as one rigid body it does not have to fall entirely in one asymmetric unit.

Formula unit: C_6H_6, IZAM = 2

Rigid bodies: NRB = 6, IRBA = 1

Rigid body	Atoms included	Origin IZ	Axes IU	IV	IW	Variables Translations x	y	z
1	1	1	0			1	1	1
2	2	1	0			1	1	1
3	3	2	0			1	1	1
4	4	1	0			1	1	1
5	5	2	0			1	1	1
6	6	3	0			1	1	1

The choice of origin atom may not be particularly important, but we have elected to make each successive atom ride on its previously introduced neighbor. This may affect the rate of energy minimization, but will have no effect on the final structure or vibrational frequencies. The several Cartesian axis systems parallel the crystal axes.

Connection table: NCT = 6. Must generate all bond distances, angles, and torsion angles for full molecule.

IACT	ICT				IDZ				IAZ						ITBR			
1	27	2	4	0	a	a	b	0	c	d	0	d	0	0	e	e	0	0
2	1	3	5	0	a	a	b	0	c	d	0	d	0	0	e	e	0	0
3	2	25	6	0	a	a	b	0	c	d	0	d	0	0	e	e	0	0
25	3	26	28	0	a	a	b	0	c	d	0	d	0	0	e	e	0	0
26	25	27	29	0	a	a	b	0	c	d	0	d	0	0	e	e	0	0
27	26	1	30	0	a	a	b	0	c	d	0	d	0	0	e	e	0	0

Specification of conformation energy terms:

(a) C-C bond stretch term

(b) C-H bond stretch term

(c) C-C-C bond angle bend

(d) C-C-H bond angle bend

(e) X-C-C-X torsion angles (four of them about each bond)

Some of the entries in IDZ and ITBR are irrelevant, because the program does not use both distances 1-2 and 2-1, for example.

Example 5.2.3

Substance: o-Terphenyl, $C_{18}H_{14}$

Treatment: Three-segment molecule with only ring-ring torsion permitted

Phase: Crystal

Reference to structure: Brown and Levy (1979).

Unit cell: Orthorhombic, variables: a, b, c

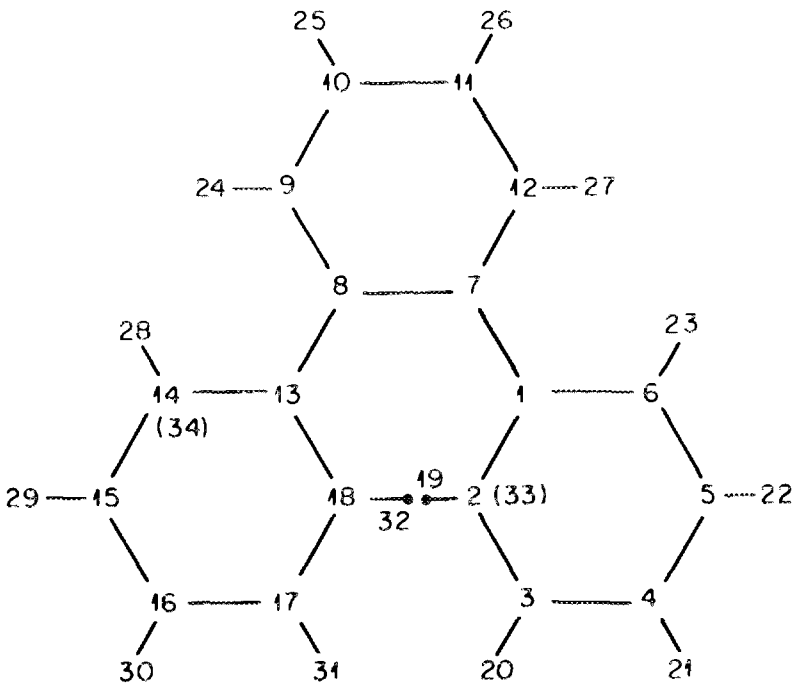
Symmetry: $P2_12_12_1$ (No. 19), NS = 4

Sequence of cards:

x	y	z
½-x	-y	½+z
½+x	½-y	-z
-x	½+y	½-z

Reciprocal lattice symmetry: ICENT = 2, HXNEG = 0, HYNEG = 0, HZNEG = 0. REJECT terms with HY = HZ = 0 and HX ≠ 2n or HX = HZ = 0 and HY ≠ 2n or HX = HY = 0 and HZ ≠ 2n, because they are zero. There are so few of these terms that it may not be worthwhile to program subroutine REJECT.

Atom numbers: NA = 34



Extra atoms 33 and 34, which coincide with atoms 2 and 14, will be used to define the segmented body coordinate systems.

Formula unit: $C_{18}H_{14}$, IZAM = 0

Rigid bodies: NRB = 3, IRBA = 0

Rigid body	Includes atoms	Origin IZ	Axes IU	Axes IV	Axes IW	Variables: Rotations x	Rotations y	Rotations z	Translations x	Translations y	Translations z
1	1, 7-13, 24-27,33,34	7	0			1	1	1	1	1	1
2	2-6, 19-23	1	7	1	33	1	0	0	0	0	0
3	14-18, 28-32	13	8	13	34	1	0	0	0	0	0

The choice of origin for rigid body 1 is not important. See Section 3.4 for the definition of the coordinate systems of rigid bodies 2 and 3. They could have been defined without using extra atoms, but these are desirable for the more complicated five-segment model of Example 5.2.4.

Connection table: NCT = 18

IACT	ICT				IDZ	IAZ						ITRB			
1	2	6	7	0		0	a	0	a	0	0	b	b	c	0
2	1	3	19	0								b	0	0	0
3	2	4	20	0											
4	3	5	21	0											
5	4	6	22	0											
6	5	1	23	0								0	b	0	0
7	12	8	1	0		0	a	0	a	0	0	b	b	c	0
8	7	9	13	0		0	a	0	a	0	0	b	b	c	0
9	8	10	24	0								b	0	0	0
10	9	11	25	0											
11	10	12	26	0											
12	11	7	27	0											
13	18	14	8	0		0	a	0	a	0	0	b	b	c	0
14	13	15	28	0								b	0	0	0
15	14	16	29	0											
16	15	17	30	0											
17	16	18	31	0											
18	17	13	32	0								0	b	0	0

Specification of conformation energy terms:

(a) Ring-link in-plane angle term. Needed only for five-segment model of Example 5.2.4.

(b) Ring-link out-of-plane torsion angles. Needed only for five-segment model of Example 5.2.4.

(c) Ring-ring torsion angle term.

Some of the entries in ITBR are irrelevant because the program does not generate conformation angles about both 1-7 and 7-1, for example.

Example 5.2.4

Substance: o-Terphenyl, $C_{18}H_{14}$

Treatment: Five-segment model permitting both in-plane and out-of-plane ring-link bends as well as ring-ring torsion

Phase: Crystal

Reference: Brown and Levy (1979).

Unit cell, Symmetry, Reciprocal lattice symmetry, Atom numbers, and Formula unit: See Example 5.2.3

Rigid bodies: NRB = 5, IRBA = 0

Rigid body	Includes atoms	Origin IZ	Axes IU	IV	IW	Variables: Rotations x	y	z	Translations x	y	z
1	7-8, 24-27	7	0			1	1	1	1	1	1
2	1, 33	7	10	7	8	0	1	1	0	0	0
3	2-6, 19-23	1	7	1	33	1	1	1	0	0	0
4	13, 34	8	11	8	9	0	1	1	0	0	0
5	14-18, 28-32	13	8	13	34	1	1	1	0	0	0

See Section 3.4 for the definition of the Cartesian axes. Note that with these definitions the ring-ring torsions are x-rotations, the out-of-plane ring-link bends are y-rotations, and the in-plane ring-link bends are z-rotations.

Connection table: See Example 5.2.3.

Example 5.2.5

Substance: 1,1'-Binaphthyl, $C_{20}H_{14}$

Treatment: Segmented molecule with only ring-ring torsion permitted

Phase: Crystal

Reference to structure: Kerr and Robertson (1969).

Unit cell: Monoclinic, variables: a, b, c, cosβ

Symmetry: C2/c (No. 15), NS = 8

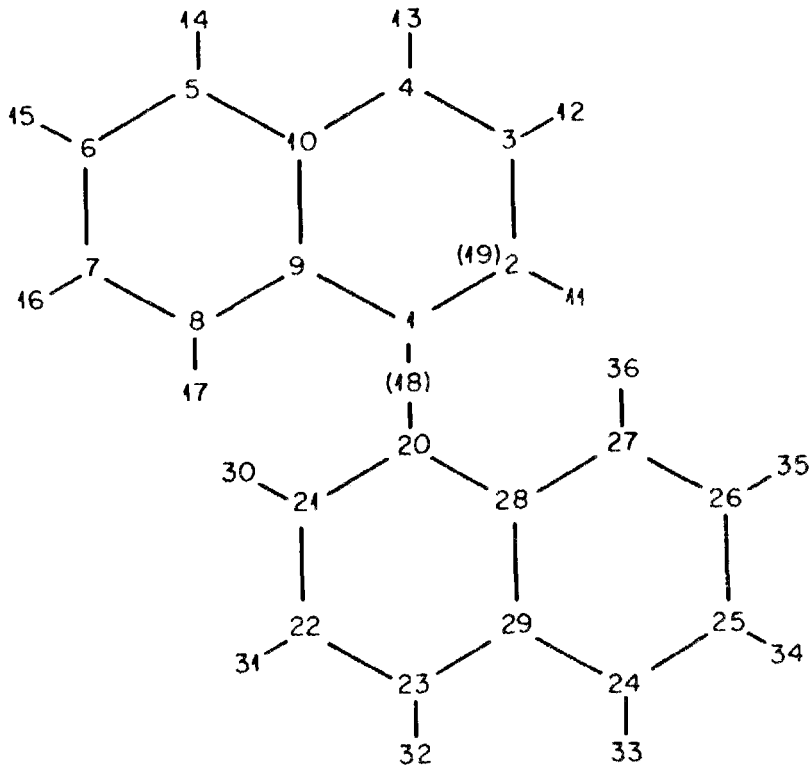
Sequence of cards:

x	y	z
-x	y	½-z
½+x	½+y	z
½-x	½+y	½-z
-x	-y	-z
x	-y	½+z
½-x	½-y	-z
½+x	½-y	½+z

For convenience the second card has been selected as the twofold axis which generates the second half of the molecule from the input atoms. (This would be required if the molecule was to be treated as one rigid body with IRSC = 2.)

Reciprocal lattice symmetry: ICENT = 1, HXNEG = 1, HYNEG = 0, HZNEG = 0. REJECT terms with HX + HY ≠ 2n or with HY = 0 and HZ ≠ 2n. These terms are zero.

Atom numbers: NA = 19



The molecule is located on a twofold axis at x = 0, z = 1/4. Atom 18 is an extra atom situated on this axis and used as a segment origin. Atom 19 is an extra atom which coincides with atom 2. It is used to define a segment coordinate system.

Formula unit: $C_{20}H_{14}$, IZAM = 2

Rigid bodies: NRB = 2, IRBA = 0

Rigid body	Includes atoms	Origin IZ	Axes IU	IV	IW	Variables: Rotations x	y	z	Translations x	y	z
1	1, 18, 19	18	0			0	1	0	0	1	0
2	2-17	1	18	1	19	1	0	0	0	0	0

Note that rigid body 1 is constrained to rotate about the twofold or translate along it. Rigid body 2 rides on rigid body 1 and rotates about the 1-20 direction which is also the 1-20 bond direction. The second half of the molecule is generated by symmetry from these segments.

Connection table: NCT = 20

IACT	ICT				IDZ	IAZ	ITBR			
1	2	9	20	0			0	0	a	0
2	1	3	11	0						
3	2	4	12	0						
4	3	10	13	0						
5	10	6	14	0						
6	5	7	15	0						
7	6	8	16	0						
8	7	9	17	0						
9	1	8	10	0						
10	4	5	9	0						
20	21	28	1	0			0	0	a	0
21	20	22	30	0						
22	21	23	31	0						
23	22	29	32	0						
24	29	25	33	0						
25	24	26	34	0						
26	25	27	35	0						
27	26	28	36	0						
28	20	27	29	0						
29	23	24	28	0						

Specification of conformation energy terms:

(a) Ring-ring torsion angles (four of them)

Because no distances or angles are varied in this model, the only internal energy terms needed are for the torsion angles. In fact, only those two cards for backbone atoms 1 and 20 need be included; the rest are optional.

5.3 Isolated Molecules

Example 5.3.1

Substance: Propane, C_3H_8

Treatment: Flexible molecule constrained to C_{2v} symmetry

Phase: Isolated molecule

Reference to structure: Gayles and King (1965).

See also: Test Problem 3A

Unit cell: Cartesian Ångstrom system, a = b = c = 1, $\cos\alpha = \cos\beta = \cos\gamma = 0$, all cell parameters fixed.

Symmetry: C_{2v}, analogous to Pmm2 (No. 25). NS = 4

Sequence of cards:	x	y	z
	x	-y	z
	-x	y	z
	-x	-y	z

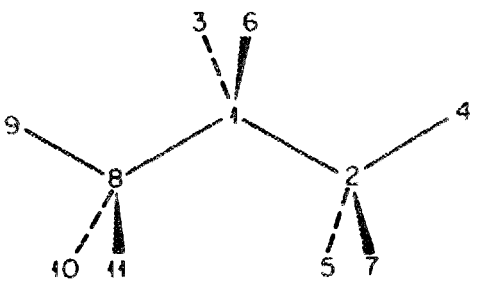
Reciprocal lattice symmetry: Irrelevant. No reciprocal lattice sums are made for an isolated molecule.

Atom input: NA = 5

No.	Name	x	y	z
1	C1	0	0	0
2	C2	1.26808	0	-0.84891
3	H1	0	0.87588	0.65883
4	H21	2.16177	0	-0.22315
5	H22	1.31300	0.88090	-1.49101

For this symmetry the origin of z is arbitrary. It has been taken at C1.

Atom numbers:



These atoms are generated by the symmetry cards.

Formula unit: C_3H_8, IZAM = 0

Rigid bodies: NRB = 5, IRBA = 1

Rigid body	Atoms included	Origin IZ	Axes IU	IV	IW	Variables Translations x	y	z
1	1	1	0			0	0	1
2	2	2	0			1	0	1
3	3	3	0			0	1	1
4	4	4	0			1	0	1
5	5	5	0			1	1	1

In minimizing the energy it would be permissible to hold the z of atom 1 fixed since it forms a redundant linear combination with the z coordinates of the other atoms. It is also satisfactory to vary it because the principal component analysis (see Section 6.2) will generate a zero eigenvalue and omit the corresponding eigenvector.

For a dynamic calculation all the z coordinates must be varied. Fixing z for atom 1 would be equivalent to assigning it infinite mass.

Connection table: NCT = 3

IACT	ICT				IDZ				IAZ						ITBR			
1	2	8	3	6	a	a	b	b	c	d	d	d	d	e	f	f	0	0
2	1	4	5	7	a	b	b	b	d	d	d	e	e	e	f	0	0	0
8	1	9	10	11	a	b	b	b	d	d	d	e	e	e	f	0	0	0

Specification of conformation energy terms:

(a) C-C bond stretch term

(b) C-H bond stretch term

(c) C-C-C bond angle bend

(d) C-C-H bond angle bend

(e) H-C-H bond angle bend

(f) X-C-C-X torsion angles

Some of the entries in IDZ and ITBR are irrelevant, because the program does not use both distances 1-2 and 2-1, for example.

Example 5.3.2

Substance: Ethane, C_2H_6

Treatment: Flexible staggered molecule constrained to D_{3d} symmetry

Phase: Isolated molecule

Reference to structure: Shaw, Lepard and Welsh (1965).

See also: Test Problem 3A

Unit cell: Hexagonal Ångstrom system, a = b = c = 1, $\cos\alpha = \cos\beta = 0$, $\cos\gamma = -0.5$, all cell parameters fixed.

Symmetry: D_{3d}, analogous to special positions 6k of $P\bar{3}1m$ (No. 162).

NS = 6

Sequence of cards:

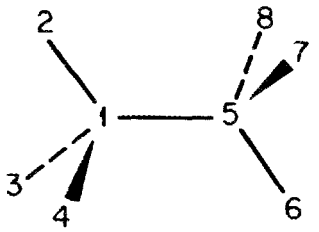
x	0	z
0	x	z
-x	-x	z
-x	0	-z
0	-x	-z
x	x	-z

Reciprocal lattice symmetry: Irrelevant. No reciprocal lattice sums are made for an isolated molecule.

Atom input: NA = 2

No.	Name	x	y	z
1	C	0	0	0.76700
2	H	1.02162	0	1.16110

Atom numbers:



These atoms are generated by the symmetry cards.

Formula unit: C_2H_6, IZAM = 2

Rigid bodies: NRB = 2, IRBA = 1

Rigid body	Atoms included	Origin IZ	Axes IU	IV	IW	Variables Translations x	y	z
1	1	1	0			0	0	1
2	2	2	0			1	0	1

Since symmetry is constrained to D_{3d} there are only three variables. These variable coordinates determine the three internal parameters: C-C distance, C-H distance, and C-C-H bond angle.

Connection table: NCT = 2

IACT	ICT				IDZ				IAZ						ITBR			
1	5	2	3	4	a	b	b	b	c	c	c	d	d	d	e	0	0	0
5	1	6	7	8	a	b	b	b	c	c	c	d	d	d	e	0	0	0

Specification of conformation energy terms:

(a) C-C bond stretch term

(b) C-H bond stretch term

(c) C-C-H bond angle bend

(d) H-C-H bond angle bend

(e) H-C-C-H torsion angles. This term is irrelevant for this example but is required for Example 5.3.3.

Example 5.3.3

Substance: Ethane, C_2H_6

Treatment: Flexible staggered molecule with initial symmetry D_{3d} but with the symmetry constraints relaxed for dynamical calculations

Phase: Isolated molecule

Reference to structure: Shaw, Lepard and Welsh (1965).

See also: Test Problem 3B

Unit cell: See Example 5.3.2.

Symmetry: D_{3d}, analogous to general positions of $P\bar{3}1m$ (No. 162).

NS = 12

Sequence of cards:

x	y	z
-y	x-y	z
y-x	-x	z
y-x	y	-z
-y	-x	-z
x	x-y	-z
-x	-y	-z
y	y-x	-z
x-y	x	-z
x-y	-y	z
y	x	z
-x	y-x	z

Note that only the first six cards are needed to generate all the atoms of the molecule. The remaining six are optionally included to aid in identifying the characters of the vibrations.

Atom input: Same as Example 5.3.2 except that NA = 2, IRSC = 6 which generates NA = 8.

Atom numbers and formula unit: See Example 5.3.2

Rigid bodies: NRB = 8, IRBA = 1

Rigid body	Includes atoms	Origin IZ	Axes IU	IV	IW	Variables Translations x	y	z
1	1	1	0			1	1	1
2	2	2	0			1	1	1
3	3	3	0			1	1	1
4	4	4	0			1	1	1
5	5	5	0			1	1	1
6	6	6	0			1	1	1
7	7	7	0			1	1	1
8	8	8	0			1	1	1

Note that we permit three degrees of freedom for each of the eight atoms. This means that six of the 24 vibrational modes will have zero frequency. It is not permissible to hold one atom fixed as that would be equivalent to assigning infinite mass to that atom.

Connection table: See Example 5.3.2.

5.4 Ionic Crystals

Example 5.4.1

Substance: Sodium chloride, NaCl

Treatment: Monatomic ions

Phase: Crystal

Reference to structure: See, for example, Wyckoff (1963).

See also: Test Problems 1A and 1B.

Unit cell: Cubic, variable: a, ISETA = 2

Symmetry: Fm3m (No. 225), NS = 4.

Sequence of cards:

x	y	z
x	½+y	½+z
½+x	y	½+z
½+x	½+y	z

The program only requires those symmetry operations needed to generate all atoms in one unit cell. These cards require ICENT = 2.

Reciprocal lattice symmetry: ICENT = 2, HXNEG = 0, HYNEG = 0, HZNEG = 0. REJECT terms with HX + HY ≠ 2n or HY + HZ ≠ 2n since they are zero. See subroutine REJECT included in Test Problems.

Atom input: NA = 2

No.	Name	x	y	z
1	Na	0	0	0
2	Cl	½	½	½

Formula unit: NaCl, IZAM = 0

Rigid bodies: NRB = 2, IRBA = 1

Rigid body	Includes atoms	Origin IZ	Axes IU	IV	IW	Variables Translations x	y	z
1	1	1	0			0	0	0
2	2	2	0			0	0	0

Because the ions are located in special symmetry positions no translations are permitted.

Example 5.4.2

Substance: Potassium sulfate, K_2SO_4

Treatment: K^+ ions and rigid $SO_4^=$ ion

Phase: Crystal

Reference to structure: See, for example, Wyckoff (1963).

Unit cell: Orthorhombic, variables: a, b, c

Symmetry: Pnma (No. 62), NS = 8

Sequence of cards:

x	y	z
x	½-y	z
½+x	y	½-z
½+x	½-y	½-z
-x	-y	-z
-x	½+y	-z
½-x	-y	½+z
½-x	½+y	½+z

Note that cards have been grouped in pairs related by the mirror plane at y = 0.25. This is so that the entire $SO_4^{=}$ ion will fall in the basic asymmetric unit when symmetry constraints are relaxed.

Reciprocal lattice symmetry: ICENT = 1, HXNEG = 0, HYNEG = 0, HZNEG = 0. REJECT terms with HX = 0 and HY + HZ ≠ 2n or HZ = 0 and HX ≠ 2n since they would be zero.

Atom input: NA = 6, IRSC = 2, generates NA = 7

No.	Name	x	y	z
1	K1	0.6768	0.25	0.4182
2	K2	-0.0115	0.25	-0.2954
3	S	0.2358	0.25	0.4155
4	O1	0.0315	0.25	0.4032
5	O2	0.2970	0.25	0.5579
6	O3	0.2997	0.0410	0.3484

Note that K1 and K2 are two crystallographic kinds of potassium atoms. These and S, O1, and O2 are in the mirror plane at y = 0.25. Because O3 is off this plane it occurs twice as often as the others, thus completing the $SO_4^{=}$ ion.

Formula unit: K_2SO_4, IZAM = 0

Rigid bodies: NRB = 3, IRBA = 0

Rigid body	Includes atoms	Origin IZ	Axes IU	IV	IW	Variables: Rotations x	y	z	Translations x	y	z
1	1	1	0			0	0	0	1	0	1
2	2	2	0			0	0	0	1	0	1
3	3-7	3	0			0	1	0	1	0	1

Because each rigid body is on the mirror plane at y = 0.25 only x and z translations are permitted, and the $SO_4^=$ ion can rotate only about the y axis.

Connection table: NCT = 1

IACT	ICT			
3	4	5	6	7

This table is optional but may be included to calculate bond distances and angles in the $SO_4^=$ ion.

6. MATHEMATICAL METHODS

6.1 Introduction

In Section 2.1 we described the operation of WMIN in the various modes which adjust either the energy parameters or the structural parameters of the model. In this chapter we will go into more detail on the mathematical methods which are used. It is hoped that an understanding of these methods will enable the user to obtain satisfactory results with fewer failures and false starts. We begin with a general presentation of the method of least squares as it is used in WMIN and then proceed to describe the particulars of modes 0, 1, 2, 3, and 4.

6.2 Method of Least Squares and Principal Component Analysis

For convenience we will first define a number of symbols to be used in the following discussion:

$\underset{\sim}{y}^{(0)}$, a vector of m observed quantities. In WMIN these quantities are $\partial W/\partial p_i$, the derivatives of energy with respect to the structural parameters for the known structure. They are "observed" to be zero since the structure is stable.

$\underset{\sim}{x}^{(1)}$, a vector of n trial parameters to be varied. For mode 0 these are usually the energy parameters q_i; for mode 1 they are structural parameters.

$\underset{\sim}{y}^{(1)}$, a vector of m quantities calculated from the trial parameters $\underset{\sim}{x}^{(1)}$. These are the values of $\partial W/\partial p_i$ calculated from the p_i's and q_i's of the model.

$\underset{\sim}{x}^{(2)}$, a vector of n improved parameters to be obtained.

$\underset{\sim}{B}$, an m*n matrix of derivatives with $B_{ij} = \partial y_i^{(1)}/\partial x_j^{(1)}$. In WMIN we have $B_{ij} = \partial^2 W/\partial p_i \partial q_j$ for mode 0 or $B_{ij} = \partial^2 W/\partial p_i \partial p_j$ for MODE = 1.

$\underset{\sim}{w}$, an m*m weight matrix. If the observations $\underset{\sim}{y}^{(0)}$ are independent then $\underset{\sim}{w}$ is diagonal and $w_{ii} = 1/\sigma^2(y_i^{(0)})$. For equal weighting we can set $w_{ii} = 1$. For careful work in mode 0 we must have $\underset{\sim}{w} = \underset{\sim}{V}^{-1}$ where $\underset{\sim}{V}$ is the m*m variance-covariance matrix of $\underset{\sim}{y}^{(0)}$. Its calculation will be discussed below.

$\underset{\sim}{s}$, an n*n diagonal scaling matrix chosen so that the diagonal elements of $\underset{\sim}{s}\,\tilde{\underset{\sim}{B}}\,\underset{\sim}{w}\,\underset{\sim}{B}\,\underset{\sim}{s}$ are unity. This is accomplished by making $s_{ii} = 1/\sqrt{(\tilde{\underset{\sim}{B}}\,\underset{\sim}{w}\,\underset{\sim}{B})_{ii}}$.

$\underset{\sim}{A} = \underset{\sim}{s}\ \tilde{\underset{\sim}{B}}\ \underset{\sim}{w}\ \underset{\sim}{B}\ \underset{\sim}{s}$, the scaled and weighted matrix of the normal equations.

$\underset{\sim}{\Lambda}$, the n*n diagonal matrix with elements λ_i which are the eigenvalues of $\underset{\sim}{A}$.

$\underset{\sim}{U}$, the n*n orthogonal matrix of eigenvectors of $\underset{\sim}{A}$. Each column represents one eigenvector which is normalized to unity. We have $\underset{\sim}{A} = \underset{\sim}{U}\ \underset{\sim}{\Lambda}\ \tilde{\underset{\sim}{U}}$ and $\underset{\sim}{A}^{-1} = \underset{\sim}{U}\ \underset{\sim}{\Lambda}^{-1}\tilde{\underset{\sim}{U}}$.

$\underset{\sim}{c} = \tilde{\underset{\sim}{U}}\ \underset{\sim}{s}^{-1}(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)})$, the vector of principal components.

$\underset{\sim}{g} = \tilde{\underset{\sim}{U}}\ \underset{\sim}{s}\ \tilde{\underset{\sim}{B}}\ \underset{\sim}{w}\ (\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)})$, the transformed vector of observations.

Now let us develop the method of least squares to obtain the improved parameters $\underset{\sim}{x}^{(2)}$. The observational equations are

$$\underset{\sim}{B}(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)}) = (\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)}) \tag{1}$$

and weighting we have

$$\underset{\sim}{w}\ \underset{\sim}{B}(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)}) = \underset{\sim}{w}(\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)}) \ . \tag{2}$$

In WMIN $\underset{\sim}{y}^{(0)} = \underset{\sim}{0}$ and could be omitted from the equations, but we will carry it along for generality.

If $n \neq m$ then we must use the method of least squares:

$$\tilde{\underset{\sim}{B}}\ \underset{\sim}{w}\ \underset{\sim}{B}(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)}) = \tilde{\underset{\sim}{B}}\ \underset{\sim}{w}(\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)}) \ . \tag{3}$$

For some purposes it is desirable to scale the parameters using $\underset{\sim}{s}$ as defined above:

$$\underset{\sim}{s}\ \tilde{\underset{\sim}{B}}\ \underset{\sim}{w}\ \underset{\sim}{B}\ \underset{\sim}{s}\ \underset{\sim}{s}^{-1}(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)}) = \underset{\sim}{s}\ \tilde{\underset{\sim}{B}}\ \underset{\sim}{w}(\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)}) \ . \tag{4}$$

Using the symbol $\underset{\sim}{A}$ for the least squares matrix we have:

$$\underset{\sim}{A}\ \underset{\sim}{s}^{-1}(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)}) = \underset{\sim}{s}\ \tilde{\underset{\sim}{B}}\ \underset{\sim}{w}(\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)}) \ . \tag{5}$$

Often these equations are solved by inverting $\underset{\sim}{A}$ so that

$$\underset{\sim}{s}^{-1}(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)}) = \underset{\sim}{A}^{-1}\ \underset{\sim}{s}\ \tilde{\underset{\sim}{B}}\ \underset{\sim}{w}(\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)}) \ , \tag{6}$$

but if $\underset{\sim}{A}$ is singular or ill-conditioned this procedure fails. We will use instead the method of principal component analysis. Determine the eigenvalues and eigenvectors of $\underset{\sim}{A}$ and substitute $\underset{\sim}{U}\,\underset{\sim}{\Lambda}\,\underset{\sim}{\tilde{U}}$ for $\underset{\sim}{A}$:

$$\underset{\sim}{U}\,\underset{\sim}{\Lambda}\,\underset{\sim}{\tilde{U}}\,\underset{\sim}{s}^{-1}(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)}) = \underset{\sim}{s}\,\underset{\sim}{\tilde{B}}\,\underset{\sim}{w}(\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)}) \tag{7}$$

or, since $\underset{\sim}{U}^{-1} = \underset{\sim}{\tilde{U}}$,

$$\underset{\sim}{\tilde{U}}\,\underset{\sim}{s}^{-1}(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)}) = \underset{\sim}{\Lambda}^{-1}\underset{\sim}{\tilde{U}}\,\underset{\sim}{s}\,\underset{\sim}{\tilde{B}}\,\underset{\sim}{w}(\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)}) \ . \tag{8}$$

Using our earlier definitions we may write

$$\underset{\sim}{c} = \underset{\sim}{\Lambda}^{-1}\,\underset{\sim}{g} \ . \tag{9}$$

Now since $\underset{\sim}{\Lambda}$ is diagonal with elements λ_i its inverse $\underset{\sim}{\Lambda}^{-1}$ is also diagonal with elements λ_i^{-1}, and we have n independent equations

$$c_i = \lambda_i^{-1}\,g_i \ . \tag{10}$$

Each c_i is a linear combination of the parameter changes $(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)})$ and, since it depends on only one element of g_i and the corresponding λ_i^{-1}, it is known as a <u>principal component</u> of the parameter changes.

A well determined matrix $\underset{\sim}{A}$ will have all of its eigenvalues of comparable size. A singular matrix, on the other hand, will have at least one eigenvalue equal to zero, and a poorly determined matrix will have one or more eigenvalues which are small compared to the others. If λ_i is small or zero this means that the linear combination of parameters represented by c_i is poorly determined. A small λ_i means a large λ_i^{-1} so c_i will be large and will cause the large parameter changes typical of a problem that is failing to converge. The availability of the eigenvalues and eigenvectors in principal component analysis permits several possible remedies for this situation.

First, the eigenvectors associated with small eigenvalues can be examined to learn which linear combinations of x_i are poorly determined. The problem can then be repeated holding some of the offending parameters constant.

Second, an automatic procedure is possible in which the principal components c_i associated with small eigenvalues are omitted. This is

done most simply by replacing λ_i^{-1} with zero if λ_i is small or zero. Let $\overset{*}{\Lambda}^{-1}$ be the diagonal matrix with λ_i^{-1} so modified. Then the parameter changes are

$$(x^{(2)} - x^{(1)}) = s\, U\, \overset{*}{\Lambda}^{-1}\, \tilde{U}\, s\, \tilde{B}\, w(y^{(0)} - y^{(1)}) \ . \tag{11}$$

When this method is used it is important to remember that the ill-conditioned problem has been made to appear well-behaved by applying constraints. In general these constraints will not be obvious from the parameter changes which result.

Third, following a procedure suggested by Marquardt (1963), a small constant may be added to each diagonal element of matrix A. This has the effect of adding that constant to each eigenvalue λ_i. Small eigenvalues are thus increased proportionally more than large ones and the large parameter changes that they would cause are effectively damped.

We will now consider two special cases which are relevant to the subsequent discussion. Consider first the well-behaved problem for which no principal components are omitted. In this case $\overset{*}{\Lambda}^{-1} = \Lambda^{-1}$ and

$$U\, \overset{*}{\Lambda}^{-1}\, \tilde{U} = U\, \Lambda^{-1}\, \tilde{U} = A^{-1} = s^{-1}(\tilde{B}\, w\, B)^{-1} s^{-1} \ . \tag{12}$$

Then Equation (11) becomes

$$(x^{(2)} - x^{(1)}) = s\, s^{-1}(\tilde{B}\, w\, B)^{-1}\, s^{-1}\, s\, \tilde{B}\, w(y^{(0)} - y^{(1)}) \tag{13}$$

or

$$(x^{(2)} - x^{(1)}) = (\tilde{B}\, w\, B)^{-1}\, \tilde{B}\, w(y^{(0)} - y^{(1)}) \tag{14}$$

so that <u>when no principal components are omitted scaling has no effect on the parameter changes</u>. Nevertheless, WMIN scales the matrix before determining the principal components unless the user specifies otherwise (by setting SLIM at a negative value).

Next we consider the case when n = m, that is the number of variables is equal to the number of observations. Then since B is square it may have an inverse, and

$$(\tilde{B}\, w\, B)^{-1} = B^{-1}\, w^{-1}\, \tilde{B}^{-1} \ . \tag{15}$$

Then from Equation (14) we have

$$(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)}) = \underset{\sim}{B}^{-1}\ \underset{\sim}{w}^{-1}\ \tilde{\underset{\sim}{B}}^{-1}\ \tilde{\underset{\sim}{B}}\ \underset{\sim}{w}(\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)}) \ , \tag{16}$$

or

$$(\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)}) = \underset{\sim}{B}^{-1}(\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)}) \ , \tag{17}$$

so that weighting makes no difference to the result when the number of variables equals the number of observations. Furthermore, in this case, the least-squares procedure gives results identical to those obtained by solving the observational equations directly. In general for the minimization of energy with modes 1 or 4 we have $n = m$, because the variables are the structural parameters and the observations are the derivatives with respect to these parameters. Therefore, in these modes no weight matrix is needed and the observational equations may be solved directly, a procedure known as Newton's method. For mode 0, on the other hand, the number of variable energy parameters will usually be less than the number of observations. In this case the method of least squares must be used and the results will depend on the weighting scheme.

6.3 Calculation of the Weight Matrix

Inclusion of a weight matrix $\underset{\sim}{w}$ will in general affect the parameter changes in mode 0. We know that $\underset{\sim}{w} = \underset{\sim}{V}^{-1}$ where $\underset{\sim}{V}$ is the variance-covariance matrix associated with the observations $\underset{\sim}{y}^{(0)}$. These observations are the derivatives of the energy with respect to the structural parameters, that is $y_i^{(0)} = \partial W/\partial p_i$, and they are assumed to be zero. Errors in the observed structural parameters, however, would imply errors in these derivatives.

Now in general, if $\underset{\sim}{f}$ is a vector of quantities derived from parameters $\underset{\sim}{p}$, the variance-covariance matrix associated with $\underset{\sim}{f}$ is given by

$$\underset{\sim}{V}_f = \tilde{\underset{\sim}{D}}\ \underset{\sim}{V}_p\ \underset{\sim}{D} \tag{18}$$

where $\underset{\sim}{V}_p$ is the variance-covariance matrix of $\underset{\sim}{p}$ and $\underset{\sim}{D}$ is a matrix with $D_{ij} = \partial f_j/\partial p_i$. Now if we identify $\underset{\sim}{y}^{(0)}$ with $\underset{\sim}{f}$ we have $D_{ij} = \partial^2 W/\partial p_i \partial p_j$,

and we may take $\underset{\sim}{V}_p$ as the diagonal matrix with elements $V_{pii} = \sigma^2(p_i)$. Our weight matrix is then

$$\underset{\sim}{w} = (\tilde{\underset{\sim}{D}}\ \underset{\sim}{V}_p\ \underset{\sim}{D})^{-1} \ . \tag{19}$$

In WMIN we calculate the elements D_{ij} from a model for W which may not be very good in the initial stages of parameter adjustment. Use of the weight matrix may therefore cause difficulties unless it is postponed to the final stages of refinement.

6.4 Inclusion of the Experimental Energy as an Observation

The experimental energy, if it is available, may be used as an observation in the least-squares adjustment of energy parameters for mode 0. It can be especially effective in establishing an energy scale for an atom-atom potential. On the other hand, there is no appropriate way to use the experimental energy in other modes of WMIN where the energy of the model is being minimized.

In the least-squares problem we can let the experimental energy $W^{(0)} = y_1{}^{(0)}$ and the calculated energy $W^{(1)} = y_1{}^{(1)}$. Then $\underset{\sim}{B}$ is a one-row matrix with $B_{1j} = \partial W^{(1)}/\partial q_j$, the derivatives of the calculated energy with respect to the variable energy parameters. We may use a scalar weight $w = 1/\sigma^2(W^{(0)})$. Then the contribution of this one observation to the least-squares equation is

$$\tilde{\underset{\sim}{B}}\ w\ \underset{\sim}{B}\ (\underset{\sim}{x}^{(2)} - \underset{\sim}{x}^{(1)}) = \tilde{\underset{\sim}{B}}\ w\ (W^{(0)} - W^{(1)}) \ . \tag{20}$$

As $\underset{\sim}{B}$ is a one-row matrix we see that inclusion of the observation causes a single term to be added to each element of the matrix and vector of the least-squares normal equations.

6.5 Calculation of the Derivatives

All derivatives of the energy W with respect to the parameters p_i (or q_i) are made numerically using the following expressions:

$$\partial W/\partial p_i = [W(p_i + \Delta p_i) - W(p_i - \Delta p_i)]/2\Delta p_i \ , \tag{21}$$

$$\partial^2 W/\partial p_i{}^2 = [W(p_i + \Delta p_i) + W(p_i - \Delta p_i) - 2W(p_i)]/\Delta^2 p_i \ , \tag{22}$$

and

$$\partial^2 W/\partial p_i \partial p_j = [W(p_i + \Delta p_i, p_j + \Delta p_j) + W(p_i, p_j)$$

$$- W(p_i + \Delta p_i, p_j) - W(p_i, p_j + \Delta p_j)]/\Delta p_i \Delta p_j \ . \qquad (23)$$

Here the parameter increments Δp_i are quantities small enough to give a good approximation to the derivative but large enough to produce an energy change ΔW with a reasonable number of significant figures. The increments for the standard structural parameters are built into the program, but the increments for the common parameters PC or extra parameters PX must be provided by the user as input data. A rule of thumb is that Δp_i can be about 10^{-3} or 10^{-4} times p_i or, alternatively, Δp_i can be about 10^{-1} times $\sigma(p_i)$, an estimated standard error for p_i.

The above expression for the first derivatives would be exact if the energy were a linear function of the parameters. Similarly, the expressions for the second derivatives would be exact if the energy were a quadratic function of the parameters.

One important advantage of using numerical derivatives is the ease with which constraints can be applied. After a parameter is incremented, two subroutines, SETA and CNSTRN, are entered before the energy is recalculated. SETA establishes the constraints between unit cell parameters for crystals of high symmetry. For a cubic crystal, for example, it sets b = a and c = a so that when the program increments cell parameter a it automatically increments b and c also. The quantity $\partial W/\partial a$ thus calculated represents the derivative subject to the constraint that a cubic cell is maintained. Subroutine CNSTRN is a user's routine which allows almost any other desired constraints to be established in a similar way.

The use of numerical derivatives also permits great flexibility in the form of the potential energy functions. User routines REPL and GPOT permit the introduction of atom-atom potentials of almost any desired form. The routines need calculate only the energy of the interaction, and the numerical derivatives are obtained automatically.

6.6 Adjustment of Energy Parameters Using Mode 0

Mode 0 uses all of the mathematical methods described above to minimize the first derivatives of the energy by adjusting the energy

parameters of the model. We will describe how the procedures are implemented, and we will discuss the program output at the various stages. Test Problem 3A, Section 10.3, illustrates the output from mode 0 when observations from two substances are combined.

Five input parameters which will be mentioned below appear on the overall control card. These are the weight indicator IWGT, the parameter limit indicator IPLM, the acceptable ratio of eigenvalues ARE, the scaling limit SLIM, and the Marquardt compromise constant CMPR.

After reading the input and making preliminary calculations for each substance involved, the program prints a list of all NP parameters with their names NAMP, values P, and increments DP. The substance number associated with each parameter is given by ISBP where zero designates the common parameters. Non-zero values for KP and KQ indicate observations and variables, respectively, and DKT is the fractional shift to be applied if this kind of damping is specified (see Section 8.1). SP is the standard error which may be assigned to each parameter and used to generate the weight matrix if IWGT $\neq$ 0. PMN and PMX are lower and upper limits on the allowed ranges of the variable parameters. These are set and used only if IPLM $\neq$ 0.

The program proceeds to treat one substance at a time entering WCALC to obtain the energy W and then using the numerical procedures of Equations (21) to (23) to obtain the first derivatives DW and the second derivatives DDWIJ. DW is negated and stored in the vector DYC which represents $(\underset{\sim}{y}^{(0)} - \underset{\sim}{y}^{(1)})$. DDWIJ is stored in the appropriate element of BTR, the matrix $\underset{\sim}{B}$ of Section 6.2. If a weight matrix is to be calculated DDWIJ is also stored in UMAT, a matrix which represents $\underset{\sim}{D}$ of Section 6.3. In obtaining these derivatives care has been taken to avoid the duplication of any energy calculations. Other time saving features will be described in Chapter 7.

If the experimental energy is to be used as an observation the program prints WOWC and the vector DWDQ which represent $(W^{(0)} - W^{(1)})$ and $\partial W/\partial q_j$, respectively, as described in Section 6.4. These quantities are then used to compute AM and VM, the contributions which are added to AN and VN, the matrix and vector of the least squares normal equations.

If IWGT $\neq$ 0 the program computes and prints the weight matrix WMAT according to Equation (19). Next the first and second derivatives of

the energy are printed. The column DYC lists the derivatives $-\partial W/\partial p_i$, the quantities which the program will try to reduce to zero. The second derivatives from matrix BTR are labelled appropriately.

Also printed are the discrepancy factors SDWS and RDWS which are the weighted or unweighted sum of squares of derivatives DYC for one substance and its square root, respectively. The program then uses DYC, BTR, and WMAT (if included) to compute AM and VM, the contributions of this substance which are added to AN and VN, the matrix and the vector of the least squares normal equations, Equation (3) above.

After making these calculations for each substance, the program prints the overall discrepancy factors. SDWST is the weighted or unweighted sum of squares of the derivatives DYC and the energy differences WOWC. RDWST is SQRT(SDWST), and SIGMA is SQRT(SDWST/DGF) where DGF is NO-NV, the number of degrees of freedom.

The program then prepares to solve the normal equations by the method of principal component analysis described in Section 6.2. The scaling matrix SAN, the $\underset{\sim}{s}$ of Equation (4), is computed from the diagonal elements of matrix AN and printed. A diagonal element less than the input scaling limit SLIM causes the corresponding element of SAN to be set to zero. (The scaling matrix will be omitted, i.e., set to unity, if SLIM is read as a negative number.)

The matrix AN and vector VN are then scaled and CMPR is added to each diagonal element to implement Marquardt's compromise. We then compute the eigenvalues, EVAL and eigenvectors EVEC of matrix AN. These are the matrices $\underset{\sim}{\Lambda}$ and $\underset{\sim}{U}$ of Equation (7). These are printed in a way which makes it easy to examine each principal component to determine the contribution of each variable. Referring to the output of Test Problem 3A, Section 10.3, we see that the eigenvalues range from 2.01 to 0.264, a relatively narrow span, so the problem is well determined. The largest EVAL corresponds to a component which includes mostly the variables DCC and AHCH, and, since their coefficients have the same sign, we can say that this component is mostly the <u>sum</u> of these variables. The smallest EVAL, on the other hand, includes these same variables but with coefficients of opposite sign. We conclude, therefore, that it is the <u>difference</u> of these variables which is less well determined.

Two other outputs may be of less interest. These are the scaled eigenvectors and the matrix $\tilde{U}\,s\,\tilde{B}\,w$ of Equation (8) which shows how each principal component depends on the observations. Examining the output of Test Problem 3A we see that the column for principal component 4 has large values corresponding to observations 29 and 48. Presumably, it is these observations which have the largest effect in determining this principal component.

The parameter changes are now calculated according to Equation (11). Using the acceptable ratio of eigenvalues ARE to set the eigenvalue limit ELIM, the matrix $\tilde{U}\,\overset{*}{\Lambda}^{-1}\,\tilde{U}$ is generated and stored in AN. If fewer than NV principal components are used the number NVU is printed out. Parameter changes are computed and scaled, and a standard error is calculated from the diagonal element of the inverse matrix. These quantities are printed together with the old and new values of the parameters.

If the parameter limit indicator IPLM is not zero, then each new parameter is tested against the lower and upper limits, PMN and PMX. If any parameter has moved outside this range, then the number of principal components used is reduced by one and the entire calculation of parameter changes is repeated.

This complete procedure is repeated for a total of NC cycles of refinement. Then one more cycle is made to calculate the energy W, its first derivatives DYC, and the discrepancy factors for the final parameters. A summary of the parameters after each cycle is printed at the end of the run.

6.7 Energy Minimization by Newton's Method, Mode 1

For energy minimization by Newton's method the variables are the structural parameters and the observations are the derivatives with respect to these parameters. We have shown in Section 6.2 that, under these circumstances, the observational equations (1) may be solved directly and that weighting has no effect on the result. In mode 1, therefore, WMIN does not normally calculate a weight matrix or use the method of least squares. The user may override this decision, however, by setting the least squares indicator ILSQ non-zero, but this would only be done for test purposes.

In mode 1 the common parameters are fixed so each substance is treated separately. Test Problem 2A of Section 10.2 shows typical output in this mode. The program calculates the energy W and its first and second derivatives, DQ and DDWIJ, as before. The experimental energy WOBS may be printed, but it is not used in the calculation. The output column DYC again lists the negatives of the first derivatives, and the second derivatives are appropriately labelled.

Because the observational equations are to be solved directly, the matrix BTR (which is symmetric in this case) and vector DYC are simply copied into locations AN and VN. Then the method of principal component analysis is used just as in mode 0 for determining the parameter changes.

In this mode the printed eigenvalues EVAL give information about the stability of the model. If all eigenvalues are positive the structure is near an energy minimum. One or more negative eigenvalues would indicate that the model is near a maximum or a saddle point. One or more zero eigenvalues would indicate that redundant parameters have been included as variables. In this case the principal components might represent the rotations or translations of an isolated molecule or coordinates along a polar crystal axis. Principal components with negative or zero eigenvalues will usually be omitted automatically, depending on the value of input parameter ARE, the acceptable range of eigenvalues.

Parameter changes and errors are calculated and printed as in mode 0. For a stable model which is behaving correctly the derivatives DYC and the discrepancy factor RDWS should become very small after several cycles. Oscillating models can sometimes be brought to convergence by damping with fractional shifts. This is done by selecting the input values of KP, as described in Section 8.1. Models which are far from equilibrium may not converge at all with mode 1, and preliminary adjustment with modes 2 or 3 is recommended in those cases.

6.8 Method of Steepest Descents, Mode 2

The energy minimization procedure using Newton's method, mode 1, works very well when the model is already close to a local minimum. In other situations it may not work at all. Because Newton's method

attempts to minimize the first derivatives of the energy, it may well locate a local maximum or a saddle point in the energy. If the starting parameters happen to represent a saddle point, Newton's method cannot move off of this point toward a minimum. For this reason two other methods of minimizing the energy have been included in WMIN. Section 6.9 describes mode 3, a modified Rosenbrock search technique which works very well. For traditional reasons the program also includes a method of steepest descents procedure, mode 2, which is described in this section. In practice this mode may not be needed, because the energy of any model can be minimized by the combined use of modes 1 and 3. For this reason no example of mode 2 is included in the test problems.

For the method of steepest descents WMIN calculates the energy W and its first derivatives DW. These first derivatives define a gradient vector in parameter space, the direction in which the energy decreases most rapidly. The program makes a step search along this vector, recalculating the energy for each parameter set. The results of each trial may be printed (depending on IPRT, see Section 7.3) so that the user may follow the search procedure. Stepping continues as long as the new energy WXN is less than the previous lowest value WXL. Then a limited binary search for a minimum is made in which the step size is halved four times. The old and new parameters are printed with their changes and the program goes back to recalculate W and DW on the next cycle.

The initial step size for the search is determined by input parameter XDRD from the overall control card. A trial value of 0.01 is recommended, but some experimentation with this parameter may be needed. Too small a step size will increase the search time unduly. Too large a step may move the model completely out of the starting region to a different local minimum.

6.9 Modified Rosenbrock Search, Mode 3

In mode 3 the program minimizes the energy using a very simple search technique based on the ideas of Rosenbrock (1960). No derivatives are used; only the energy W is calculated for various trial values of the parameters. The procedure takes longer to reach a final minimum than does Newton's method, but it will always move toward a lower

energy, even from a saddle point. In practice it will often be desirable to start an energy minimization using mode 3, and then to switch to mode 1 for a final parameter adjustment.

In mode 3 the NC cycles of adjustment are each divided into NSTG stages where NC and NSTG are input integers on the overall control card. Another input constant EPSC, which is also read from this card, will be mentioned below.

At the start of a cycle the energy W is calculated and various outputs are printed just as in other modes. It then begins the first stage of the search. Each stage is divided into an exploratory search and a vector search. The exploratory search adjusts one parameter at a time starting with the first variable and working down the parameter list. For variable parameter P(I) a change is made of EPS(I) = EPSC * DP(I). EPSC is an input parameter of perhaps 10.0 so that the initial parameter change is larger than the DP(I) used for derivative calculations in the other modes. Using the modified parameter the program calculates WTR, a trial value of the energy. If WTR is less than or equal to the current energy WCUR the trial is called a <u>success</u>, and WCUR is set to WTR. If, on the other hand, WTR is greater than WCUR the trial is called a <u>failure</u>, and parameter P(I) is reset to its previous value.

If the first trial for parameter P(I) is a success then the program increases the increment EPS(I) by a factor of 3.0, changes the parameter again, and calculates a new energy WTR. This is again compared with WCUR to determine the success or failure of the new trial, and the process is repeated until a failure occurs. Note that a failure must occur eventually as we pass the energy minimum.

Alternatively, if the first trial for parameter P(I) is a failure then the program halves the increment EPS(I) and changes its sign so that the next step will move P(I) in the opposite direction. A new trial is made and the process is repeated until a success is obtained. Such a success must eventually occur even if a minimum energy has already been reached, because for a small enough parameter shift the energy change will become either negative or zero.

The exploratory search for each parameter continues only until at least one success and at least one failure have been achieved. Then

the program moves on to the next variable parameter and repeats the procedure.

When all the variable parameters have been adjusted in the exploratory search the program proceeds to make a vector search in which all variables are adjusted simultaneously. The direction taken is that of the vector VBEST made up of the net parameter changes from the exploratory search. Each parameter is changed by an amount EPSL * VBEST(I) where EPSL is initially set at 0.25. The procedure is exactly analogous to that used for the exploratory search. A success causes EPSL to be increased by a factor of 3.0; a failure causes it to be halved and negated. One failure and one success ends the vector search and terminates the stage. Exploratory searches followed by a vector search are repeated NSTG times in each cycle.

An important feature of this search procedure is that the values of EPS(I), the increments for each parameter, are automatically adjusted to optimum size and direction. This adjustment continues throughout the energy minimization with the current values of EPS(I) being carried over from stage to stage and from cycle to cycle. As the minimum is approached the values of EPS(I) get smaller and so do the parameter changes, which are the elements of VBEST. When the sum of the squares of these changes, VBSQ, becomes almost zero the search is terminated with a printed message.

Test Problem 2B, Section 10.2, illustrates the output from a mode 3 energy minimization. The initial calculation of the energy produces the same output as the other modes. The results of each trial calculation may also be printed (depending on IPRT, see Section 7.3). These include the parameter number I, the increment EPS(I), the parameter value P(I), and the trial energy WTR. This output will enable the user to follow the course of the search, if necessary. At the end of each cycle the old and new parameters are printed together with their changes.

6.10 Calculation of Vibrational Frequencies and Normal Modes, Mode 4

The operation of mode 4 was described briefly in Section 2.5. Most of these calculations are made in subroutine WDYN which is shown schematically in Figure 2.5. We will now describe the computational methods in

more detail. Output from a mode 4 calculation is shown in Test Problem 3B, Section 10.3.

The matrix equation to be solved is

$$\underset{\sim}{B}\ \underset{\sim}{U} = \underset{\sim}{K}\ \underset{\sim}{U}\ \underset{\sim}{\Lambda} \tag{24}$$

where $\underset{\sim}{B}$ is the potential energy matrix with elements $B_{ij} = \partial^2 W/\partial p_i \partial p_j$ and $\underset{\sim}{K}$ is the kinetic energy matrix with elements $K_{ij} = \partial^2 T/\partial \dot{p}_i \partial \dot{p}_j$, the derivatives of the kinetic energy T with respect to the generalized velocities $\dot{p}_i$. $\underset{\sim}{B}$ and $\underset{\sim}{K}$ are both symmetric and correspond to the matrices $\underset{\sim}{F}$ and $\underset{\sim}{G}^{-1}$ often used in spectroscopic calculations (Eyring, Walter and Kimball, 1944; Wilson, Decius and Cross, 1955). Solving Equation (24) produces the eigenvalue and eigenvector matrices $\underset{\sim}{\Lambda}$ and $\underset{\sim}{U}$. Matrix $\underset{\sim}{\Lambda}$ is diagonal with elements λ_i related to the vibrational frequencies so that

$$\nu_i = \sqrt{\lambda_i}/2\pi \ . \tag{25}$$

Each column of the eigenvector matrix $\underset{\sim}{U}$ describes one normal mode of vibration in terms of the dynamic variables p_i.

We will choose as these dynamic variables the rigid-body rotations and translations which are the structural parameters p_i of Sections 6.6 and 6.7. The crystal lattice parameters, however, are not used as variables since they would correspond to low frequency elastic vibrations of the crystal. With this limitation, the matrix $\underset{\sim}{B}$ is just the matrix BTR which is computed numerically as in mode 1.

The kinetic energy of the system is

$$T = \frac{1}{2} \sum_k m_k \sum_{\ell=1}^{3} \dot{x}^2_{\ell k} \tag{26}$$

where k numbers the atoms in the formula unit, m_k is the mass of each atom, and $\dot{x}_{\ell k}$, $\ell = 1,2,3$, is a Cartesian component of velocity for atom k. Noting that $\partial \dot{x}_{\ell k}/\partial \dot{p}_i = \partial x_{\ell k}/\partial p_i$, we can express the required kinetic energy derivatives as

$$K_{ij} = \sum_k m_k \sum_{\ell=1}^{3} (\partial x_{\ell k}/\partial p_i)(\partial x_{\ell k}/\partial p_j) \ . \tag{27}$$

The coordinate derivatives are obtained numerically according to the expression

$$\partial x_{\ell k}/\partial p_i = [x_{\ell k}(p_i + \Delta p_i) - x_{\ell k}(p_i - \Delta p_i)]/2\Delta p_i \ . \tag{28}$$

When mode 4 is specified WMIN performs NC cycles of energy minimization, just as in mode 1, and then enters subroutine WDYN. Derivatives of the Cartesian coordinates with respect to each dynamical variable are calculated according to Equation (28) and stored in arrays DXQ, DYQ, and DZQ. For this purpose each dynamic variable P is incremented or decremented in turn and WCAL is entered with break indicator IBK set nonzero. This causes WCAL to obtain Cartesian coordinates XYZC for each atom and to exit at that point, omitting the energy calculation. To simplify the interpretation of the output, each atom is referred to the same Cartesian system, namely that defined for the first rigid body in the list. The values of DXQ, DYQ, and DZQ are printed as output in a way which allows users to visualize the dynamic variables which they have defined. In Test Problem 3B we have set IPRT to omit this output which would be particularly simple in this case because each atom is treated as a separate rigid body and referred to the same axes.

The derivatives DXQ, DYQ, and DZQ are then used, together with the atomic masses AMASS, to calculate the matrix AKE, which is the kinetic energy matrix $\underset{\sim}{K}$, according to Equation (27). Any lattice parameters which were varied in the first cycles are removed from matrix BTR, and these two symmetric matrices are printed. The program then solves Equation (24) storing the eigenvalues λ_i in EVAL and the eigenvectors $\underset{\sim}{U}$ in the location of BTR, and these quantities are also printed.

Each eigenvalue and eigenvector represent one normal mode of vibration. The program takes each of these modes in sequence, beginning with the largest eigenvalue, and presents the results in the following way. The frequency FREQ in Kaisers (cm^{-1}) is calculated from Equation (25). The relative Cartesian displacements XYZD of each atom are computed

from the eigenvector and the derivatives DXQ, DYQ, and DZQ, and these displacements are printed. Again they are all referred to the same Cartesian system, that defined for the first rigid body.

The symmetry of the vibration can be determined by examining the atomic displacements involved, but this is not always a trivial task. The program therefore proceeds to compute for each symmetry operation a quantity called CHAR which is related to the group theoretical character of that vibration. This is done by first computing UU, the sum of the squares of all atomic displacements. Then it applies the symmetry operation to both the atomic coordinates and to the displacements. For each atom, after locating the symmetry related one, the transformed displacements are compared with the original ones. This is done by accumulating for all the atoms the inner product US of the transformed displacements with the original ones. CHAR is then set to US/UU. Thus a vibration which is symmetric with respect to a symmetry operation will produce a CHAR of +1, and an antisymmetric vibration generates a CHAR of -1. Degenerate modes may produce intermediate values, the significance of which will be described below. (If a symmetry equivalent atom cannot be found because of an error in the problem set up, the program sets CHAR to a large number which serves as in error indicator.)

The interpretation of the output of CHAR is best explained by reference to the output of Test Problem 3B, Section 10.3, which refers to the isolated molecule of ethane, C_2H_6, as described in Section 5.3.3. Ethane has point symmetry D_{3d} ($\bar{3}m$), and, although only six symmetry cards are needed to generate the molecule, the test problem includes cards for all twelve symmetry operations of the point group so that the corresponding values of CHAR can be computed. Table 6.1 lists the character table for D_{3d}. (See, for example, Wilson, Decius, and Cross (1955) or Eyring, Walter, and Kimball (1944).)

Examining the test output we see that for FREQ(1) the value of CHAR(7) corresponding to inversion i, is -1. This identifies the mode as a u-type vibration. Values of +1 and -1 corresponding to the C_3 and C_2 symmetry operations, respectively, establish the symmetry of the mode as A_{2u}, and the remaining values of CHAR corroborate this. For FREQ(2), on the other hand, we find that all values of CHAR are +1, so this represents a totally symmetric A_{1g} vibration.

Table 6.1. Characters of Group D_{3d}

	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$	Rotations and translations
A_{1g}	1	1	1	1	1	1	
A_{2g}	1	1	-1	1	1	-1	R_z
E_g	2	-1	0	2	-1	0	(R_x, R_y)
A_{1u}	1	1	1	-1	-1	-1	
A_{2u}	1	1	-1	-1	-1	1	T_z
E_u	2	-1	0	-2	1	0	(T_x, T_y)

We note that the values of FREQ(3) and FREQ(4) are very nearly the same, so we identify these as a degenerate pair. Presumably their frequencies would be identical if it were not for round-off errors in our numerical procedures. In order to compare the results with Table 6.1 it is necessary to add corresponding values of CHAR under FREQ(3) and FREQ(4). Thus for the identity operation E we have a character of 1 + 1 = 2, for C_3 we obtain -0.5 - 0.5 = -1, for C_2 we have 0.537 - 0.537 = 0, and for i we get -1 - 1 = -2. We can then identify the pair of vibrations as belonging to symmetry species E_u. The remaining normal modes in the output can be identified in a similar way.

In order to generate the desired vibrational modes for a system it is usually necessary to relax the symmetry constraints as described in Section 3.3. This is because any distortion of our model is always required to conform to the symmetry imposed. Comparison of the treatment of ethane in Test Problems 3A and 3B shows that relaxing the symmetry constraints increases the number of atoms NA and also increases the number of independent variables. The number of normal modes calculated is, of course, equal to the number of these variables.

In the case of an isolated molecule, the inclusion of three variables for each atom means that six redundant parameters have been introduced corresponding to the molecular rotations and translations. These will appear as zero frequencies in the resulting normal modes. Examining the output of Test Problem 3B we find that the final six modes, FREQ(19) to

FREQ(24), have small values for the frequencies. Examining the atomic displacements and the values of CHAR we can identify FREQ(19) as the A_{2g} rotation about z and FREQ(20) and FREQ(21) as the degenerate pair of E_g rotations about x and y. FREQ(23) is the A_{2u} translation in the z direction, and FREQ(22) and FREQ(24) are the degenerate E_u translations in the x and y directions.

Failure of the program to produce exactly zero frequencies for these redundant modes is a measure of the precision of the numerical derivatives used in setting up the matrix $\underset{\sim}{B}$. Probably the situation is aggravated in this test problem because our Cartesian variables do not have the three-fold symmetry of the ethane molecule. In any case, the largest redundant frequency is of the order of one percent of the highest frequency calculated. Presumably we can expect a similar percentage accuracy in the calculation of the low frequency external modes involving large rigid bodies.

It might be assumed that one could omit the redundant translations from the problem by holding one atom fixed. Such a procedure would indeed reduce the number of dynamic variables and eliminate the three translations, but the calculated frequencies and normal modes would be incorrect since one atom would be fixed. The procedure would be equivalent to assigning infinite mass to that atom.

On the other hand, it is permissible to apply symmetry constraints to the model if only certain vibrational modes are desired. Thus if the frequencies of ethane are calculated without relaxing the symmetry constraints of Test Problem 3A, then there are only three dynamic variables and only the three totally symmetric A_{1g} vibrational modes will be calculated. Care must be taken with this procedure, however. The propane molecule, C_3H_8, as described in Section 5.3.1 has 10 structural parameters, but one z-coordinate is redundant. In minimizing the energy of propane only 9 variables need be used, but to calculate the totally symmetric vibrations in mode 4 all 10 dynamic variables must be included. Fixing one atom would again be equivalent to assigning it infinite mass and would produce incorrect results.

Similar considerations apply to the calculation of the vibrational modes in crystals. If we relax all constraints so that the only symmetry

imposed on the model is that of the unit cell translations, then we will calculate all of the optical modes of the crystal. These are the modes in which every unit cell is vibrating in phase, sometimes known as the modes with k = 0. These optical modes include three zero-frequency crystal translations but no crystal rotations. WMIN can be used for calculating modes with other k values only by doubling or multiplying the size of the unit cell. This procedure may be practical for some purposes, but it will increase the required computing time considerably.

7. SPECIAL PROGRAM FEATURES

7.1 Dynamic Dimensioning of Arrays

WMIN uses 133 arrays with dimensions which depend on the particular problem under study. The broad range of such problems makes it inconvenient or wasteful to use fixed dimension statements. A dynamic dimensioning system has therefore been provided in program MAIN which sets up the storage at run time based on 16 input integers LIM.

Storage for each of the 133 arrays is allocated in one master array S using the pointer list K so that the arrays start at S(K(1)), S(K(2)), and so on to S(K(133)). These locations are passed to eleven major subroutines of the program as subroutine arguments. Inside these subroutines the arrays are renamed with the mnemonic symbols used throughout this report. MAIN calls each of these routines only once, and for this initializing entry the subroutine names have the suffix I added to become WDYNI, WPREI, WCALCI, etc. Each of these routines also has an entry point WDYN, WPRE, WCALC, etc. used for all later calls. Some such calls require no additional arguments; others require a few.

A directory to the arrays as allocated is printed at the start of each problem, and the test problem output, Section 10, provides some examples which may be illustrative. The overall storage array S is taken as NST 8-byte words. Its size is established by subroutine MASTER, and it may be enlarged at run time by recompiling only that small routine. The pointer array K, which contains the starting location of each of the 133 arrays, is calculated from the 16 input integers, LIM. For this purpose two preset arrays, L1 and L2, specify the two quantities LIM(L1(I)) and LIM(L2(I)) which are multiplied to compute the dimension of array I. Thus the array BTR is dimensioned NVMAX*NOSMAX. The array LIM also contains preset integers from 0 to 12 in locations LIM(20) to LIM(32), and these are needed for computing the sizes of arrays such as ACZ dimensioned 9*NRBMAX or AMASS dimensioned 1*NKAMAX. In computing K the program uses a third preset array, ITYPE, which specifies whether each array consists of 8-byte or 4-byte words.

The printed directory lists the array name, the names of the limits which determine its dimensions, its size in words, the word size in

bytes, and the hexadecimal address of each array in the overall storage array S. The latter is useful if it is necessary to locate an array in a program dump.

This dynamic dimensioning procedure is probably the one feature of WMIN which is most likely to cause difficulties when different computers or different operating systems are used. The author is interested in discussing with users any problems which may arise and any modifications which prove useful on particular machines.

7.2 Bypassing Duplicate Calculations

Most of the computer time used by WMIN involves the repeated calculation of the energy in subroutines WCALC and GCWX. Often these calculations are made following a change in only one or two parameters so that many of the energy terms would remain unchanged. Two mechanisms included in WMIN to avoid the repeated calculation of such unchanged terms will be described below. This description may be of no interest to the casual user of the program, but any programmer making modifications to WCALC or GCWX should be aware of these features. They are included in the flowcharts, Figures 2.3 and 2.4.

The first time-saving procedure involves bypassing the calculation of direct lattice energy terms which are predicted to be unchanged from their previous values. Each such term depends on certain constants and on possible variables which are the common parameters PC, the lattice parameters A, the extra parameters PX, and the coordinates, XC, YC, and ZC, of the atoms in the cell. On each entry to WCALC the values of these variables are saved in arrays PCSV, ASV, PXSV, XCSV, YCSV, and ZCSV, respectively. On each entry after the first their current values are compared with the saved values and indicators are set to zero if no change has occurred. If the lattice parameters are unchanged then ICA is set to zero and the initial unit cell calculations are bypassed. Indicator ICCAX is set to zero if PC, A, and PX are all unchanged, and the array element ICC(K) is zero if atom K has not been displaced. The calculation of the unit cell sums SQK, SPLK, and SPPK are bypassed if ICCAX is zero. In the fast direct lattice sum the computation of the terms between atoms I and J is bypassed if ICC(I), ICC(J), and ICCAX are

all zero. In this case the previously saved terms RSV, VSV, and CSV are added to WR, SVDW, and SG, respectively. This bypass does not occur if user routine GPOT is being used, because the energy terms could depend on the positions of atoms other than I and J in that case.

Similarly, in subroutine GCWX, if ICCAX is zero and if the atoms involved in a distance, bond angle, or torsion angle have not moved, then the calculation is bypassed and the saved term WSV is added to WX.

The second time-saving feature comes into play only in mode 0 when derivatives with respect to the common parameters PC are being calculated. This involves bypassing the entire reciprocal lattice sum, the direct lattice sum, or the calculation of extra energy in CWX or GCWX, depending on the nature of the common parameter which has been modified.

For each common parameter PC the user provides an indicator KPC, the kind of common parameter. A KPC of 1 indicates that the parameter affects Coulomb or van der Waals energy and thus the values of both the reciprocal and direct lattice sums. A KPC of 2 describes a parameter such as a repulsion which affects only the direct lattice sum. A parameter used only by CWX, GCWX, or WCNF for the calculation of internal energy is designated with KPC = 3. Any other type of common parameter must have KPC = 0, a value which prevents any bypassing.

During the calculation of numerical derivatives the program makes repeated entries to WCALC after having incremented either one or two parameters, P(I) and P(J). The function subroutine IBYPAS uses arguments I and J together with the array KPC to generate a bypass indicator IBY which is an argument for subroutine WCALC. IBY is assigned values from 0 to 7, and the three bits of its binary representation specify which parts of the energy calculation are to be bypassed, as is shown in Table 7.1. The program also uses the indicator IBYP which is IBY + 1. Note that no bypassing occurs if zero is used for the argument IBY.

As WMIN loops through the parameters calculating numerical derivatives, the indices I and J specify the parameters which have been incremented. I is the index of the inner loop and changes most rapidly; J is the index of the outer loop and changes more slowly. Subroutine IBYPAS uses arguments I and J together with indicators KPC to set IBY according to the following rules:

Table 7.1 Definition of bypass indicators IBY and IBYP

IBY decimal	IBY binary	IBYP decimal	Reciprocal lattice sum	Direct lattice sum	Intra-molecular energy
0	000	1	Compute	Compute	Compute
1	001	2	Compute	Compute	Bypass
2	010	3	Compute	Bypass	Compute
3	011	4	Compute	Bypass	Bypass
4	100	5	Bypass	Compute	Compute
5	101	6	Bypass	Compute	Bypass
6	110	7	Bypass	Bypass	Compute
7	111	8	Bypass	Bypass	Bypass

1) No bypassing occurs unless J is the same as its previous value JP. (If only one parameter P(I) has been changed the argument J is fixed at zero so this condition is satisfied.)

2) No bypassing occurs unless $I \leq NPC$ so that P(I) is a common parameter.

3) No section of the calculation is bypassed unless it is permitted by KPC(I) which describes parameter P(I).

4) No section of the calculation is bypassed if rule (3) forced its calculation on the preceding entry. This is determined from KPC(IP) where IP is the preceding value of I.

The net effect of these rules is that a section of WCALC is bypassed only if it is certain that its result will be the same as that calculated on the previous entry. The improved efficiency applies only to mode 0 as that is the only situation in which the common parameters are varied. It is also clear that the maximum improvement occurs if energy parameters of the same kind are grouped together in the common parameter list.

7.3 Control of Printed Output

Program WMIN can provide copious output including almost all the intermediate quantities and matrices used in the calculation. This output may be valuable in the initial stages of a problem or when unforeseen

Table 7.2. Effect of print indicator IPRT in controlling amount of output.

KEY: P = Printed; FL = Printed on first and last cycles; F = Printed on first cycle; 0 = Not printed.

Output item	Value of IPRT					
	0	1	2	3	4	5
Dynamic dimensions of arrays	P	P	P	P	P	P
All input mirrored as output	P	P	P	P	P	P
List of atoms in cell, formula unit, bonded contacts	P	P	P	P	P	0
Initial parameter list	P	P	P	P	0	0
Count of observations and variables	P	P	P	P	P	0
Direct and reciprocal terms in energy	P	P	FL	F	0	0
List of interatomic distances	P	P	FL	F	0	0
Intramolecular bond distances and angles	P	P	FL	F	0	0
Individual terms in the energy	P	P	P	P	P	0
Energy mapping, mode -1	P	P	P	P	P	P
Derivatives of the energy	P	P	P	P	0	0
Weight matrix	P	P	FL	F	0	0
Agreement factors	P	P	P	P	P	0
Computing time analysis and recommendations	P	P	FL	F	0	0
Scalefactors for modes 0 and 1	P	FL	F	0	0	0
Eigenvalues and eigenvectors, modes 0 and 1	P	P	FL	F	0	0
Scaled eigenvectors and other matrices	P	FL	F	0	0	0
Individual steps in steepest descent, mode 2	P	FL	F	0	0	0
Individual steps in Rosenbrock search, mode 3	P	FL	F	0	0	0
Parameter changes, modes 0, 1, 2, 3, or 4	P	P	P	0	0	0
Dynamic variables, mode 4	P	P	P	0	0	0
Matrices, engenvalues, and engenvectors, mode 4	P	P	0	0	0	0
Normal mode frequencies, displacements, and characters	P	P	P	P	P	0
Revised atom coordinates, modes 1, 2, 3, or 4	P	P	P	P	P	P
Summary on standard output	P	P	P	P	P	0
Summary on auxiliary output	P	P	P	P	P	P

difficulties are encountered. On the other hand, it may be wasteful or inconvenient for routine work. A print indicator IPRT has therefore been provided which is set by the user to a value from 0 to 5. An IPRT of 0 causes all output to be printed, a value of 3 for IPRT may be suitable for normal problems, and an IPRT of 5 severely limits the output. Table 7.2 lists the items which will be printed for various values of this indicator.

7.4 Timing Measurements and Optimization

Most of the machine time for these computations is used by the energy calculating subroutine WCALC, and it is desirable to know how this time is divided between the various parts of the calculation. We have therefore defined nine sections of program in WCALC and established arrays of nine counters NT and nine timers LT. At the end of each pass through a section its counter NT is incremented and the elapsed time for that section is added to its timer LT. These times are determined by the system subroutine ICLOCK which returns central processor time in units of 0.01 seconds. On each cycle, after all entries to WCALC have been made, the program enters subroutine TIMOUT which prints for each of the nine sections the number of passes, the elapsed time for all passes, and the average time per pass.

For the calculation of Coulomb or van der Waals energy using direct and reciprocal lattice sums, subroutine TIMOUT also computes and prints optimum values of the summation limits, the Ewald constant, and the predicted computing time for six different levels of precision. This is done in the following way:

We can assume that the computing time t is given by

$$t = C_f Q_{lim}^3 + C_g r_{lim}^3 \qquad (1)$$

where Q_{lim} and r_{lim} are the summation limits in reciprocal and direct space, respectively. TIMOUT determines the constants C_f and C_g from the elapsed times measured for the sums. In general these will depend on the particular problem under study and on the computer being used.

As we have seen in Section 4.2.1, the limits required for a given precision depend on the value of the Ewald constant K. Increasing K

makes it necessary to include more terms in the reciprocal lattice sum and fewer in the direct lattice sum. The total time t can be optimized by choosing K correctly and setting the limits accordingly.

It is clear that the direct and reciprocal lattice sums should be computed to the same precision, since the poorest one determines the error of their sum. We will assume that the precision of each sum is proportional to the modification functions erfc(a) and $\exp(-b^2)$, respectively, of Equation (2), Section 4, when a and b have their maximum values. Defining

$$\alpha = r_{lim} K \tag{2}$$

and

$$\beta = Q_{lim}/K \tag{3}$$

we see that we should choose α and β so that

$$\mathrm{erfc}(\sqrt{\pi}\,\alpha) = \exp(-\pi\beta^2) = \Delta \tag{4}$$

where Δ is a small number which measures the desired precision. In TIMOUT values of α and β are stored in preset arrays AL and BT for six values of Δ, each a factor of ten smaller than the preceding one. Although these tabulated constants are based on the modification functions for the Coulomb energy, they seem to work fairly well for optimizing calculations including van der Waals terms.

Given α and β and the measured constants C_f and C_g we can rewrite Equation (1) as

$$t = C_f(\beta K)^3 + C_g(\alpha/K)^3 \ . \tag{5}$$

Minimizing t with respect to K yields

$$K = \sqrt[6]{C_g/C_f}\ \sqrt{\alpha/\beta}\ , \tag{6}$$

$$Q_{lim} = \sqrt[6]{C_g/C_f}\ \sqrt{\alpha\beta}\ , \tag{7}$$

and

$$r_{lim} = \sqrt[6]{C_f/C_g}\ \sqrt{\alpha\beta}\ . \tag{8}$$

The predicted time, which is divided equally between the two sums, is given by

$$t = 2\sqrt{C_f C_g}\ (\alpha\beta)^{3/2} \ . \tag{9}$$

TIMOUT prints these four quantities as PRK, PRQ, PRR, and PRT, respectively, for each of six values of Δ.

After a preliminary run for a new calculation it will usually improve the efficiency to reset the limits QLIM and RLIM, perhaps using two values for each, together with the corresponding Ewald constant CK. On subsequent runs the times for each sum should be comparable and the total time should be close to that predicted. It should be noted, however, that the optimum conditions may change if symmetry constraints are relaxed or if different modes are used.

8. INSTRUCTIONS FOR PROBLEM SETUP

```
      SUBROUTINE INSTRU                                                 INST   5
C     ******************************************************************INST  10
C                                                                       INST  15
C   8.1 DATA INPUT FOR WMIN                                             INST  20
C                                                                       INST  25
C       ALL INPUT FORMATS ARE IW OR FW.0 UNLESS OTHERWISE NOTED.        INST  30
C                                                                       INST  35
C  *    RECENT MODIFICATIONS ARE MARKED WITH AN ASTERISK (*).           INST  40
C                                                                       INST  45
C       IN MAKING UP THE DATA FOR A PROBLEM IT MAY BE DESIRABLE TO      INST  50
C       CONSIDER FIRST INPUTS (11) TO (35), THEN INPUTS (2) TO (10),    INST  55
C       AND FINALLY INPUT (1).                                          INST  60
C                                                                       INST  65
C  *  1) DYNAMIC DIMENSIONS USED TO SET UP ARRAY STORAGE. IF IBPC.EQ.1  INST  70
C       THESE DIMENSIONS MUST BE THE SAME AS FOR THE PREVIOUS JOB.      INST  75
C                                                                       INST  80
C        CARD 1                                                 MINIMUM INST  85
C        COLS                UPPER LIMIT ON -                    VALUE  INST  90
C        1- 9  NPCMAX - THE NUMBER OF COMMON PARAMETERS            0   INST  95
C       10-18  NAMAX  - ATOMS IN THE ASYMMETRIC UNIT               1   INST 100
C       19-27  NKAMAX - KINDS OF ATOMS                             1   INST 105
C       28-36  NSMAX  - SYMMETRY CARDS                             1   INST 110
C       37-45  NRBMAX - RIGID BODIES IN ASYMMETRIC UNIT            1   INST 115
C       46-54  NPXMAX - EXTRA PARAMETERS FOR ONE SUBSTANCE         0   INST 120
C       55-63  NCTMAX - CARDS IN MOLECULAR CONNECTION TABLE        1   INST 125
C       64-72  NBCMAX - BONDED CONTACTS GENERATED FROM             1   INST 130
C                       MOLECULAR CONNECTION TABLE                     INST 135
C        CARD 2                                                        INST 140
C        COLS                                                          INST 145
C        1- 9  MMAX    - DISTANCES, ANGLES, CONFORMATION ANGLES     0 INST 150
C                       GENERATED FROM CONNECTION TABLE AND            INST 155
C                       CONTRIBUTING TO THE ENERGY                     INST 160
C       10-18  NFSMAX - NUMBER OF RECIPROCAL LATTICE POINTS.         0 INST 165
C                       ZERO IF CK.EQ.0 OR IMOL.EQ.1                   INST 170
C       19-27  NGSMAX - NUMBER OF INTERATOMIC VECTORS.               0 INST 175
C                       ZERO FOR SINGLE ENERGY CALCULATION             INST 180
C       28-36  NPSMAX - PARAMETERS FOR ONE SUBSTANCE.                  INST 185
C                                   FOR IRBA.EQ.0   6+6*NRB+NPX        INST 190
C                                   FOR IRBA.EQ.1   6+3*NRB+NPX        INST 195
C       37-45  NPMAX  - TOTAL PARAMETERS.   FOR MODE 0     NPC+SUM(NPS) INST 200
C                                 FOR OTHER MODES       NPC+NPSMAX     INST 205
C       46-54  NOSMAX - OBSERVATIONS FOR ONE SUBSTANCE             1   INST 210
C       55-63  NOMAX  - TOTAL OBSERVATIONS. FOR MODE 0         SUM(NOS) INST 215
C                                   FOR OTHER MODES          NOSMAX   INST 220
C       64-72  NVMAX  - NUMBER OF VARIABLES.                       1   INST 225
C                          FOR MODE 0 USE TOTAL VARIABLES.             INST 230
C                          FOR OTHER MODES USE MAX FOR ONE SUBSTANCE.  INST 235
C                                                                      INST 240
C     2) OVERALL TITLE CARD                                            INST 245
C        COLS                                                          INST 250
C        1-72  TITLE. ANY 72 HOLLERITH CHARACTERS                      INST 255
C                                                                      INST 260
C     3) OVERALL CONTROL CARD                                          INST 265
C        COLS                                                          INST 270
C        1- 3  MODE OF REFINEMENT                                      INST 275
C                 0 - ADJUST ENERGY PARAMETERS SPECIFIED BY KQC AND    INST 280
C                     KQS USING STRUCTURAL PARAMETERS SPECIFIED BY KPS INST 285
C                     AS OBSERVATIONS. THIS PROCEDURE CONVERGES ONLY   INST 290
C                     WHEN THE PARAMETERS ARE NEARLY CORRECT. IT MAY   INST 295
C                     BE DESIRABLE TO DEDUCE INITIAL VALUES OF         INST 300
C                     POTENTIAL PARAMETERS BY MAPPING WITH MODE -1 OR  INST 305
C                     BY ADJUSTING THE STRUCTURE WITH MODE 3.          INST 310
C                 1 - MINIMIZE ENERGY USING NEWTON'S METHOD TO ADJUST  INST 315
C                     STRUCTURAL PARAMETERS SPECIFIED BY KPS.          INST 320
C                     KQC AND KQS ARE IGNORED. THIS METHOD WILL NOT    INST 325
C                     CONVERGE IF THE STRUCTURE IS VERY FAR FROM THE   INST 330
C                     MINIMUM. IT MAY BE PREFERABLE TO USE MODE 3      INST 335
C                     FIRST.                                           INST 340
C                 2 - MINIMIZE ENERGY USING METHOD OF STEEPEST         INST 345
C                     DESCENTS TO ADJUST STRUCTURAL PARAMETERS         INST 350
C                     SPECIFIED BY KPS. KQC AND KQS ARE IGNORED.       INST 355
C                     MODE 3 IS PROBABLY PREFERABLE.                   INST 360
C                 3 - MINIMIZE ENERGY USING ROSENBROCK SEARCH TO       INST 365
C                     ADJUST STRUCTURAL PARAMETERS SPECIFIED BY KPS.   INST 370
C                     KQC AND KQS ARE IGNORED. THIS SEARCH ALWAYS      INST 375
C                     REDUCES THE ENERGY, EVEN WHEN STARTING FROM A    INST 380
C                     SADDLE POINT. IT MAY BE SLOW TO ATTAIN FINAL     INST 385
C                     CONVERGENCE, AND THEREFORE SHOULD BE FOLLOWED    INST 390
C                     BY MODE 1.                                       INST 395
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C                 4 - MINIMIZE ENERGY AS FOR MODE.EQ.1. THEN CALCULATE INST 400
C                     VIBRATIONAL FREQUENCIES AND NORMAL MODES.        INST 405
C                     VIBRATIONAL VARIABLES ARE SPECIFIED BY KPS BUT   INST 410
C                     LATTICE PARAMETERS ARE FIXED. IF NC.EQ.0 ONLY    INST 415
C                     THE FREQUENCIES AND NORMAL MODES ARE CALCULATED. INST 420
C                -1 - MAP ENERGY AS A FUNCTION OF 1, 2, OR 3           INST 425
C                     PARAMETERS.                                      INST 430
C          4- 6  NC, THE NUMBER OF CYCLES OF REFINEMENT. 3 TO 5 MAY BE INST 435
C                     SATISFACTORY. IF NC.EQ.0 ENERGY W AND FIRST      INST 440
C                     DERIVATIVES WILL BE CALCULATED.                  INST 445
C          7- 9  NPC, THE NUMBER OF COMMON PARAMETERS. THESE ARE ENERGY INST 450
C                     PARAMETERS WHICH MAY BE COMMON TO ALL SUBSTANCES.INST 455
C                     THEY ARE DEFINED BY USER'S SUBROUTINE CNSTRN.    INST 460
C         10-12  ILSQ, LEAST SQUARES INDICATOR.                        INST 465
C                 1 - FORCES PROGRAM TO USE LEAST SQUARES.             INST 470
C                 0 - ALLOWS PROGRAM TO SOLVE LINEARIZED               INST 475
C                     EQUATIONS WHEN VARIABLES ARE THE SAME AS THE     INST 480
C                     OBSERVATIONS. USE 0.                             INST 485
C         13-15  IWGT, THE WEIGHT INDICATOR.                           INST 490
C                 1 - A WEIGHT MATRIX IS USED FOR LEAST SQUARES.       INST 495
C                 0 - NO WEIGHTING IS USED. USE 0 INITIALLY.           INST 500
C         16-18  IPLM, THE PARAMETER LIMIT INDICATOR.                  INST 505
C                 0 - LIMITS PCMN, PCMX, ETC. ARE IGNORED.             INST 510
C                 1 - PARAMETER CHANGES WHICH EXCEED THESE LIMITS      INST 515
C                     ARE PREVENTED FOR MODE 0, 1, OR 4.               INST 520
C         19-21  IPRT, THE OUTPUT PRINT INDICATOR.                     INST 525
C                 0 - PROGRAM PRINTS ALL INTERMEDIATE RESULTS.         INST 530
C                 5 - PROGRAM PRINTS MINIMUM OUTPUT.                   INST 535
C                     USE 0 INITIALLY AND INCREASE IT LATER.           INST 540
C         22-24  NSTG, THE NUMBER OF STAGES PER CYCLE FOR MODE 3.      INST 545
C                     5 MAY BE SUITABLE. IGNORED FOR OTHER MODES.      INST 550
C         25-27  IBPC, COMMON PARAMETER BYPASS INDICATOR.              INST 555
C                 0 - COMMON PARAMETERS ARE READ FROM CARDS.           INST 560
C                 1 - USE COMMON PARAMETERS LEFT FROM PREVIOUS         INST 565
C                     CALCULATION. DO NOT CHANGE DYNAMIC DIMENSIONS    INST 570
C                     IN THIS CASE.                                    INST 575
C         28-36  ARE (FORMAT E9.0), ACCEPTABLE RATIO OF EIGENVALUES.   INST 580
C                 0.0001 MAY BE SATISFACTORY. FOR ILL-CONDITIONED      INST 585
C                     PROBLEMS THIS VALUE IS USED TO PREVENT BLOW-UP   INST 590
C                     BY HOLDING POORLY DETERMINED EIGENVECTORS        INST 595
C                     CONSTANT IN MODES 0, 1, OR 4.                    INST 600
C         37-45  SLIM (FORMAT E9.0), THE SCALING LIMIT.                INST 605
C                 0.000001 MAY BE SATISFACTORY. DIAGONAL ELEMENTS      INST 610
C                     SMALLER THAT SLIM ARE TREATED AS ZERO WHEN       INST 615
C                     NORMAL EQUATIONS ARE SCALED.                     INST 620
C                -1 - EQUATIONS NOT SCALED.                            INST 625
C         46-54  CMPR (FORMAT E9.0), A CONSTANT FOR MARQUARDT'S        INST 630
C                     COMPROMISE. THIS IS ADDED TO THE DIAGONAL        INST 635
C                     ELEMENTS OF THE SCALED MATRIX OF NORMAL          INST 640
C                     EQUATIONS (WHICH ARE OTHERWISE UNITY). THIS HAS  INST 645
C                     THE EFFECT OF DAMPING AN ILL-CONDITIONED PROBLEM INST 650
C                     BY ADDING CMPR TO EACH EIGENVALUE BEFORE ITS     INST 655
C                     RECIPROCAL IS TAKEN. THIS REDUCES THE            INST 660
C                     CONTRIBUTION OF EACH EIGENVECTOR, ESPECIALLY     INST 665
C                     THOSE WITH SMALL EIGENVALUES. RELEVANT ONLY IN   INST 670
C                     MODES 0, 1, OR 4.                                INST 675
C                 NON-ZERO VALUES UP TO 0.1 MAY PROVIDE SUITABLE       INST 680
C                     DAMPING.                                         INST 685
C                 0 - NO DAMPING IS APPLIED. IF IN DOUBT USE 0.        INST 690
C         55-63  XDRD, INITIAL VALUE OF XD FOR MODE 2.                 INST 695
C                 0.010 MAY BE SATISFACTORY.                           INST 700
C         64-72  EPSC, INITIAL CONSTANT FOR MODE 3.                    INST 705
C                 10.0 MAY BE SATISFACTORY.                            INST 710
C                                                                      INST 715
C     4) COMMON PARAMETER NAME CARD(S). NPC ENTRIES AT 8 PER CARD.     INST 720
C        OMIT IF NPC.EQ.0 OR IBPC.EQ.1.                                INST 725
C          COLS                                                        INST 730
C          1- 5  NOT USED.                                             INST 735
C          6- 9  NAMPC(1), ALPHANUMERIC NAME OF COMMON PARAMETER 1.    INST 740
C                     USED TO CLARIFY THE OUTPUT.                      INST 745
C         10-14  NOT USED.                                             INST 750
C         15-18  NAMPC(2)                                              INST 755
C           .       .                                                  INST 760
C           .       .                                                  INST 765
C          ETC.  NAMPC(NPC)                                            INST 770
C                                                                      INST 775
C     5) COMMON PARAMETER VALUE CARD(S). NPC ENTRIES AT 8 PER CARD.    INST 780
C        OMIT IF NPC.EQ.0 OR IBPC.EQ.1.                                INST 785
C          COLS                                                        INST 790
C          1- 9  PC(1), INITIAL VALUE OF COMMON PARAMETER 1.           INST 795
C         10-18  PC(2)                                                 INST 800
C           .       .                                                  INST 805
C           .       .                                                  INST 810
C          ETC.  PC(NPC)                                               INST 815
C                                                                      INST 820
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C      6) COMMON PARAMETER INCREMENT CARD(S). NPC ENTRIES AT 8 PER CARD.  INST 825
C         OMIT IF NPC.EQ.0 OR IBPC.EQ.1.                                  INST 830
C          COLS                                                           INST 835
C           1- 9  DPC(1). AN INCREMENT TO BE ADDED TO OR SUBTRACTED FROM  INST 840
C                        PC(1) IN CALCULATING NUMERICAL DERIVATIVES.      INST 845
C                    0.001 MAY BE SATISFACTORY.                           INST 850
C         10-18  DPC(2)                                                   INST 855
C           .       .                                                     INST 860
C           .       .                                                     INST 865
C          ETC.   DPC(NPC)                                                INST 870
C                                                                         INST 875
C      7) COMMON PARAMETER MINIMUM CARD(S). NPC ENTRIES AT 8 PER CARD.    INST 880
C   *     OMIT IF NPC.EQ.0, IBPC.EQ.1, OR IPLM.EQ.0.                      INST 885
C          COLS                                                           INST 890
C           1- 9  PCMN(1). ALGEERAIC MINIMUM ALLOWED VALUE FOR PC(1).     INST 895
C         10-18  PCMN(2)                                                  INST 900
C           .       .                                                     INST 905
C           .       .                                                     INST 910
C          ETC.   PCMN(NPC)                                               INST 915
C                                                                         INST 920
C      8) COMMON PARAMETER MAXIMUM CARD(S). NPC ENTRIES AT 8 PER CARD.    INST 925
C   *     OMIT IF NPC.EQ.0, IBPC.EQ.1, OR IPLM.EQ.0.                      INST 930
C          COLS                                                           INST 935
C           1- 9  PCMX(1). MAXIMUM ALLOWED VALUE FOR PC(1).               INST 940
C         10-18  PCMX(2)                                                  INST 945
C           .       .                                                     INST 950
C           .       .                                                     INST 955
C          ETC.   PCMX(NPC)                                               INST 960
C                                                                         INST 965
C      9) COMMON PARAMETER DESCRIPTION. USED TO SPEED UP PROGRAM IN       INST 970
C         MODE 0 WHEN PC'S ARE BEING ADJUSTED. NPC ENTRIES AT 72 PER      INST 975
C         CARD. OMIT IF NPC.EQ.0 OR IBPC.EQ.1.                            INST 980
C          COL                                                            INST 985
C           1     KPC(1). DESCRIPTION OF PC(1).                           INST 990
C                    1 - INVOLVES ONLY Q OR PL.                           INST 995
C                    2 - INVOLVES ONLY AR, BR. OR PARAMETERS USED BY REPL.INST1000
C                    3 - USED ONLY BY CWX, GCWX, OR WCNF FOR              INST1005
C                        INTRAMOLECULAR ENERGY.                           INST1010
C                    0 - STRUCTURE PARAMETER OR OTHER TYPE.               INST1015
C                        IF IN DOUBT USE 0.                               INST1020
C           2     KPC(2)                                                  INST1025
C           .       .                                                     INST1030
C           .       .                                                     INST1035
C          ETC.   KPC(NPC)                                                INST1040
C                                                                         INST1045
C     10) VARIABLE SELECTION CARD(S) FOR COMMON PARAMETERS. NPC ENTRIES   INST1050
C         AT 72 PER CARD. OMIT IF NPC.EQ.0. IF NC.EQ.0 OR MODE.NE.0       INST1055
C         (AND NPC.NE.0) THESE CARDS ARE IRRELEVANT BUT MUST BE INCLUDED.INST1060
C          COL                                                            INST1065
C           1     KQC(1). REFINEMENT INDICATOR FOR PC(1).                 INST1070
C                    0 - PC(1) IS NOT VARIED IN MODE 0.                   INST1075
C               1 TO 9 - PC(1) IS VARIED IN MODE 0 WITH DAMPING SELECTED  INST1080
C                        AS DESCRIBED IN (30) BELOW.                      INST1085
C           2     KQC(2)                                                  INST1090
C           .       .                                                     INST1095
C           .       .                                                     INST1100
C          ETC.   KQC(NPC)                                                INST1105
C                                                                         INST1110
C     ------------------------------------------------------------------INST1115
C     A COMPLETE SET OF DATA CARDS (11) TO (33) IS PROVIDED FOR EACH      INST1120
C     SUBSTANCE TO BE INCLUDED IN THE JOB.                                INST1125
C     ------------------------------------------------------------------INST1130
C                                                                         INST1135
C     11) SUBSTANCE IDENTIFICATION CARD.                                  INST1140
C          COLS                                                           INST1145
C           1- 3  ISB. SUBSTANCE IDENTIFICATION. MUST BE NON-ZERO.        INST1150
C                        MAY BE TESTED BY USER SUBROUTINES.               INST1155
C           4-71  STITLE. THE SUBSTANCE NAME.                             INST1160
C                                                                         INST1165
C     12) CONTROL CARD FOR THIS SUBSTANCE.                                INST1170
C          COLS                                                           INST1175
C           1- 3  NA. NUMBER OF ATOMS IN ASYMMETRIC UNIT (INCLUDING EXTRA INST1180
C                        ATOMS). MODIFIED BY PROGRAM IF IRSC.GT.1.        INST1185
C           4- 6  NKA. NUMBER OF CHEMICAL KINDS OF ATOMS.                 INST1190
C           7- 9  NS. NUMBER OF SYMMETRY CARDS. THIS IS THE NUMBER OF     INST1195
C                        EQUIPOINTS IN THE CELL INCLUDING THE IDENTITY    INST1200
C                        X, Y, Z (EVEN IF THE STRUCTURE IS CENTERED       INST1205
C                        OR CENTROSYMMETRIC).                             INST1210
C          10-12  ICENT. SYMMETRY INDICATOR FOR RECIPROCAL LATTICE SUMS   INST1215
C                    1 - THERE IS A CENTER OF INVERSION AT THE ORIGIN.    INST1220
C                        AND THIS CENTER RELATES THE FIRST NS/2 SYMMETRY  INST1225
C                        CARDS TO THE NS/2 LATER ONES.                    INST1230
C                    2 - STRUCTURE IS NON-CENTROSYMMETRIC OR SYMMETRY     INST1235
C                        CARDS ARE NOT IN SEQUENCE SPECIFIED ABOVE.       INST1240
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C          13-15  HXNEG, NEGATIVE INDEX INDICATOR FOR H. SEE BELOW.          INST1245
C          16-18  HYNEG, NEGATIVE INDEX INDICATOR FOR K. SEE BELOW.          INST1250
C          19-21  HZNEG, NEGATIVE INDEX INDICATOR FOR L.                     INST1255
C                    0 - OMIT NEGATIVE INDICES FROM RECIPROCAL LATTICE.      INST1260
C                    1 - INCLUDE NEGATIVE INDICES.                           INST1265
C                 OVERALL INSTRUCTIONS FOR HXNEG, HYNEG, AND HZNEG -         INST1270
C                    USE 0, 0, 0 FOR ORTHORHOMBIC, CUBIC, AND TETRAGONAL     INST1275
C                        SPACE GROUPS WITH LAUE GROUP 4/MMM.                 INST1280
C                    USE 1, 0, 0 FOR MONOCLINIC, HEXAGONAL, AND TETRAGONAL INST1285
C                        SPACE GROUPS WITH LAUE GROUP 4/M.                   INST1290
C                    USE 1, 1, 0 FOR TRICLINIC, TRIGONAL, OR RHOMBOHEDRAL    INST1295
C                        SPACE GROUPS. IF IN DOUBT USE 1, 1, 0.              INST1300
C          22-24  NRB, THE NUMBER OF RIGID BODIES IN THE ASYMMETRIC UNIT.    INST1305
C                        EACH ATOM OR GROUP WHICH TRANSLATES OR ROTATES      INST1310
C                        INDEPENDENTLY IS A RIGID BODY. (IF IRSC.GT.1        INST1315
C                        THEN NRB IS THE NUMBER OF RIGID BODIES IN THE       INST1320
C                        EXPANDED ASYMMETRIC UNIT.)                          INST1325
C          25-27  NPX, THE NUMBER OF EXTRA PARAMETERS FOR THIS SUBSTANCE.    INST1330
C                        THEY ARE DEFINED BY THE USER'S SUBROUTINE CNSTRN. INST1335
C          28-30  NRP, THE DISTANCE PRINT COUNTER. THE 10*NRP SHORTEST       INST1340
C                        DISTANCES ARE PRINTED. SET NRP NEGATIVE TO OMIT     INST1345
C                        BONDED CONTACTS FROM THE LIST.                      INST1350
C          31-33  ICMB, THE COULOMB ENERGY INDICATOR.                        INST1355
C                    0 - COULOMB ENERGY WILL NOT BE CALCULATED.              INST1360
C                    1 - COULOMB ENERGY WILL BE CALCULATED.                  INST1365
C          34-36  IVDW, THE VAN DER WAALS ENERGY INDICATOR.                  INST1370
C                    0 - VAN DER WAALS ENERGY WILL NOT BE CALCULATED.        INST1375
C                    1 - VAN DER WAALS ENERGY WILL BE CALCULATED.            INST1380
C     *    37-39  IREP, THE REPULSION ENERGY INDICATOR. REPULSION (OR        INST1385
C                        ATTRACTION) CAN BE CALCULATED IN STANDARD WAY,      INST1390
C                        BY USER'S ROUTINE REPL, AND/OR BY USER'S            INST1395
C                        ROUTINE GPOT, INCLUDE TERMS FROM -                  INST1400
C                          GPOT     REPL   STANDARD                          INST1405
C                    0 -    NO       NO       NO                             INST1410
C                    1 -    NO       NO       YES                            INST1415
C                    2 -    NO       YES      NO                             INST1420
C                    3 -    NO       YES      YES                            INST1425
C                    4 -    YES      NO       NO                             INST1430
C                    5 -    YES      NO       YES                            INST1435
C                    6 -    YES      YES      NO                             INST1440
C                    7 -    YES      YES      YES                            INST1445
C          40-42  IMOL, THE ISOLATED MOLECULE INDICATOR.                     INST1450
C                    0 - THE CALCULATION IS FOR A CRYSTAL.                   INST1455
C                    1 - THE CALCULATION IS FOR AN ISOLATED MOLECULE.        INST1460
C          43-45  NCT, THE NUMBER OF CARDS IN THE ATOM CONNECTION TABLE.     INST1465
C                        IF BOND DISTANCE, BOND ANGLE, OR CONFORMATION       INST1470
C                        ENERGY IS TO BE INCLUDED FOR A FLEXIBLE MOLECULE    INST1475
C                        THEN NCT IS THE NUMBER OF ATOMS BONDED TO MORE      INST1480
C                        THAN ONE OTHER ATOM. OTHERWISE NCT = 0.             INST1485
C          46-48  IRSC, INDICATOR FOR RELAXING SYMMETRY CONSTRAINTS.         INST1490
C                    0 OR 1 - NO RELAXATION PERFORMED. THIS IS THE           INST1495
C                        USUAL SITUATION.                                    INST1500
C                    FOR IRSC.GT.1 THE ATOM LIST WILL BE EXPANDED TO         INST1505
C                        INCLUDE ATOMS GENERATED BY THE FIRST IRSC           INST1510
C                        SYMMETRY CARDS. THESE WILL CONSTITUTE THE           INST1515
C                        REVISED ASYMMETRIC UNIT. BE SURE TO INCREASE NRB    INST1520
C                        AND ADD NEW RIGID-BODY IDENTIFIERS AND RIGID-       INST1525
C                        BODY CARDS. ALSO INCREASE NAMAX, NRBMAX, NPSMAX,    INST1530
C                        AND NPMAX, AND MODIFY SUBROUTINE REJECT.            INST1535
C          49-51  IZAM, INTEGER TO CONTROL SIZE OF FORMULA UNIT FOR WHICH    INST1540
C                        THE ENERGY IS CALCULATED.                           INST1545
C                    0 - THE PROGRAM SELECTS THE SMALLEST UNIT WHICH         INST1550
C                        CONTAINS AN INTEGRAL NUMBER OF EACH ATOM. THIS      INST1555
C                        IS ALWAYS SATISFACTORY IF NO CONFORMATION ENERGY    INST1560
C                        IS INCLUDED.                                        INST1565
C                    FOR IZAM.NE.0 IT SPECIFIES THE NUMBER OF TIMES          INST1570
C                        ATOM 1 OF THE ATOM LIST IS TO APPEAR IN THE         INST1575
C                        FORMULA UNIT.                                       INST1580
C     *    52-54  IGEM, INDICATOR FOR GEMINAL ATOMS (I.E. 1-3 ATOMS).        INST1585
C                    0 - INCLUDE NON-BONDED INTERACTION BETWEEN 1-3 ATOMS. INST1590
C                    1 - OMIT NON-BONDED INTERACTION BETWEEN 1-3 ATOMS.      INST1595
C                        IRRELEVANT IF NCT.EQ.0.                             INST1600
C     *    55-57  IRBA, INDICATOR FOR KIND OF RIGID BODIES.                  INST1605
C                    0 - RIGID BODIES MAY BE POLYATOMIC WITH ROTATION AND    INST1610
C                        TRANSLATION PERMITTED.                              INST1615
C                    1 - ONLY TRANSLATION IS PERMITTED. USUALLY USED         INST1620
C                        FOR SINGLE ATOMS.                                   INST1625
C     *    58-60  ISETA, LATTICE PARAMETER CONSTRAINT INDICATOR              INST1630
C                    0 - LATTICE IS TRICLINIC, MONOCLINIC, OR                INST1635
C                          ORTHORHOMBIC. NO CONSTRAINTS ARE APPLIED.         INST1640
C                          IF LATTICE PARAMETERS ARE NOT TREATED AS          INST1645
C                          VARIABLES OR OBSERVATIONS THEN ISETA=0 IS         INST1650
C                          ALL RIGHT FOR ANY SYMMETRY.                       INST1655
C                    1 - LATTICE IS TETRAGONAL OR HEXAGONAL. B IS            INST1660
C                          CONSTRAINED TO EQUAL A.                           INST1665
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C                 2 - LATTICE IS CUBIC. B AND C ARE CONSTRAINED          INST1670
C                       TO EQUAL A.                                      INST1675
C                 3 - LATTICE IS RHOMBOHEDRAL. B AND C ARE               INST1680
C                       CONSTRAINED TO EQUAL A, AND BETA AND GAMMA       INST1685
C                       ARE CONSTRAINED TO EQUAL ALPHA.                  INST1690
C                                                                        INST1695
C    13) CONVERGENCE CONTROL CARD.                                       INST1700
C         COLS                                                           INST1705
C          1- 9  CK, CONVERGENCE CONSTANT FOR EWALD METHOD. THIS AFFECTS INST1710
C                     THE RATE OF CONVERGENCE BUT NOT THE FINAL RESULT.  INST1715
C                 0.25 IS A SATISFACTORY INITIAL VALUE. THE PROGRAM      INST1720
C                     WILL RECOMMEND AN IMPROVED VALUE.                  INST1725
C                 0 - CAUSES RECIPROCAL LATTICE SUM TO BE BYPASSED.      INST1730
C                     IRRELEVANT IF ICMB.EQ.0 AND IVDW.EQ.0.             INST1735
C                     IF IMOL.EQ.1 THE PROGRAM SETS CK = 0.              INST1740
C        10-12  NQ, NUMBER OF LIMITS FOR RECIPROCAL SUM. 1.LE.NQ.LE.5.   INST1745
C                 2 IS SATISFACTORY.                                     INST1750
C        13-15  NR, NUMBER OF LIMITS FOR DIRECT SUM. 1.LE.NR.LE.5.       INST1755
C                 2 IS SATISFACTORY.                                     INST1760
C                                                                        INST1765
C    14) RECIPROCAL LATTICE SUM LIMITS. (INCLUDE A BLANK CARD IF BOTH    INST1770
C        ICMB.EQ.0 AND IVDW.EQ.0.)                                       INST1775
C         COLS                                                           INST1780
C          1- 9  QLIM(1), THE LIMIT OF THE FIRST SHELL IN RECIPROCAL     INST1785
C                     ANGSTROM UNITS.                                    INST1790
C                 0.5 MAY BE SATISFACTORY. THE PROGRAM WILL RECOMMEND    INST1795
C                     IMPROVED VALUES.                                   INST1800
C        10-18  QLIM(2)                                                  INST1805
C                 0.6 MAY BE SATISFACTORY.                               INST1810
C          .       .                                                     INST1815
C          .       .                                                     INST1820
C         ETC.  QLIM(NQ)                                                 INST1825
C                                                                        INST1830
C    15) DIRECT LATTICE SUM LIMITS.                                      INST1835
C         COLS                                                           INST1840
C          1- 9  RLIM(1), THE LIMIT OF THE FIRST SHELL IN ANGSTROM UNITS.INST1845
C                 5.0 MAY BE SATISFACTORY. THE PROGRAM WILL RECOMMEND    INST1850
C                     IMPROVED VALUES.                                   INST1855
C        10-18  RLIM(2)                                                  INST1860
C                 6.0 MAY BE SATISFACTORY.                               INST1865
C          .       .                                                     INST1870
C          .       .                                                     INST1875
C         ETC.  RLIM(NR)                                                 INST1880
C                                                                        INST1885
C    16) LATTICE PARAMETERS.                                             INST1890
C         COLS                                                           INST1895
C          1- 9  A(1), CELL PARAMETER A, ANGSTROMS.                      INST1900
C        10-18  A(2), CELL PARAMETER B, ANGSTROMS.                       INST1905
C        19-27  A(3), CELL PARAMETER C, ANGSTROMS.                       INST1910
C        28-36  A(4), COSINE ALPHA.                                      INST1915
C        37-45  A(5), COSINE BETA.                                       INST1920
C        46-54  A(6), COSINE GAMMA.                                      INST1925
C                                                                        INST1930
C    17) STANDARD ERRORS OF LATTICE PARAMETERS USED TO WEIGHT            INST1935
C   *    OBSERVATIONS. OMIT IF IWGT.EQ.0.                                INST1940
C         COLS                                                           INST1945
C          1- 9  SA(1), STANDARD ERROR OF A, ANGSTROMS.                  INST1950
C        10-18  SA(2), STANDARD ERROR OF B, ANGSTROMS.                   INST1955
C        19-27  SA(3), STANDARD ERROR OF C, ANGSTROMS.                   INST1960
C        28-36  SA(4), STANDARD ERROR OF COSINE ALPHA.                   INST1965
C        37-45  SA(5), STANDARD ERROR OF COSINE BETA.                    INST1970
C        46-54  SA(6), STANDARD ERROR OF COSINE GAMMA.                   INST1975
C                                                                        INST1980
C    18) SYMMETRY INFORMATION. NS CARDS, ONE FOR EACH EQUIVALENT         INST1985
C        POSITION NEEDED TO GENERATE ALL THE ATOMS IN THE CELL.          INST1990
C        THE BASIC POSITION X, Y, Z SHOULD BE INCLUDED, USUALLY FIRST.   INST1995
C        ATOMS IN SPECIAL POSITIONS ARE AUTOMATICALLY TREATED BY NOT     INST2000
C        PLACING MORE THAN ONE ATOM OF THE SAME CHEMICAL KIND ON A SITE. INST2005
C                                                                        INST2010
C        IF ICENT.EQ.1 INDICATING A CENTER OF SYMMETRY AT THE ORIGIN     INST2015
C        THEN THE FIRST NS/2 CARDS MUST REPRESENT POSITIONS NOT RELATED  INST2020
C        BY THIS CENTER.                                                 INST2025
C                                                                        INST2030
C        IF IRSC.GT.1 THE SEQUENCE OF SYMMETRY CARDS MUST BE CHOSEN      INST2035
C        SO THAT THE FIRST IRSC CARDS GENERATE THE REVISED ASYMMETRIC    INST2040
C        UNIT. IN THIS CASE IT MAY NOT BE POSSIBLE TO SET ICENT=1.       INST2045
C        FURTHERMORE, THE TRANSLATIONAL PARTS OF THE SYMMETRY OPERATIONS INST2050
C        MUST BE CHOSEN SO THAT GROUPS TO BE COMBINED AS ONE RIGID BODY  INST2055
C        ARE ADJACENT TO ONE ANOTHER.                                    INST2060
C                                                                        INST2065
C        IN MODE 4 THE SYMMETRY CARDS ARE USED TO ANALYZE THE SYMMETRY   INST2070
C        OF THE NORMAL VIBRATIONS. FOR THESE CALCULATIONS IT MAY BE      INST2075
C        DESIRABLE TO ADD REDUNDANT SYMMETRY CARDS, THAT IS CARDS        INST2080
C        WHICH REPEAT SYMMETRY ALREADY PRESENT IN THE ATOM LIST.         INST2085
C        ENOUGH CARDS MUST BE ADDED SO THAT THE SYMMETRY OPERATIONS      INST2090
C        STILL FORM A GROUP.                                             INST2095
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C                                                                       INST2100
C         COLS                                                          INST2105
C         1- 4   NAMS(J), ALPHANUMERIC SYMBOL FOR SYMMETRY OPERATION J. INST2110
C                     USED TO CLARIFY THE OUTPUT IN MODE 4. OPTIONAL.   INST2115
C         5-15   SYM( 1,J), TRANSLATIONAL PART OF X', THE TRANSFORMED   INST2120
C                     X COORDINATE.                                     INST2125
C        16-18   SYM( 2,J), COEFFICIENT OF X IN X'                      INST2130
C        19-21   SYM( 3,J), COEFFICIENT OF Y IN X'                      INST2135
C        22-24   SYM( 4,J), COEFFICIENT OF Z IN X'                      INST2140
C        25-39   SYM( 5,J), TRANSLATIONAL PART OF Y'                    INST2145
C        40-42   SYM( 6,J), COEFFICIENT OF X IN Y'                      INST2150
C        43-45   SYM( 7,J), COEFFICIENT OF Y IN Y'                      INST2155
C        46-48   SYM( 8,J), COEFFICIENT OF Z IN Y'                      INST2160
C        49-63   SYM( 9,J), TRANSLATIONAL PART OF Z'                    INST2165
C        64-66   SYM(10,J), COEFFICIENT OF X IN Z'                      INST2170
C        67-69   SYM(11,J), COEFFICIENT OF Y IN Z'                      INST2175
C        70-72   SYM(12,J), COEFFICIENT OF Z IN Z'                      INST2180
C                                                                       INST2185
C        FOR EXAMPLE, EQUIPOINT -X, Y-X, 2/3-Z, WHICH DESCRIBES A       INST2190
C        TWO-FOLD AXIS, COULD BE PUNCHED AS:                            INST2195
C  2          0 -1  0  0                0 -1  1  0       0.6666667  0  0 -1INST2200
C                                                                       INST2205
C    19) PARAMETERS FOR EACH CHEMICAL KIND OF ATOM, NKA CARDS.          INST2210
C                                                                       INST2215
C        THE NON-BONDED INTERACTION ENERGY IN KCAL/MOLE BETWEEN ATOMS   INST2220
C        OF KIND K AND KIND L SEPARATED BY R ANGSTROMS IS USUALLY       INST2225
C        CALCULATED AS                                                  INST2230
C                                                                       INST2235
C        332.17*Q(K)*Q(L)/R                                   (COULOMB) INST2240
C        -PL(K)*PL(L)/R**6                                (VAN DER WAALS) INST2245
C        +(BR(K)+BR(L))*EXP((AR(K)+AR(L)-R)/(BR(K)+BR(L)))  (REPULSION)  INST2250
C                                                                       INST2255
C        ALTERNATIVELY, THE REPULSION MAY BE CALCULATED BY USER'S       INST2260
C        SUBROUTINES REPL OR GPOT.                                      INST2265
C                                                                       INST2270
C         COLS                                                          INST2275
C         1- 4   NAMK(K), ALPHANUMERIC NAME OF ATOM KIND K.             INST2280
C         5- 9   NOT USED.                                              INST2285
C        10-18   Q(K), CHARGE ON ATOM OF KIND K IN UNITS OF PROTONS.    INST2290
C                     MAY BE LEFT BLANK AND SET BY SUBROUTINE CNSTRN.   INST2295
C                     IRRELEVANT IF ICMB.EQ.0.                          INST2300
C        19-27   PL(K), COEFFICIENT OF ATOM OF KIND K IN VAN DER WAALS  INST2305
C                     ENERGY. MAY BE LEFT BLANK AND SET BY SUBROUTINE   INST2310
C                     CNSTRN. IRRELEVANT IF IVDW.EQ.0.                  INST2315
C        28-36   AR(K), RADIUS OF ATOM FOR REPULSION ENERGY TERM.       INST2320
C                     MAY BE LEFT BLANK AND SET BY SUBROUTINE CNSTRN.   INST2325
C        37-45   BR(K), SOFTNESS COEFFICIENT IN THE REPULSION ENERGY.   INST2330
C                     MAY BE LEFT BLANK AND SET BY SUBROUTINE CNSTRN.   INST2335
C        46-54   AMASS(K), MASS OF ATOM OF KIND K IN PHYSICAL ATOMIC    INST2340
C                     WEIGHT UNITS. IRRELEVANT UNLESS MODE.EQ.4.        INST2345
C                                                                       INST2350
C    20) ATOM COORDINATE CARDS, NA CARDS, ONE FOR EACH ATOM IN THE      INST2355
C        ASYMMETRIC UNIT (INCLUDING ANY EXTRA ATOMS NEEDED TO DEFINE    INST2360
C        THE ORIGINS AND COORDINATE SYSTEMS FOR THE RIGID BODIES).      INST2365
C                                                                       INST2370
C         COLS                                                          INST2375
C         1- 4   NAME(J), ALPHANUMERIC NAME OF ATOM J. USED TO CLARIFY  INST2380
C                   THE OUTPUT.                                         INST2385
C         5- 9   IKA(J), AN INTEGER WHICH SPECIFIES THE CHEMICAL KIND   INST2390
C                   OF ATOM J. 0.LE.IKA(J).LE.NKA. IF IKA(J).EQ.0 THEN  INST2395
C                   THEN THIS IS AN EXTRA ATOM WHICH WILL BE OMITTED    INST2400
C                   FROM ALL ENERGY CALCULATIONS.                       INST2405
C        10-27   NOT USED.                                              INST2410
C        28-36   XYZ(1,J), ATOMIC COORDINATE X                          INST2415
C        37-45   XYZ(2,J), ATOMIC COORDINATE Y                          INST2420
C        46-54   XYZ(3,J), ATOMIC COORDINATE Z                          INST2425
C                   THESE ARE EXPRESSED AS FRACTIONS OF THE LATTICE     INST2430
C                   TRANSLATIONS. THEY MUST BE INCLUDED EVEN IF THEY ARE INST2435
C                   SET BY SUBROUTINE CNSTRN. BECAUSE THE PROGRAM USES  INST2440
C                   THEM TO GENERATE THE ATOMS IN ONE UNIT CELL AND TO  INST2445
C                   ESTABLISH WHICH ATOMS ARE IN SPECIAL POSITIONS.     INST2450
C                                                                       INST2455
C    21) ATOM RIGID-BODY IDENTIFIERS, NA ENTRIES AT 24 PER CARD.        INST2460
C        (IF IRSC.GT.1 THEN NA IS THE NUMBER OF ATOMS IN THE EXPANDED   INST2465
C        LIST.)                                                         INST2470
C                                                                       INST2475
C         COLS                                                          INST2480
C         1- 3   IRB(1), AN INTEGER WHICH SPECIFIES THE RIGID BODY TO   INST2485
C                   WHICH ATOM 1 BELONGS. 0.LE.IRB(J).LE.NRB. IF        INST2490
C                   IRB(J).EQ.0 THEN ATOM J BELONGS TO NO RIGID BODY    INST2495
C                   AND MUST REMAIN FIXED IN ITS INPUT POSITION.        INST2500
C         4- 6   IRB(2)                                                 INST2505
C         7- 9   IRB(3)                                                 INST2510
C          .       .                                                    INST2515
C          .       .                                                    INST2520
C         ETC.   IRB(NA)                                                INST2525
C                                                                       INST2530
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C     22) RIGID-BODY CARDS. NRB CARDS ARE INCLUDED.                      INST2535
C                                                                        INST2540
C         WHEN THE STRUCTURE IS ADJUSTED TO MINIMIZE THE ENERGY IT IS    INST2545
C         THE RIGID BODY ROTATIONS AND TRANSLATIONS WHICH ARE THE        INST2550
C         VARIABLES. NOT THE ATOM COORDINATES THEMSELVES. THE DISPLACED  INST2555
C         ATOM COORDINATES ARE GENERATED FROM THE INPUT COORDINATES BY   INST2560
C         APPLYING THE NRB RIGID BODY OPERATIONS IN THEIR INPUT SEQUENCE.INST2565
C         RIGID BODY COORDINATE AXES MAY BE REFERRED EITHER TO THE       INST2570
C         CRYSTAL AXES OR TO SPECIFIED ATOMS. SUCH ATOMS MAY EITHER BE   INST2575
C         IN THEIR INPUT POSITIONS OR IN POSITIONS GENERATED BY A        INST2580
C         PREVIOUS RIGID BODY OPERATION.                                 INST2585
C                                                                        INST2590
C         A SEGMENTED MOLECULE MAY BE DEFINED BY REFERRING THE FIRST     INST2595
C         RIGID BODY AXES TO THE CRYSTAL AXES OR TO INPUT ATOMS. THE     INST2600
C         SECOND RIGID BODY AXES MAY THEN BE DEFINED IN TERMS OF ATOMS   INST2605
C         OF THE FIRST, THE THIRD IN TERMS OF THE SECOND, ETC. BY        INST2610
C         CHOOSING THESE AXES PROPERLY, INTERATOMIC DISTANCES CAN BE     INST2615
C         FIXED AND ROTATIONS CAN BE CONSTRAINED TO BE ABOUT SPECIFIED   INST2620
C         BONDS.                                                         INST2625
C                                                                        INST2630
C         AT THE END OF EACH JOB NEW ATOMIC COORDINATES ARE PRINTED      INST2635
C         AND PUNCHED. THESE CAN BE USED AS INPUT TO THE SUBSEQUENT JOB  INST2640
C         SO THAT THE INPUT VALUES OF THE RIGID BODY ROTATIONS AND       INST2645
C         TRANSLATIONS ARE USUALLY ZERO.                                 INST2650
C                                                                        INST2655
C          COLS                                                          INST2660
C          1- 3   IZ(L), THE NUMBER OF THE ATOM (OR EXTRA ATOM) WHICH    INST2665
C                        SERVES AS THE CENTER OF ROTATION OF RIGID BODY L.INST2670
C                        FOR SINGLE ATOMS USE THE NUMBER OF THAT ATOM.   INST2675
C          4- 6   IU(L)                                                  INST2680
C          7- 9   IV(L)                                                  INST2685
C         10-12   IW(L)                                                  INST2690
C                                                                        INST2695
C                    THESE ARE THE NUMBERS OF THREE ATOMS WHICH DEFINE   INST2700
C                    THE CARTESIAN AXES OF ROTATION AND TRANSLATION FOR  INST2705
C                    RIGID BODY L.                                       INST2710
C                                                                        INST2715
C                    IF IU(L).EQ.0 THEN IV(L) AND IW(L) ARE IRRELEVANT   INST2720
C                    AND THE AXES ARE BASED ON THE CRYSTAL AXES.         INST2725
C                    X IS PARALLEL TO A, Y LIES IN THE A,B PLANE. AND    INST2730
C                    Z IS PERPENDICULAR TO THE A,B PLANE.                INST2735
C                                                                        INST2740
C                    IF IU(L).NE.0 THEN X POINTS  FROM ATOM IU(L) TOWARD INST2745
C                    ATOM IV(L), Y LIES IN THE PLANE OF THE THREE ATOMS  INST2750
C                    ON THE SIDE TOWARD IW(L), AND Z IS PERPENDICULAR    INST2755
C                    TO THE PLANE OF THE THREE ATOMS MAKING A RIGHT      INST2760
C                    HANDED COORDINATE SYSTEM.                           INST2765
C                                                                        INST2770
C  *                 FOR A DIATOMIC OR LINEAR MOLECULE NOT PARALLEL TO   INST2775
C                    THE A-AXIS SET IW(L)=0. THEN X POINTS FROM ATOM     INST2780
C                    IU(L) TOWARD ATOM IV(L), Y LIES IN THE PLANE OF X   INST2785
C                    AND THE CRYSTAL A-AXIS. AND Z IS PERPENDICULAR TO   INST2790
C                    X AND Y MAKING A RIGHT-HANDED COORDINATE SYSTEM.    INST2795
C                                                                        INST2800
C         13-18   NOT USED.                                              INST2805
C         19-27   SSR(L), THE ESTIMATED STANDARD ERROR IN RADIANS FOR THE INST2810
C                        ORIENTATION ANGLES OF RIGID BODY L.             INST2815
C                        IRRELEVANT IF IWGT.EQ.0.                        INST2820
C         28-36   STR(L), THE ESTIMATED STANDARD ERROR OF THE            INST2825
C                        TRANSLATIONAL POSITION OF RIGID RIGID BODY L IN INST2830
C                        ANGSTROM UNITS. IRRELEVANT IF IWGT.EQ.0.        INST2835
C         37-42   SXR(L), INITIAL VALUE OF ROTATION ABOUT X IN RADIANS.  INST2840
C                        USUALLY ZERO. IRRELEVANT IF IRBA.EQ.1.          INST2845
C         43-48   SYR(L), INITIAL VALUE OF ROTATION ABOUT Y IN RADIANS.  INST2850
C                        USUALLY ZERO. IRRELEVANT IF IRBA.EQ.1.          INST2855
C         49-54   SZR(L), INITIAL VALUE OF ROTATION ABOUT Z IN RADIANS.  INST2860
C                        USUALLY ZERO. IRRELEVANT IF IRBA.EQ.1.          INST2865
C         55-60   TR(1,L), INITIAL VALUE OF X TRANSLATION IN ANGSTROMS.  INST2870
C                        USUALLY ZERO.                                   INST2875
C         61-66   TR(2,L), INITIAL VALUE OF Y TRANSLATION IN ANGSTROMS.  INST2880
C                        USUALLY ZERO.                                   INST2885
C         67-72   TR(3,L), INITIAL VALUE OF Z TRANSLATION IN ANGSTROMS.  INST2890
C                        USUALLY ZERO.                                   INST2895
C                                                                        INST2900
C     23) CONNECTION TABLE FOR THE CALCULATION OF BOND-DISTANCE, BOND-   INST2905
C         ANGLE, AND CONFORMATION-ANGLE CONTRIBUTIONS TO THE ENERGY.     INST2910
C         INCLUDE NCT CARDS WHERE NCT IS THE NUMBER OF 'BACKBONE' ATOMS. INST2915
C         THAT IS THE NUMBER OF ATOMS BONDED TO MORE THAN ONE OTHER ATOM.INST2920
C         OMIT IF NCT.EQ.0.                                              INST2925
C                                                                        INST2930
C          COLS                                                          INST2935
C          1- 3   IACT(J), THE IDENTIFICATION NUMBER OF A BACKBONE ATOM. INST2940
C                        THIS IS THE NUMBER OF THE ATOM IN ARRAYS XC, ETC.INST2945
C          4- 6   NOT USED.                                              INST2950
C          7- 9   ICT(1,J), NUMBER OF AN ATOM BONDED TO IACT(J).         INST2955
C         10-12   ICT(2,J), NUMBER OF AN ATOM BONDED TO IACT(J).         INST2960
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C        13-15  ICT(3,J), NUMBER OF AN ATOM BONDED TO IACT(J).          INST2965
C        16-18  ICT(4,J), NUMBER OF AN ATOM BONDED TO IACT(J).          INST2970
C                  IF THERE ARE LESS THAN 4 ATOMS BONDED TO IACT(J)     INST2975
C                  FILL OUT THE LIST WITH ZEROS AT THE END.             INST2980
C        19-21  NOT USED.                                               INST2985
C        22-24  IDZ(1,J), DEFINITION OF POTENTIAL FOR BOND              INST2990
C                  BETWEEN ATOMS IACT(J) AND ICT(1,J).                  INST2995
C        25-27  IDZ(2,J), DEFINITION OF POTENTIAL FOR BOND              INST3000
C                  BETWEEN ATOMS IACT(J) AND ICT(2,J).                  INST3005
C        28-30  IDZ(3,J), DEFINITION OF POTENTIAL FOR BOND              INST3010
C                  BETWEEN ATOMS IACT(J) AND ICT(3,J).                  INST3015
C        31-33  IDZ(4,J), DEFINITION OF POTENTIAL FOR BOND              INST3020
C                  BETWEEN ATOMS IACT(J) AND ICT(4,J).                  INST3025
C                                                                       INST3030
C                  THESE SPECIFY THE NUMBERS OF COMMON PARAMETERS PC    INST3035
C                  USED TO CALCULATE THE BOND ENERGY. THE COMMON        INST3040
C                  PARAMETERS ARE ASSUMED TO BE IN PAIRS CONSISTING OF  INST3045
C                  A DISTANCE (ANGSTROMS) FOLLOWED BY A FORCE CONSTANT. INST3050
C                  THE BOND ENERGY (KCAL/MOLE) IS GIVEN BY:             INST3055
C                                                                       INST3060
C                  WD=50.0*PC(IDZ(I,J)+1)*(DIJ-PC(IDZ(I,J)))**2         INST3065
C                                                                       INST3070
C                  NOTE THAT WD INCLUDES A SCALE FACTOR OF 100.         INST3075
C                                                                       INST3080
C                  IF IDZ(I,J).EQ.0 THEN WD=0.                          INST3085
C                                                                       INST3090
C        34-36  NOT USED.                                               INST3095
C        37-39  IAZ(1,J), DEFINITION OF POTENTIAL FOR ANGLE             INST3100
C                  ICT(1,J) - IACT(J) - ICT(2,J).                       INST3105
C        40-42  IAZ(2,J), DEFINITION OF POTENTIAL FOR ANGLE             INST3110
C                  ICT(1,J) - IACT(J) - ICT(3,J).                       INST3115
C        43-45  IAZ(3,J), DEFINITION OF POTENTIAL FOR ANGLE             INST3120
C                  ICT(1,J) - IACT(J) - ICT(4,J).                       INST3125
C        46-48  IAZ(4,J), DEFINITION OF POTENTIAL FOR ANGLE             INST3130
C                  ICT(2,J) - IACT(J) - ICT(3,J).                       INST3135
C        49-51  IAZ(5,J), DEFINITION OF POTENTIAL FOR ANGLE             INST3140
C                  ICT(2,J) - IACT(J) - ICT(4,J).                       INST3145
C        52-54  IAZ(6,J), DEFINITION OF POTENTIAL FOR ANGLE             INST3150
C                  ICT(3,J) - IACT(J) - ICT(4,J).                       INST3155
C                                                                       INST3160
C                  THESE SPECIFY THE NUMBERS OF COMMON PARAMETERS PC    INST3165
C                  USED TO CALCULATE ANGLE BENDING ENERGY. THE COMMON   INST3170
C                  PARAMETERS ARE ASSUMED TO BE IN PAIRS CONSISTING OF  INST3175
C                  AN ANGLE (DEGREES) FOLLOWED BY A FORCE CONSTANT.     INST3180
C                  THE BENDING ENERGY (KCAL/MOLE) IS GIVEN BY:          INST3185
C                                                                       INST3190
C                  WA=0.5*PC(IAZ(I,J)+1)*(AIJK-PC(IAZ(I,J)))**2         INST3195
C                                                                       INST3200
C                  IF IAZ(I,J).EQ.0 THEN WA=0.                          INST3205
C                                                                       INST3210
C        55-57  NOT USED.                                               INST3215
C        58-60  ITBR(1,J), DEFINITION OF POTENTIAL FOR ALL TORSION      INST3220
C                  ANGLES ABOUT BOND IACT(J) - ICT(1,J).                INST3225
C        61-63  ITBR(2,J), DEFINITION OF POTENTIAL FOR ALL TORSION      INST3230
C                  ANGLES ABOUT BOND IACT(J) - ICT(2,J).                INST3235
C        64-66  ITBR(3,J), DEFINITION OF POTENTIAL FOR ALL TORSION      INST3240
C                  ANGLES ABOUT BOND IACT(J) - ICT(3,J).                INST3245
C        67-69  ITBR(4,J), DEFINITION OF POTENTIAL FOR ALL TORSION      INST3250
C                  ANGLES ABOUT BOND IACT(J) - ICT(4,J).                INST3255
C                                                                       INST3260
C                  IF ITBR(I,J).EQ.0 THEN WCF=0.                        INST3265
C                                                                       INST3270
C *                IF ITBR(I,J).LT.0 USER SUBROUTINE WCNF IS CALLED.    INST3275
C                  THE VALUE OF ITBR IS PASSED TO WCNF AS AN INDICATOR. INST3280
C                                                                       INST3285
C                  OTHERWISE ITBR(I,J) SPECIFIES THE NUMBER OF THE      INST3290
C                  FIRST OF TWO COMMON PARAMETERS PC USED TO CALCULATE  INST3295
C                  THE ENERGY FOR EACH TORSION ANGLE ABOUT THIS BOND.   INST3300
C                  THIS ENERGY IS                                       INST3305
C                                                                       INST3310
C                  WCF=PC(ITBR(I,J))*WRAG(PI/180*CNF.PC(ITBR(I,J)+1))   INST3315
C                  WHERE WRAG IS A WRAP-AROUND GAUSSIAN FUNCTION.       INST3320
C                  SEE SUBROUTINE WRAG FOR FURTHER DESCRIPTION.         INST3325
C                                                                       INST3330
C     24) EXTRA PARAMETER NAME CARD(S). NPX ENTRIES AT 8 PER CARD.      INST3335
C         OMIT IF NPX.EQ.0.                                             INST3340
C          COLS                                                         INST3345
C          1- 5  NOT USED.                                              INST3350
C          6- 9  NAMPX(1), ALPHANUMERIC NAME OF EXTRA PARAMETER 1.      INST3355
C                   USED TO CLARIFY THE OUTPUT.                         INST3360
C        10-14  NOT USED.                                               INST3365
C        15-18  NAMPX(2)                                                INST3370
C          .       .                                                    INST3375
C          .       .                                                    INST3380
C         ETC.  NAMPX(NPX)                                              INST3385
C                                                                       INST3390
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C     25) EXTRA PARAMETER VALUE CARD(S). NPX ENTRIES AT 8 PER CARD.
C         OMIT IF NPX.EQ.0.
C          COLS
C          1- 9  PX(1), INITIAL VALUE OF EXTRA PARAMETER 1.
C         10-18  PX(2)
C           .      .
C           .      .
C          ETC.  PX(NPX)
C
C     26) EXTRA PARAMETER INCREMENT CARD(S). NPX ENTRIES AT 8 PER CARD.
C         OMIT IF NPX.EQ.0.
C          COLS
C          1- 9  DPX(1), AN INCREMENT TO BE ADDED TO OR SUBTRACTED FROM
C                        PX(1) IN CALCULATING NUMERICAL DERIVATIVES.
C                    0.001 MAY BE SATISFACTORY.
C         10-18  DPX(2)
C           .      .
C           .      .
C          ETC.  DPX(NPX)
C
C     27) EXTRA PARAMETER MINIMUM CARD(S). NPX ENTRIES AT 8 PER CARD.
C    *    OMIT IF NPX.EQ.0 OR IPLM.EQ.0.
C          COLS
C          1- 9  PXMN(1), ALGEBRAIC MINIMUM ALLOWED VALUE FOR PX(1).
C         10-18  PXMN(2)
C           .      .
C           .      .
C          ETC.  PXMN(NPX)
C
C     28) EXTRA PARAMETER MAXIMUM CARD(S). NPX ENTRIES AT 8 PER CARD.
C    *    OMIT IF NPX.EQ.0 OR IPLM.EQ.0.
C          COLS
C          1- 9  PXMX(1), MAXIMUM ALLOWED VALUE FOR PX(1).
C         10-18  PXMX(2)
C           .      .
C           .      .
C          ETC.  PXMX(NPX)
C
C     29) OBSERVED ENERGY FOR THIS SUBSTANCE. ALWAYS INCLUDE ONE CARD.
C         A BLANK CARD IS SATISFACTORY IF THE LATTICE ENERGY IS UNKNOWN.
C          COLS
C          1- 3  KPWS, OBSERVATION SELECTION INTEGER FOR OBSERVED ENERGY.
C                    0 - ENERGY NOT USED AS AN OBSERVATION.
C                    1 - ENERGY USED AS AN OBSERVATION FOR MODE 0.
C                   -1 - ENERGY USED AS AN OBSERVATION FOR MODE 0 ONLY
C                        IF WOBS.GT.WCALC. THIS MIGHT BE USED WHEN THE
C                        CALCULATION IS FOR A STRUCTURE OTHER THAN THE
C                        OBSERVED ONE.
C          4- 9  NOT USED.
C         10-18  WOBS, THE OBSERVED LATTICE ENERGY IN KCAL/MOLE FOR ONE
C                        FORMULA UNIT, (A NEGATIVE NUMBER).
C         19-27  SIGWO, THE STANDARD ERROR OF WOBS. IRRELEVANT IF
C                        IWGT.EQ.0. IF IWGT.EQ.1 AND KPWS.NE.0 THEN SIGWO
C                        MUST BE NON-ZERO.
C
C     30) STRUCTURAL PARAMETER SELECTION CARD(S). NPS ENTRIES AT 72 PER
C         CARD MUST ALWAYS BE INCLUDED. EACH ENTRY CORRESPONDS TO ONE
C         OF THE NPS PARAMETERS FOR THIS SUBSTANCE IN A LIST WHICH THE
C         PROGRAM SETS UP AS FOLLOWS:
C
C         PARAMETER      DESCRIPTION                  NUMBER INCLUDED
C
C          A(1)          LATTICE PARAMETERS                 6
C           .
C           .
C          A(6)
C
C          SXR(1)        ROTATIONS FOR RIGID              3 OR 0
C    *     SYR(1)        BODY 1. OMIT IF IRBA.EQ.1.
C          SZR(1)
C          TR(1,1)       TRANSLATIONS FOR                   3
C          TR(2,1)       RIGID BODY 1.
C          TR(3,1)
C          SXR(2)        SAME FOR                         6 OR 3
C            .           RIGID BODY 2.
C            .
C          TR(3,2)
C            .                                                     TOTAL OF
C            .                                                     6*NRB OR
C          TR(3,NRB)                                               3*NRB
C
C          PX(1)         EXTRA PARAMETERS                   NPX
C          PX(2)         DEFINED BY USER'S
C            .           SUBROUTINE CNSTRN
C            .
C          PX(NPX)
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C          COL                                                          INST3830
C           1     KPS(1), SELECTION INTEGER FOR PARAMETER P(1).         INST3835
C                   0 - NOT A OBSERVATION OR VARIABLE.                  INST3840
C              1 TO 9 - AN OBSERVATION OR VARIABLE.                     INST3845
C           2     KPS(2)                                                INST3850
C           .       .                                                   INST3855
C           .       .                                                   INST3860
C          ETC.   KPS(NPS)                                              INST3865
C                                                                       INST3870
C       THESE ENTRIES SELECT THE STRUCTURAL PARAMETERS WHICH WILL BE    INST3875
C       USED AS OBSERVATIONS FOR MODE 0 OR AS VARIABLES IN MODES 1, 2,  INST3880
C       3, OR 4. WHEN THEY DEFINE VARIABLES THE NON-ZERO VALUES ALSO    INST3885
C       SPECIFY FRACTIONAL SHIFTS USED FOR DAMPING IN MODES 1 OR 4.     INST3890
C       IF PD(L) IS THE CALCULATED SHIFT FOR PARAMETER L THEN THE       INST3895
C       SHIFT APPLIED IS DKT*PD(L) WHERE DKT DEPENDS ON KPS(L) AS       INST3900
C       FOLLOWS:                                                        INST3905
C                 KPS        DKT              KPS        DKT            INST3910
C                  1        1.000              6        0.100           INST3915
C                  2        0.630              7        0.063           INST3920
C                  3        0.400              8        0.040           INST3925
C                  4        0.250              9        0.025           INST3930
C                  5        0.160                                       INST3935
C                                                                       INST3940
C       THE NUMBER OF NON-ZERO KPS(L)'S IS NOS, THE NUMBER OF           INST3945
C       OBSERVATIONS FOR THIS SUBSTANCE. THIS AND THE TOTAL NUMBER OF   INST3950
C       OBSERVATIONS, NO, MUST NOT EXCEED THE DIMENSIONS SPECIFIED.     INST3955
C                                                                       INST3960
C    31) VARIABLE SELECTION CARD(S) FOR MODE 0. NPS ENTRIES AT 72 PER   INST3965
C       CARD ARE ALWAYS INCLUDED. IF MODE.NE.0 OR NC.EQ.0 THESE CARDS   INST3970
C       ARE IRRELEVANT BUT MUST BE INCLUDED.                            INST3975
C                                                                       INST3980
C          COL                                                          INST3985
C           1     KQS(1), SELECTION INTEGER FOR PARAMETER P(1).         INST3990
C                   0 - NOT A VARIABLE FOR MODE 0.                      INST3995
C              1 TO 9 - A VARIABLE FOR MODE 0.                          INST4000
C           2     KQS(2)                                                INST4005
C           .       .                                                   INST4010
C           .       .                                                   INST4015
C          ETC.   KQS(NPS)                                              INST4020
C                                                                       INST4025
C       THESE ENTRIES ARE ANALOGOUS TO THOSE FOR KPS ABOVE. THEY ARE    INST4030
C       USUALLY ZERO EXCEPT IN THE SPECIAL CASE WHEN A STRUCTURAL       INST4035
C       PARAMETER IS TO BE VARIED IN MODE 0. NON-ZERO VALUES SPECIFY    INST4040
C       DAMPING AS DESCRIBED ABOVE FOR KPS.                             INST4045
C                                                                       INST4050
C    32) MAPPING CARDS. OMIT UNLESS MODE.EQ.-1.                         INST4055
C                                                                       INST4060
C       IN MODE -1 THE PROGRAM STEPS THROUGH A SERIES OF VALUES FOR     INST4065
C       EACH OF THREE SPECIFIED PARAMETERS AND CALCULATES THE ENERGY    INST4070
C       OF THE SYSTEM FOR EACH SET. EACH VARIABLE PARAMETER IS DEFINED  INST4075
C       BY ONE CARD. IF LESS THAN THREE VARIABLES ARE NEEDED THEN KPI,  INST4080
C       KPJ, AND/OR KPK CAN BE SET TO -1. ALL OTHER PARAMETERS ARE      INST4085
C       FIXED AT THEIR INPUT VALUES.                                    INST4090
C                                                                       INST4095
C       CAUTION - EACH CALCULATION IS MADE USING THE LIST OF INTER-     INST4100
C       ATOMIC CONTACTS SET UP INITIALLY FROM THE INPUT STRUCTURE. THE  INST4105
C       MAPPING VARIABLES MUST NOT ALTER THE STRUCTURE DRASTICALLY      INST4110
C       BECAUSE NEW CONTACTS WHICH BECOME IMPORTANT MAY NOT BE IN       INST4115
C       THE LIST.                                                       INST4120
C                                                                       INST4125
C        CARD 1                                                         INST4130
C        COLS                                                           INST4135
C        1- 3  KPI, KIND OF PARAMETER FOR OUTER LOOP.                   INST4140
C                -1 - NO PARAMETER. REMAINDER OF CARD IS IRRELEVANT.    INST4145
C                 0 - A COMMON PARAMETER.                               INST4150
C                 1 - A PARAMETER OF THIS SUBSTANCE.                    INST4155
C        4- 6  MPI, THE PARAMETER NUMBER. IF KPI.EQ.1 THEN MPI = 1      INST4160
C                   FOR LATTICE PARAMETER A(1), ETC.                    INST4165
C        7- 9  NOT USED.                                                INST4170
C       10-18  PINI, INITIAL VALUE OF PARAMETER FOR OUTER LOOP.         INST4175
C       19-27  PDLI, POSITIVE INCREMENT FOR PARAMETER OF OUTER LOOP.    INST4180
C       28-36  PLMI, UPPER LIMIT FOR PARAMETER OF OUTER LOOP.           INST4185
C                                                                       INST4190
C        CARD 2                                                         INST4195
C        COLS                                                           INST4200
C        1- 3  KPJ, KIND OF PARAMETER FOR MIDDLE LOOP.                  INST4205
C                -1 - NO PARAMETER. REMAINDER OF CARD IS IRRELEVANT.    INST4210
C                 0 - A COMMON PARAMETER.                               INST4215
C                 1 - A PARAMETER OF THIS SUBSTANCE.                    INST4220
C        4- 6  MPJ, THE PARAMETER NUMBER. IF KPJ.EQ.1 THEN MPJ = 1      INST4225
C                   FOR LATTICE PARAMETER A(1), ETC.                    INST4230
C        7- 9  NOT USED.                                                INST4235
C       10-18  PINJ, INITIAL VALUE OF PARAMETER FOR MIDDLE LOOP.        INST4240
C       19-27  PDLJ, POSITIVE INCREMENT FOR PARAMETER OF MIDDLE LOOP.   INST4245
C       28-36  PLMJ, UPPER LIMIT FOR PARAMETER OF MIDDLE LOOP.          INST4250
C                                                                       INST4255
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C        CARD 3                                                          INST4260
C        COLS                                                            INST4265
C         1- 3  KPK, KIND OF PARAMETER FOR INNER LOOP.                   INST4270
C                -1 - NO PARAMETER. REMAINDER OF CARD IS IRRELEVANT.     INST4275
C                 0 - A COMMON PARAMETER.                                INST4280
C                 1 - A PARAMETER OF THIS SUBSTANCE.                     INST4285
C         4- 6  MPK, THE PARAMETER NUMBER. IF KPK.EQ.1 THEN MPK = 1      INST4290
C                   FOR LATTICE PARAMETER A(1), ETC.                     INST4295
C         7- 9  NOT USED.                                                INST4300
C        10-18  PINK, INITIAL VALUE OF PARAMETER FOR INNER LOOP.         INST4305
C        19-27  PDLK, POSITIVE INCREMENT FOR PARAMETER OF INNER LOOP.    INST4310
C        28-36  PLMK, UPPER LIMIT FOR PARAMETER OF INNER LOOP.           INST4315
C                                                                        INST4320
C       REPEAT CARDS 1, 2, AND 3 AS MANY TIMES AS DESIRED. (ALL          INST4325
C       PARAMETERS ARE RESET TO THEIR INPUT VALUES AFTER EACH            INST4330
C       TRIPLE LOOP.)                                                    INST4335
C                                                                        INST4340
C    33) MAPPING TERMINATION CARD. INCLUDE ONE BLANK CARD IF MODE.EQ.-1. INST4345
C                                                                        INST4350
C    34) REPEAT INPUTS (11) TO (33) FOR EACH ADDITIONAL SUBSTANCE TO BE  INST4355
C        INCLUDED IN THE JOB.                                            INST4360
C                                                                        INST4365
C    35) JOB TERMINATION CARD. ONE BLANK CARD. ANOTHER SET OF DATA       INST4370
C        STARTING WITH CARD (1) MAY FOLLOW.                              INST4375
C                                                                        INST4380
C     ******************************************************************INST4385
C                                                                        INST4390

C     8.2            USER SUBROUTINES FOR WMIN                           INST4395
C                                                                        INST4400
C     THE FOLLOWING ROUTINES ARE DESIGNED TO BE MODIFIED BY THE USER     INST4405
C     FOR EACH PARTICULAR PROBLEM. IMPLICIT AND DIMENSION STATEMENTS     INST4410
C     MUST BE INCLUDED AS THEY ARE IN THE DUMMY SUBROUTINES PROVIDED.    INST4415
C     COMMON STATEMENTS MAY BE NEEDED.                                   INST4420
C                                                                        INST4425
C     FOR SOME OF THESE ROUTINES THE LOCATIONS OF ARRAYS WITH DYNAMIC    INST4430
C     DIMENSIONS ARE PASSED TO THE SUBROUTINE BY A SINGLE CALL FROM      INST4435
C     THE MAIN PROGRAM TO AN INITIALIZING ENTRY. IF ADDITIONAL SUCH      INST4440
C     ARRAYS ARE NEEDED IT WILL BE NECESSARY TO MODIFY THE CALLING       INST4445
C     STATEMENT IN THE MAIN PROGRAM APPROPRIATELY.                       INST4450
C                                                                        INST4455
C     ------------------------------------------------------------------INST4460
C                                                                        INST4465
C     SUBROUTINE CNSTRI(AR,BR,PC,PL,Q,SXR,SYR,SZR,TR)                    INST4470
C     ENTRY CNSTRN                                                       INST4475
C                                                                        INST4480
C     THE PURPOSE OF CNSTRN IS TO DEFINE THE COMMON PARAMETERS, PC, OR   INST4485
C     EXTRA PARAMETERS, PX, BY USING THEM TO SET OTHER VARIABLES. THE    INST4490
C     ROUTINE MAY ALSO BE USED TO ESTABLISH ANY DESIRED CONSTRAINTS.     INST4495
C                                                                        INST4500
C     CNSTRI IS CALLED ONCE FROM MAIN TO PASS THE LOCATIONS OF THE       INST4505
C     ARRAYS LISTED ABOVE.                                               INST4510
C                                                                        INST4515
C     USER ROUTINE CNSTRN IS CALLED NEAR THE END OF WPRE, WHICH IS       INST4520
C     ENTERED ONCE FOR EACH SUBSTANCE, AND NEAR THE BEGINNING OF WCALC.  INST4525
C     WHICH IS ENTERED ONCE FOR EACH ENERGY CALCULATION.                 INST4530
C                                                                        INST4535
C     ON ENTRY, PARAMETERS PC, A, SXR, SYR, SZR, TR, AND PX HAVE BEEN    INST4540
C     SET FROM THE OVERALL PARAMETER LIST. SUBROUTINE SETA HAS BEEN      INST4545
C     ENTERED AND THE VARIABLES OF COMMON/AB/ HAVE BEEN CALCULATED.      INST4550
C                                                                        INST4555
C     THE SUBROUTINE MAY SET POTENTIAL PARAMETERS Q, PL, AR, OR BR IN    INST4560
C     TERMS OF COMMON PARAMETERS PC. THE CHARGES OR COORDINATES OF       INST4565
C     FRACTIONAL ATOMS CONSTITUTING A DIPOLE MAY BE SET FROM THE EXTRA   INST4570
C     PARAMETERS PX. OTHER TYPES OF CONSTRAINTS MAY BE ESTABLISHED BY    INST4575
C     SETTING CERTAIN VARIABLES IN TERMS OF OTHERS. IF THE CALCULATION   INST4580
C     INVOLVES MORE THAN ONE SUBSTANCE THEN CNSTRN SHOULD TEST ISB TO    INST4585
C     IDENTIFY THE CURRENT SUBSTANCE. COMMON BLOCKS MAY BE INCLUDED FOR  INST4590
C     ISB AND ANY OTHER VARIABLES NOT DIMENSIONED DYNAMICALLY. SEE THE   INST4595
C     TEST PROBLEMS FOR EXAMPLES.                                        INST4600
C                                                                        INST4605
C     ------------------------------------------------------------------INST4610
C                                                                        INST4615
C     SUBROUTINE CWXI(PC,PX,Q,TR,XC,YC,ZC)                               INST4620
C     ENTRY CWX                                                          INST4625
C                                                                        INST4630
C     THE PURPOSE OF CWX IS TO CALCULATE WX, ANY EXTRA CONTRIBUTION TO   INST4635
C     THE ENERGY WHICH IS DESIRED BY THE USER. EXAMPLES MIGHT BE THE     INST4640
C     INTERNAL ENERGY OF POLARIZATION OR ANY CONFORMATIONAL ENERGY NOT   INST4645
C     CALCULATED BY GCWX.                                                INST4650
C                                                                        INST4655
C     CWXI IS CALLED ONCE FROM MAIN TO PASS THE LOCATIONS OF THE         INST4660
C     ARRAYS LISTED ABOVE.                                               INST4665
C                                                                        INST4670
C     USER ROUTINE CWX IS CALLED FROM WCALC JUST BEFORE GCWX IS ENTERED. INST4675
C     THIS OCCURS ONCE FOR EACH ENERGY CALCULATION.                      INST4680
C                                                                        INST4685
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C     ON ENTRY THE EXTRA ENERGY WX HAS BEEN SET TO ZERO. SUBROUTINE      INST4690
C     CNSTRN HAS BEEN CALLED. ATOM COORDINATES XC, YC, AN ZC ARE         INST4695
C     AVAILABLE.                                                         INST4700
C                                                                        INST4705
C     THE SUBROUTINE SHOULD SET WX AS DESIRED BY THE USER. THE UNITS OF  INST4710
C     ENERGY ARE KCAL/MOLE FOR THE FORMULA UNIT CONSISTING OF ZAM(I)     INST4715
C     ATOMS OF EACH KIND. FUNCTIONS DST, ANG, AND CONF ARE AVAILABLE FORINST4720
C     THE CALCULATION OF DISTANCES, ANGLES, AND CONFORMATION ANGLES.     INST4725
C     THE CURRENT SUBSTANCE CAN BE DETERMINED BY TESTING ISB. COMMON     INST4730
C     BLOCKS MUST BE INCLUDED FOR WX, ISB, AND OTHER VARIABLES NOT       INST4735
C     DIMENSIONED DYNAMICALLY.                                           INST4740
C                                                                        INST4745
C     ------------------------------------------------------------------INST4750
C                                                                        INST4755
C  *  FUNCTION GPOTI(AR,BR,IACT,ICT,ISC,JAC,PC,PL,PX,Q,SYM,XC,YC,ZC)     INST4760
C     ENTRY GPOT(ISB,I,J,IA,JA,IK,JK,GX,GY,GZ,DX,DY,DZ,R)                INST4765
C                                                                        INST4770
C     GPOT SERVES THE SAME PURPOSE AS REPL BUT MORE ARGUMENTS ARE        INST4775
C     AVAILABLE TO IT. COMPLICATED ATOM PAIR POTENTIALS WHICH DEPEND     INST4780
C     ON THE ANGLES MADE WITH ADJACENT ATOMS CAN BE COMPUTED.            INST4785
C                                                                        INST4790
C     GPOTI IS CALLED ONCE FROM MAIN TO PASS THE LOCATIONS OF THE        INST4795
C     ARRAYS LISTED ABOVE.                                               INST4800
C                                                                        INST4805
C     USER ROUTINE GPOT IS CALLED FROM WCALC IN THE DIRECT LATTICE       INST4810
C     SUMMATIONS IF THE INPUT IREP.EQ.4, 5, 6, OR 7. THERE WILL BE ONE   INST4815
C     ENTRY FOR EACH ATOM PAIR INCLUDED. FUNCTION GPOT IS NOT CALLED     INST4820
C     FOR BONDED PAIRS OR FOR ATOM PAIRS IN THE SAME RIGID BODY. IT IS   INST4825
C     NOT CALLED FOR GEMINAL ATOM PAIRS IF IGEM.EQ.1.                    INST4830
C                                                                        INST4835
C     ON ENTRY ISB INDICATES THE CURRENT SUBSTANCE, I AND J ARE THE      INST4840
C     ATOM NUMBERS (IN THE FULL UNIT CELL) OF THE NON-BONDED PAIR, IA    INST4845
C     AND JA ARE THEIR NUMBERS IN THE ASYMMETRIC UNIT, IK AND JK ARE     INST4850
C     THEIR CHEMICAL KINDS. GX, GY, AND GZ ARE THE UNIT CELL TRANS-      INST4855
C     LATIONS FOR ATOM J, AND DX, DY, AND DZ ARE THE COMPONENTS OF       INST4860
C     THE ATOM-ATOM VECTOR IN THE CRYSTAL SYSTEM. R IS THE DISTANCE.     INST4865
C                                                                        INST4870
C     THE USER'S PROGRAM MUST SET GPOT TO THE VALUE OF THE POTENTIAL     INST4875
C     ENERGY IN KCAL/MOLE FOR THE PAIR.                                  INST4880
C                                                                        INST4885
C     ------------------------------------------------------------------INST4890
C                                                                        INST4895
C     SUBROUTINE MASTER(NST)                                             INST4900
C                                                                        INST4905
C     THE PURPOSE OF MASTER IS TO PERMIT THE USER TO INCREASE THE        INST4910
C     OVERALL STORAGE AVAILABLE FOR ARRAYS WITH DYNAMIC DIMENSIONS.      INST4915
C                                                                        INST4920
C     MASTER IS CALLED ONCE FROM MAIN.                                   INST4925
C                                                                        INST4930
C     THE USER MAY INCREASE THE DIMENSION OF ARRAY S AND SET NST         INST4935
C     ACCORDINGLY.                                                       INST4940
C                                                                        INST4945
C     ------------------------------------------------------------------INST4950
C                                                                        INST4955
C     SUBROUTINE REJECT(ISB,HX,HY,HZ,IREJ)                               INST4960
C                                                                        INST4965
C     THE PURPOSE OF REJECT IS TO BYPASS THE STRUCTURE FACTOR            INST4970
C     CALCULATION FOR SPACE GROUP ABSENCES AND THUS TO SPEED UP THE      INST4975
C     RECIPROCAL LATTICE SUM FOR COULOMB AND VAN DER WAALS ENERGY OF     INST4980
C     CRYSTALS. OMITTING THIS ROUTINE SHOULD HAVE NO EFFECT ON THE       INST4985
C     NUMERICAL RESULTS.                                                 INST4990
C                                                                        INST4995
C     REJECT IS CALLED ONCE FOR EACH RECIPROCAL LATTICE POINT ON THE     INST5000
C     FIRST ENERGY CALCULATION OF EACH CYCLE. IT IS NEVER CALLED IF      INST5005
C     IMOL.EQ.1.OR.CK.EQ.0.OR.(ICMB.EQ.0.AND.IVDW.EQ.0).                 INST5010
C                                                                        INST5015
C     ON ENTRY ISB INDICATES THE SUBSTANCE. HX, HY, AND HZ ARE THE       INST5020
C     INDICES OF THE RECIPROCAL LATTICE POINT (REAL*4). IREJ IS ZERO.    INST5025
C                                                                        INST5030
C     THE SUBROUTINE SHOULD TEST THE INDICES HX, HY, AND HZ AND SET      INST5035
C     IREJ=1 FOR A COMBINATION WHICH DESCRIBES A SPACE GROUP ABSENCE.    INST5040
C     SEE THE TEST PROBLEMS FOR AN EXAMPLE.                              INST5045
C                                                                        INST5050
C     CAUTION- WHEN SYMMETRY CONSTRAINTS ARE RELAXED THEN SUBROUTINE     INST5055
C     REJECT MUST BE ALTERED APPROPRIATELY OR OMITTED.                   INST5060
C                                                                        INST5065
C     ------------------------------------------------------------------INST5070
C                                                                        INST5075
C     FUNCTION REPLI(AR,BR,PC,PL,PX,Q)                                   INST5080
C     ENTRY REPL(ISB,IK,JK,R)                                            INST5085
C                                                                        INST5090
C     THE PURPOSE OF REPL IS TO ALLOW THE USER FLEXIBILITY IN            INST5095
C     CHOOSING THE FORM OF THE ATOM-ATOM REPULSION (OR ATTRACTION)       INST5100
C     POTENTIAL.                                                         INST5105
C                                                                        INST5110
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C     REPLI IS CALLED ONCE FROM MAIN TO PASS THE LOCATIONS OF THE        INST5115
C     ARRAYS LISTED ABOVE.                                               INST5120
C                                                                        INST5125
C     USER ROUTINE REPL IS CALLED FROM WCALC IN THE DIRECT LATTICE       INST5130
C     SUMMATIONS IF THE INPUT IREP.EQ.2. 3. 5, OR 7. THERE WILL BE ONE   INST5135
C     ENTRY FOR EACH ATOM PAIR INCLUDED. FUNCTION REPL IS NOT CALLED     INST5140
C     FOR BONDED PAIRS OR FOR ATOM PAIRS IN THE SAME RIGID BODY. IT IS   INST5145
C     NOT CALLED FOR GEMINAL ATOM PAIRS IF IGEM.EQ.1.                    INST5150
C                                                                        INST5155
C     ON ENTRY ISB INDICATES THE CURRENT SUBSTANCE, IK AND JK DEFINE     INST5160
C     THE CHEMICAL KINDS OF ATOMS IN THE PAIR, AND R IS THE CALCULATED   INST5165
C     INTERATOMIC DISTANCE.                                              INST5170
C                                                                        INST5175
C     THE USER'S PROGRAM MUST SET REPL TO THE VALUE OF THE REPULSION     INST5180
C     ENERGY IN KCAL/MOLE FOR THE PAIR.                                  INST5185
C                                                                        INST5190
C     ------------------------------------------------------------------INST5195
C                                                                        INST5200
C     SUBROUTINE WCNFI(IKA,JAC,PC)                                       INST5205
C     ENTRY WCNF(IA,JA,KA,LA,CNF,ITKJ,WCF)                               INST5210
C                                                                        INST5215
C     THE PURPOSE OF WCNF IS TO ALLOW THE USER COMPLETE FREEDOM TO       INST5220
C     SPECIFY THE POTENTIAL ASSOCIATED WITH AN INTRAMOLECULAR TORSION    INST5225
C     ANGLE.                                                             INST5230
C                                                                        INST5235
C     WCNFI IS CALLED ONCE FROM MAIN TO PASS THE LOCATIONS OF THE        INST5240
C     ARRAYS LISTED ABOVE.                                               INST5245
C                                                                        INST5250
C     USER ROUTINE WCNF IS CALLED FROM GCWX ONCE FOR EACH OF THE         INST5255
C     TORSION ANGLES ABOUT TWO ATOMS SPECIFIED IN THE CONNECTION TABLE   INST5260
C     AS IACT(J) AND ICT(I,J). WCNF IS CALLED ONLY IF ITBR(I,J).LT.0.    INST5265
C                                                                        INST5270
C     ON ENTRY IA, JA, KA, AND LA ARE THE NUMBERS OF THE ATOMS WHICH     INST5275
C     DEFINE THE CONFORMATION ANGLE. CNF IS THE ANGLE IN DEGREES.        INST5280
C     ITKJ IS THE INPUT INTEGER ITBR(I,J), A NEGATIVE NUMBER. ITS VALUE  INST5285
C     MAY BE SPECIFIED BY THE USER AS AN INDICATOR. THE ENERGY WCF HAS   INST5290
C     NOT BEEN CLEARED.                                                  INST5295
C                                                                        INST5300
C     THE USER'S PROGRAM MUST COMPUTE WCF, THE ENERGY IN KCAL/MOLE       INST5305
C     ASSOCIATED WITH THIS ONE CONFORMATION ANGLE. NOTE THAT THERE       INST5310
C     MAY BE AS MANY AS NINE SUCH TORSION ANGLES ABOUT A GIVEN ATOM      INST5315
C     PAIR.                                                              INST5320
C                                                                        INST5325
C     ******************************************************************INST5330
C                                                                        INST5335

C     8.3            COMPILING AND TESTING WMIN                          INST5340
C                                                                        INST5345
C  1) THE PROGRAM AS DISTRIBUTED CONSISTS OF A SINGLE FILE CONTAINING    INST5350
C        A) FORTRAN SOURCE PROGRAMS MAIN TO WRAG,                        INST5355
C        B) INSTRUCTIONS AND GLOSSARY,                                   INST5360
C        C) DUMMY LIBRARY ROUTINES ICLOCK AND IDAY,                      INST5365
C        D) FORTRAN USER ROUTINES FOR THE TEST PROBLEMS,                 INST5370
C        E) DATA FOR THE TEST PROBLEMS.                                  INST5375
C     THESE ITEMS SHOULD BE SAVED ON A BACK-UP TAPE, LISTED, AND THEN    INST5380
C     SEPARATED, EITHER BY EDITING THEM INTO INDIVIDUAL FILES OR BY      INST5385
C     PUNCHING CARDS WHICH CAN BE DIVIDED UP.                            INST5390
C                                                                        INST5395
C  2) ROUTINES MAIN TO WRAG SHOULD BE COMPILED TO YIELD AN OBJECT        INST5400
C     PROGRAM. (SUBROUTINES WMIN AND WCALC MAY REQUIRE MORE THAN THE     INST5405
C     USUAL MEMORY REGION FOR COMPILATION.)                              INST5410
C                                                                        INST5415
C  3) DURING THE LOADING PROCESS THE PROGRAM WILL CALL FOR LIBRARY       INST5420
C     ROUTINES ICLOCK AND IDAY. THE DUMMY ROUTINES PROVIDED CAN BE       INST5425
C     USED TEMPORARILY, IF NECESSARY.                                    INST5430
C                                                                        INST5435
C  4) THE PROGRAM ALSO CALLS DERFC, THE DOUBLE-PRECISION ERROR FUNCTION  INST5440
C     COMPLEMENT, AND OTHER STANDARD ARITHMETIC FUNCTIONS.               INST5445
C                                                                        INST5450
C  5) DURING EXECUTION THE PROGRAM OFTEN CALLS THE EXPONENTIAL FUNCTION  INST5455
C     DEXP WITH LARGE NEGATIVE ARGUMENTS. ON SOME SYSTEMS THIS WILL      INST5460
C     CAUSE EXPONENT UNDERFLOW. THE USER SHOULD ARRANGE TO HAVE THE      INST5465
C     RESULT REPLACED BY ZERO AFTER EXPONENT UNDERFLOW. DEPENDING ON     INST5470
C     THE INSTALLATION, THIS CAN BE DONE BY                              INST5475
C        A) ADDING CALL ERRSET(208,256,-1,0,1) TO MAIN,                  INST5480
C        B) USING THE OPTION PARM.GO='EU=-1', OR                         INST5485
C        C) USING A VERSION OF DEXP WHICH SETS UNDERFLOW TO ZERO.        INST5490
C                                                                        INST5495
C  6) THE PROGRAM USES THE FOLLOWING DATA SET REFERENCE NUMBERS, AND     INST5500
C     THE APPROPRIATE DATA DEFINITION CARDS SHOULD BE PROVIDED.          INST5505
C                                                                        INST5510
```

```
C                                          REFERENCE NUMBERS
C          DESCRIPTION                  SYMBOL    VALUE      SET BY
C
C       STANDARD INPUT USING              --        5        SYSTEM
C       READ STATEMENTS
C
C       STANDARD OUTPUT USING             --        6        SYSTEM
C       PRINT STATEMENTS
C
C       CARD OUTPUT USING                 --        7        SYSTEM
C       PUNCH STATEMENTS
C
C       INTERMEDIATE STORAGE (A)          ND       20         MAIN
C       FOR EACH SUBSTANCE
C
C       INTERMEDIATE STORAGE (B)          NB       21         MAIN
C       FOR EACH SUBSTANCE
C
C       SUMMARY OF RESULTS PRINTED       NSP        6         MAIN
C       ON STANDARD STREAM
C
C       SUMMARY OF RESULTS PRINTED       NSD       22         MAIN
C       ON SEPARATE STREAM
C
C   7) THE USER ROUTINES MAY BE COMPILED AT RUN TIME. THEY OVERRIDE
C      THE DUMMY ROUTINES INCLUDED IN THE OBJECT PROGRAM.
C
C   8) THE TEST PROBLEMS ARE EXECUTED BY INCLUDING THE USER ROUTINES
C      PROVIDED AND READING THE TEST DATA AS INPUT. THE OUTPUT CAN BE
C      COMPARED WITH THE EXAMPLES PROVIDED.
C
C      ******************************************************************
       RETURN
       END
```

9.1 Standard Fortran Program

```
C     TOTAL NUMBER OF CARDS TRANSMITTED (FORTRAN AND TEST DATA) IS 6748 MAIN   5
C     PROGRAM WMIN                                                      MAIN  10
C                                                                       MAIN  15
C     PROGRAM TO REPRESENT CRYSTALS OR MOLECULES BY A POTENTIAL-ENERGY  MAIN  20
C     MODEL, ADJUST PARAMETERS OF THE POTENTIAL, ADJUST THE STRUCTURE   MAIN  25
C     FOR MINIMUM ENERGY, OR CALCULATE ITS VIBRATIONAL FREQUENCIES.     MAIN  30
C                                                                       MAIN  35
C     WRITTEN BY W. R. BUSING, CHEMISTRY DIVISION, OAK RIDGE NATIONAL   MAIN  40
C     LABORATORY, P. O. BOX X, OAK RIDGE, TENNESSEE 37830               MAIN  45
C                                                                       MAIN  50
C     REVISED DECEMBER 1980                                             MAIN  55
C     SEE SUBROUTINE INSTRU FOR DATA INPUT INSTRUCTIONS.                MAIN  60
C     SEE SUBROUTINE GLOSS FOR DEFINITIONS OF SYMBOLS                   MAIN  65
C                                                                       MAIN  70
C     CALLING PROGRAM TO PROVIDE DIMENSIONING OF ARRAYS AT RUN TIME     MAIN  75
      IMPLICIT REAL*8(A-H,O-Z)                                          MAIN  80
      REAL*8 NAMLIM,NAMARY                                              MAIN  85
      DIMENSION NAMLIM(32),LIM(32),NAMARY(133),L1(133),L2(133)          MAIN  90
     1,(TYPE(133),NWORD(133),K(134),KADR(133)                           MAIN  95
      DATA NAMLIM/6HNPCMAX,6H NAMAX,6HNKAMAX,6H NSMAX,6HNRBMAX,6HNPXMAX MAIN 100
     1  ,6HNCTMAX,6HNBCMAX,6H  MMAX,6HNFSMAX,6HNGSMAX,6HNPSMAX,6H NPMAX MAIN 105
     2  ,6HNOSMAX,6H NOMAX,6H NVMAX,6H      ,6H      ,6H      ,6H    0 MAIN 110
     3  ,6H    1  ,6H    2  ,6H    3  ,6H    4  ,6H    5  ,6H    6  ,6H    7 MAIN 115
     4  ,6H    8  ,6H    9  ,6H   10  ,6H   11  ,6H   12  /              MAIN 120
      DATA LIN/20*0,1,2,3,4,5,6,7,8,9,10,11,12/                         MAIN 125
      DATA NAMARY/6H  ACZ ,6H  AKE ,6H   AM ,6H AMASS,6H   AN ,6H   AR  MAIN 130
     1  ,6H   BR ,6H  BTR ,6H CHAR ,6H CMBT ,6H  CSV ,6H   DP ,6H   DPC MAIN 135
     2  ,6H  DPX ,6H   DW ,6H DWDQ ,6H  DXQ ,6H  DYC ,6H  DYQ ,6H   DZQ MAIN 140
     3  ,6H  EPS ,6H  ERR ,6H EVAL ,6H EVEC ,6H  FMC ,6H FREQ ,6H   GMT MAIN 145
     4  ,6H  GXT ,6H  GYT ,6H  GZT ,6H  HMT ,6H  HXT ,6H  HTY ,6H   HZT MAIN 150
     5  ,6H IACT ,6H IASV ,6H  IAT ,6H  IAZ ,6H  ICC ,6H  ICT ,6H   IDZ MAIN 155
     6  ,6H  IKA ,6H IOUT ,6H  IRB ,6H IRBC ,6H ISBP ,6H  ISC ,6H   ISV MAIN 160
     7  ,6H ITBR ,6H   IU ,6H   IV ,6H   IW ,6H   IZ ,6H  JAC ,6H  JASV MAIN 165
     8  ,6H  JAT ,6H JOTS ,6H JOUT ,6H  JSV ,6H KASV ,6H   KP ,6H   KPC MAIN 170
     9  ,6H  KPS ,6H   KQ ,6H  KQC ,6H  KQS ,6H LASV ,6H LBCI ,6H  LBCJ MAIN 175
     A  ,6H   LI ,6H   MJ ,6H NAME ,6H NAMK ,6H NAMP ,6H NAMPC,6H  NAMPX MAIN 180
     B  ,6H NAMS ,6H NOBS ,6H NOSS ,6H NOUT ,6H    P ,6H PBASE,6H   PC MAIN 185
     C  ,6H PCMN ,6H PCMX ,6H PCSV ,6H   PD ,6H   PL ,6H  PMN ,6H  PMX MAIN 190
     D  ,6H   PS ,6H  PSV ,6H   PX ,6H PXMN ,6H PXMX ,6H PXSV ,6H    Q MAIN 195
     E  ,6H RFPT ,6H  RSV ,6H   RT ,6H  SAN ,6H  SMC ,6H   SP ,6H  SPW MAIN 200
     F  ,6H SRBT ,6H  SSR ,6H  STR ,6H  SXR ,6H  SYM ,6H  SYR ,6H  SZR MAIN 205
     G  ,6H TMAT ,6H   TQ ,6H   TR ,6H UMAT ,6H VBEST,6H VDWT ,6H   VM MAIN 210
     H  ,6H   VN ,6H  VSV ,6H WMAT ,6H   WN ,6H   WP ,6H  WSV ,6H   XC MAIN 215
     I  ,6H  XYZ ,6H XYZC ,6H XYZD ,6H XYZN ,6H XYZR ,6H   YC ,6H  ZAM MAIN 220
     J  ,6H   ZC  /                                                     MAIN 225
      DATA L1/        29.      20.      16.      21.      16.      21 MAIN 230
     1 .      21.      16.      21.      21.      21.      21.      21 MAIN 235
     2 .      21.      21.      21.      16.      21.      16.      16 MAIN 240
     3 .      21.      21.      21.      16.       2.      21.      21 MAIN 245
     4 .      21.      21.      21.      21.      21.      21.      21 MAIN 250
     5 .      21.      21.      21.      26.       2.      24.      24 MAIN 255
     6 .      21.      21.      21.       2.      21.       2.      21 MAIN 260
     7 .      24.      21.      21.      21.      21.       2.      21 MAIN 265
     8 .      21.      21.      21.      21.      21.      21.      21 MAIN 270
     9 .      21.      21.      21.      21.      21.      21.      21 MAIN 275
     A .      21.      21.      21.      21.      21.      21.      21 MAIN 280
     B .      21.      21.      21.      21.      21.      21.      21 MAIN 285
     C .      21.      21.      21.      21.      21.      21.      21 MAIN 290
     D .      22.      21.      21.      21.      21.      21.      21 MAIN 295
     E .      21.      21.      21.      21.       2.      21.      21 MAIN 300
     F .      21.      21.      21.      21.      32.      21.      21 MAIN 305
     G .      14.      21.      23.      14.      21.      21.      21 MAIN 310
     H .      21.      21.      14.      21.      21.      21.       2 MAIN 315
     I .      23.      23.      23.      23.      23.       2.      21 MAIN 320
     J .       2/                                                      MAIN 325
      DATA L2/         5.      20.      16.       3.      16.       3 MAIN 330
     1 .       3.      14.       4.      11.      11.      13.       1 MAIN 335
     2 .       6.      13.      16.       2.      15.       2.       2 MAIN 340
     3 .      13.      16.      16.      16.       4.      16.      11 MAIN 345
     4 .      11.      11.      11.      10.      10.      10.      10 MAIN 350
     5 .       7.       9.      11.       7.       4.       7.       7 MAIN 355
     6 .       2.      16.       2.       4.      13.       5.       9 MAIN 360
     7 .       7.       5.       5.       5.       5.       5.       9 MAIN 365
     8 .      11.      14.      15.       9.       9.      13.       1 MAIN 370
     9 .      12.      13.       1.      12.       9.       8.       8 MAIN 375
     A .      13.      13.       2.       3.      13.       1.       6 MAIN 380
     B .       4.      15.      14.      16.      13.      13.       1 MAIN 385
     C .       1.       1.       1.      16.       3.      13.      13 MAIN 390
     D .      16.      13.       6.       6.       6.       6.       3 MAIN 395
     E .      11.      11.      11.      16.       4.      13.      14 MAIN 400
     F .      11.       5.       5.       5.       4.       5.       5 MAIN 405
     G .      14.      16.       5.      14.      13.      11.      16 MAIN 410
     H .      16.      11.      14.      13.      13.       9.       4 MAIN 415
     I .       2.       2.       2.       2.       2.       4.       2 MAIN 420
     J .       4/                                                      MAIN 425
      DATA ITYPE/      8.       8.       8.       8.       8.       8 MAIN 430
     1 .       8.       8.       8.       4.       8.       8.       8 MAIN 435
     2 .       8.       8.       8.       8.       8.       8.       8 MAIN 440
     3 .       8.       8.       8.       8.       4.       8.       8 MAIN 445
     4 .       4.       4.       4.       4.       4.       4.       4 MAIN 450
     5 .       4.       4.       4.       4.       4.       4.       4 MAIN 455
     6 .       4.       4.       4.       4.       4.       4.       4 MAIN 460
     7 .       4.       4.       4.       4.       4.       4.       4 MAIN 465
     8 .       4.       4.       4.       4.       4.       4.       4 MAIN 470
     9 .       4.       4.       4.       4.       4.       4.       4 MAIN 475
     A .       4.       4.       4.       4.       4.       4.       4 MAIN 480
     B .       4.       4.       4.       4.       8.       8.       8 MAIN 485
     C .       8.       8.       8.       8.       8.       8.       8 MAIN 490
     D .       8.       8.       8.       8.       8.       8.       8 MAIN 495
     E .       4.       8.       4.       8.       4.       8.       8 MAIN 500
     F .       4.       8.       8.       8.       8.       8.       8 MAIN 505
     G .       8.       8.       8.       8.       8.       4.       8 MAIN 510
     H .       8.       8.       8.       8.       8.       8.       8 MAIN 515
     I .       8.       8.       8.       8.       8.       8.       8 MAIN 520
     J .       8/                                                      MAIN 525
C     /MAX/ USED BY MAIN, WMIN, WDYN, WPRE, WCALC, AND GCWX             MAIN 530
      COMMON/MAX/NPCMAX,NAMAX,NKAMAX,NSMAX,NRBMAX,NPXMAX,NCTMAX,NBCMAX  MAIN 535
     1,MMAX,NFSMAX,NGSMAX,NPSMAX,NPMAX,NOSMAX,NOMAX,NVMAX,ND,NB,NSD,NSP MAIN 540
C                                                                       MAIN 545
C     DIMENSION OF OVERALL STORAGE ARRAY S IS SET IN SUBROUTINE MASTER  MAIN 550
      COMMON/S/S(1)                                                     MAIN 555
      CALL MASTER(NST)                                                  MAIN 560
C                                                                       MAIN 565
C     READ AND PRINT LIMITS                                             MAIN 570
    5 READ 10,(LIM(I),I=1,16)                                           MAIN 575
   10 FORMAT(8I9)                                                       MAN 580
      DO 15 I=2,16                                                      MAIN 585
      IF(I.EQ.6.OR.I.EQ.9.OR.I.EQ.10.OR.I.EQ.11) GO TO 15               MAIN 590
      IF(LIM(I).EQ.0) LIM(I)=1                                          MAIN 595
   15 CONTINUE                                                          MAIN 600
      PRINT 20,(NAMLIM(I),I= 1, 8),(LIM(I),I= 1, 8)                     MAIN 605
     1          ,(NAMLIM(I),I= 9,16),(LIM(I),I= 9,16)                  MAIN 610
   20 FORMAT('1DYNAMIC DIMENSIONS FOR WMIN'                             MAIN 615
     1/'0',8(2X,A6)/X,9I8/'0',8(2X,A6)/X,8I8)                           MAIN 620
C                                                                       MAIN 625
C     PUT LIMITS IN COMMON/MAX/                                         MAIN 630
      NPCMAX=LIM( 1)                                                    MAIN 635
      NAMAX =LIM( 2)                                                    MAIN 640
      NKAMAX=LIM( 3)                                                    MAIN 645
      NSMAX =LIM( 4)                                                    MAIN 650
      NRBMAX=LIM( 5)                                                    MAIN 655
      NPXMAX=LIM( 6)                                                    MAIN 660
      NCTMAX=LIM( 7)                                                    MAIN 665
      NBCMAX=LIM( 8)                                                    MAIN 670
      MMAX  =LIM( 9)                                                    MAIN 675
      NFSMAX=LIM(10)                                                    MAIN 680
      NGSMAX=LIM(11)                                                    MAIN 685
      NPSMAX=LIM(12)                                                    MAIN 690
      NPMAX =LIM(13)                                                    MAIN 695
      NOSMAX=LIM(14)                                                    MAIN 700
      NOMAX =LIM(15)                                                    MAIN 705
      NVMAX =LIM(16)                                                    MAIN 710
C                                                                       MAIN 715
C     SET DATA SET REFERENCE NUMBERS                                    MAIN 720
      ND=20                                                             MAIN 725
      NB=21                                                             MAIN 730
      NSD=22                                                            MAIN 735
      NSP=6                                                             MAIN 740
C                                                                       MAIN 745
C     SPECIAL TREATMENT OF AUXILIARY MATRICES TMAT AND UMAT             MAIN 750
      LL=14                                                             MAIN 755
      IF(NVMAX.GT.NOSMAX) LL=16                                         MAIN 760
      L1(112)=LL                                                        MAIN 765
      L1(115)=LL                                                        MAIN 770
      L2(112)=LL                                                        MAIN 775
      L2(115)=LL                                                        MAIN 780
C                                                                       MAIN 785
C     COMPUTE LOCATIONS FOR VARIABLES                                   MAIN 790
      K(1)=1                                                            MAIN 795
      DO 60 I=1,133                                                     MAIN 800
      NWORD(I)=LIM(L1(I))*LIM(L2(I))                                    MAIN 805
      IF(ITYPE(I).EQ.8) GO TO 40                                        MAIN 810
      IF(MOD(NWORD(I),2).NE.0) NWORD(I)=NWORD(I)+1                      MAIN 815
      K(I+1)=K(I)+NWORD(I)/2                                            MAIN 820
      GO TO 50                                                          MAIN 825
   40 K(I+1)=K(I)+NWORD(I)                                              MAIN 830
   50 KADR(I)=8*(K(I)-1)                                                MAIN 835
   60 CONTINUE                                                          MAIN 840
      KST=K(134)-1                                                      MAIN 845
      KDIFF=IABS(NST-KST)                                               MAIN 850
      KBYTE=KDIFF/128                                                   MAIN 855
C                                                                       MAIN 860
C     PRINT DIRECTORY                                                   MAIN 865
      I2=0                                                              MAIN 870
   70 I1=I2+1                                                           MAIN 875
      I2=I1+9                                                           MAIN 880
      IF(I2.GT.133) I2=133                                              MAIN 885
      PRINT 75,(I,I=I1,I2)                                              MAIN 890
   75 FORMAT('0',11X,10I11)                                             MAIN 895
      PRINT 80,(NAMARY(I),I=I1,I2)                                      MAIN 900
   80 FORMAT(' ARRAY',6X,10(5X,A6))                                     MAIN 905
      PRINT 90,(NAMLIM(L1(I)),I=I1,I2)                                  MAIN 910
   90 FORMAT(' DIMEN-',5X,10('    (',A6))                              MAIN 915
      PRINT 95,(NAMLIM(L2(I)),I=I1,I2)                                  MAN 920
   95 FORMAT('  SIONS',6X,10('  *',A6,')'))                             MAN 925
      PRINT 100,(NWORD(I),I=I1,I2)                                      MAIN 930
  100 FORMAT(' WORDS',6X,10I11)                                         MAIN 935
      PRINT 110,(ITYPE(I),I=I1,I2)                                      MAIN 940
  110 FORMAT(' BYTES/WORD ',10I11)                                      MAIN 945
      PRINT 120,(KADR(I),I=I1,I2)                                       MAIN 950
  120 FORMAT(' HEX ADDRESS',10Z11)                                      MAIN 955
      IF(I2.NE.133) GO TO 70                                            MAIN 960
C                                                                       MAIN 965
C     PRINT TOTAL STORAGE USED AND TEST FOR OVERFLOW                    MAIN 970
      PRINT 130,KST,NST                                                 MAIN 975
  130 FORMAT('0',I8,' 8-BYTE STORAGE LOCATIONS HAVE BEEN REQUESTED. THE MAIN 980
     1PROGRAM IS DIMENSIONED FOR',I8)                                   MAIN 985
      IF(KST.LE.NST) GO TO 150                                          MAIN 990
      PRINT 140,KDIFF,KBYTE                                             MAIN 995
  140 FORMAT('0COMMON/S/ AND NST MUST BE INCREASED BY',I6,' WORDS. THIS MAIN1000
     1WILL ADD',I4,'K BYTES TO THE REGION USED.')                       MAIN1005
      CALL EXIT                                                         MAIN1010
  150 PRINT 160,KDIFF,KBYTE                                             MAIN1015
  160 FORMAT('0COMMON/S/ AND NST MAY BE DECREASED BY',I6,' WORDS. THIS WMAIN1020
     2ILL REDUCE THE REGION USED BY',I4,'K BYTES.')                     MAIN1025
                                                                        MAIN1030
C     MAKE INITIAL CALLS TO PASS ARRAY LOCATIONS TO SUBPROGRAMS         MAIN1035
C     CALL WDYNI (S(K(2)),S(K(4)),S(K(8)),S(K(9)),S(K(12)),S(K(17))     MAIN1040
     1,S(K(19)),S(K(20)),S(K(23)),S(K(26)),S(K(42)),S(K(43)),S(K(64))   MAIN1045
     2,S(K(72)),S(K(77)),S(K(80)),S(K(81)),S(K(109)),S(K(113)),S(K(119))MAIN1050
     3,S(K(126)),S(K(127)),S(K(128)),S(K(129)),S(K(132)))               MAIN1055
      CALL WPREI (S(K(1)),S(K(4)),S(K(6)),S(K(7)),S(K(12)),S(K(14))     MAIN1060
     1,S(K(25)),S(K(35)),S(K(38)),S(K(40)),S(K(41)),S(K(42)),S(K(44))   MAIN1065
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     2,S(K(45)),S(K(46)),S(K(47)),S(K(49)),S(K(50)),S(K(51)),S(K(52))    MAIN1070
     3,S(K(53)),S(K(54)),S(K(57)),S(K(63)),S(K(64)),S(K(66)),S(K(68))    MAIN1075
     4,S(K(69)),S(K(72)),S(K(73)),S(K(74)),S(K(76)),S(K(77)),S(K(79))    MAIN1080
     5,S(K(81)),S(K(88)),S(K(89)),S(K(90)),S(K(93)),S(K(94)),S(K(95))    MAIN1085
     6,S(K(97)),S(K(102)),S(K(103)),S(K(106)),S(K(107)),S(K(108))        MAIN1090
     7,S(K(109)),S(K(110)),S(K(111)),S(K(114)),S(K(125)),S(K(126))       MAIN1095
     8,S(K(131)),S(K(132)),S(K(133)),S(K(61))                            MAIN1100
      DUMMY=WCALC1 (S(K(1)),S(K(6)),S(K(7)),S(K(10)),S(K(11)),S(K(25))   MAIN1105
     1,S(K(27)),S(K(28)),S(K(29)),S(K(30)),S(K(31)),S(K(32)),S(K(33))    MAIN1110
     2,S(K(34)),S(K(37)),S(K(39)),S(K(42)),S(K(44)),S(K(45)),S(K(47))    MAIN1115
     3,S(K(50)),S(K(51)),S(K(52)),S(K(53)),S(K(54)),S(K(56)),S(K(68))    MAIN1120
     4,S(K(69)),S(K(72)),S(K(81)),S(K(83)),S(K(86)),S(K(88)),S(K(93))    MAIN1125
     5,S(K(96)),S(K(97)),S(K(98)),S(K(99)),S(K(100)),S(K(105)),S(K(108))MAIN1130
     6,S(K(109)),S(K(110)),S(K(111)),S(K(114)),S(K(117)),S(K(120))       MAIN1135
     7,S(K(125)),S(K(126)),S(K(127)),S(K(130)),S(K(131)),S(K(132))       MAIN1140
     8,S(K(133))                                                         MAIN1145
      CALL GCWXI (S(K(35)),S(K(36)),S(K(38)),S(K(39)),S(K(40)),S(K(41))  MAIN1150
     1,S(K(48)),S(K(49)),S(K(55)),S(K(59)),S(K(60)),S(K(67)),S(K(83))    MAIN1155
     2,S(K(124)),S(K(54)),S(K(72))                                       MAIN1160
      CALL VECI (S(K(125)),S(K(131)),S(K(133)))                          MAIN1165
C                                                                        MAIN1170
C     THE USER MAY MODIFY THE FOLLOWING CALLS TO PASS OTHER ARRAYS       MAIN1175
      CALL CNSTRI (S(K(6)),S(K(7)),S(K(83)),S(K(88)),S(K(93)),S(K(97))   MAIN1180
     1,S(K(108)),S(K(109)),S(K(111)),S(K(114))                           MAIN1185
      CALL CWXI (S(K(83)),S(K(93)),S(K(97)),S(K(114)),S(K(125))          MAIN1190
     1,S(K(131)),S(K(133)))                                              MAIN1195
      DUMMY=REPLI (S(K(6)),S(K(7)),S(K(83)),S(K(88)),S(K(93)),S(K(97)))  MAIN1200
      DUMMY=GPOTI (S(K(6)),S(K(7)),S(K(35)),S(K(40)),S(K(47)),S(K(54))   MAIN1205
     1,S(K(83)),S(K(88)),S(K(93)),S(K(97)),S(K(109)),S(K(125))           MAIN1210
     2,S(K(131)),S(K(133))                                               MAIN1215
      CALL WCNFI (S(K(42)),S(K(54)),S(K(83)))                            MAIN1220
C                                                                        MAIN1225
C     ENTER WMIN WITH ARRAY LOCATIONS AS ARGUMENTS                       MAIN1230
      CALL WMIN (S(K(1)),S(K(3)),S(K(4)),S(K(5)),S(K(6)),S(K(7))         MAIN1235
     1,S(K(8)),S(K(12)),S(K(13)),S(K(15)),S(K(16)),S(K(18)),S(K(21))     MAIN1240
     2,S(K(22)),S(K(23)),S(K(24)),S(K(25)),S(K(26)),S(K(35)),S(K(38))    MAIN1245
     3,S(K(40)),S(K(41)),S(K(42)),S(K(43)),S(K(44)),S(K(45)),S(K(46))    MAIN1250
     4,S(K(47)),S(K(49)),S(K(50)),S(K(51)),S(K(52)),S(K(53)),S(K(54))    MAIN1255
     5,S(K(57)),S(K(58)),S(K(61)),S(K(62)),S(K(63)),S(K(65)),S(K(68))    MAIN1260
     6,S(K(69)),S(K(70)),S(K(71)),S(K(72)),S(K(73)),S(K(74)),S(K(75))    MAIN1265
     7,S(K(77)),S(K(76)),S(K(79)),S(K(80)),S(K(81)),S(K(82)),S(K(83))    MAIN1270
     8,S(K(84)),S(K(85)),S(K(87)),S(K(88)),S(K(89)),S(K(90)),S(K(91))    MAIN1275
     9,S(K(92)),S(K(93)),S(K(97)),S(K(101)),S(K(102)),S(K(103))          MAIN1280
     A,S(K(104)),S(K(109)),S(K(112)),S(K(113)),S(K(115)),S(K(116))       MAIN1285
     B,S(K(118)),S(K(119)),S(K(121)),S(K(122)),S(K(123)),S(K(125))       MAIN1290
     C,S(K(126)),S(K(130)),S(K(131)),S(K(132)),S(K(133)))                MAIN1295
      GO TO 5                                                            MAIN1300
      END                                                                MAIN1305


      SUBROUTINE WMIN (ACZ,AM,AMASS,AN,AR,BR                             WMIN   5
     1,BTR,DP,DPC,DW,DWDQ,DYC,EPS                                        WMIN  10
     2,ERR,EVAL,EVEC,FMC,FREQ,IACT,IAZ                                   WMIN  15
     3,ICT,IDZ,IKA,IOUT,IRBS,IRSC,ISBP                                   WMIN  20
     4,ISC,ITBR,IU,IV,IW,IZ,JAC                                          WMIN  25
     5,JOTS,JOUT,KP,KPC,KQ,KQC,LBCI                                      WMIN  30
     6,LBCJ,LI,MJ,NAME,NAMK,NAMP,NAMPC                                   WMIN  35
     7,NAMS,NOBS,NOSS,NOUT,P,PBASE,PC                                    WMIN  40
     8,PCMN,PCMX,PD,PL,PMN,PMX,PS                                        WMIN  45
     9,PSV,PX,Q,SAN,SMC,SP                                               WMIN  50
     A,SYM,SYMTMAT,TQ,UMAT,VBEST                                         WMIN  55
     B,VM,VN,WMAT,WN,WP,XC                                               WMIN  60
     C,XYZ,XYZR,YC,ZAM,ZC)                                               WMIN  65
      IMPLICIT REAL*8(A-H,O-Z)                                           WMIN  70
      DIMENSION ACZ(9,1),AM(1),AMASS(1),AN(1),AR(1),BR(1)                WMIN  75
     1,BTR(1),DP(1),DPC(1),DW(1),DWDQ(1),DYC(1),EPS(1)                   WMIN  80
     2,ERR(1),EVAL(1),EVEC(1),FMC(1),FREQ(1),IACT(1),IAZ(6,1)            WMIN  85
     3,ICT(4,1),IDZ(4,1),IKA(1),IOUT(1),IRBS(1),ISBP(1)                  WMIN  90
     4,ISC(1),ITBR(4,1),IU(1),IV(1),IW(1),IZ(1),JAC(1)                   WMIN  95
     5,JOTS(1),JOUT(1),KP(1),KPC(1),KQ(1),KQC(1),LBCI(1)                 WMIN 100
     6,LBCJ(1),LI(1),MJ(1),NAME(1),NAMK(1),NAMP(1),NAMPC(1)              WMIN 105
     7,NAMS(1),NOBS(1),NOSS(1),NOUT(1),P(1),PBASE(1),PC(1)               WMIN 110
     8,PCMN(1),PCMX(1),PD(1),PL(1),PMN(1),PMX(1),PS(9,1)                 WMIN 115
     9,PSV(1),PX(1),Q(1),SAN(1),SMC(1),SP(1)                             WMIN 120
     A,SPW(1),SYM(12,1),TMAT(1),TQ(1),UMAT(1),VBEST(1)                   WMIN 125
     B,VM(1),VN(1),WMAT(1),WN(1),WP(1),XC(1)                             WMIN 130
     C,XYZ(3,1),XYZR(3,1),YC(1),ZAM(1),ZC(1)                             WMIN 135
C     /DOUBL/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, TIMOUT              WMIN 140
      COMMON/DUBL/A(6),AC(9),ACB(9),ASV(6),CA(9),CAD(9),CK               WMIN 145
     1,CKKCAL,CRA(9),DAA,DATE,FKCAL,WR,PI,PICK,PICKZ,PIDKSQ              WMIN 150
     2,PINHZ,QLIM(5),QMAX,RDWSS(9),RLIM(5),RMI(9),RMAX,RTPIZ             WMIN 155
     3,SA(6),SIGWG,SOTPDK,SOTPI,SOTPIK,TM(5),TPI,TRT(3),TW(3)            WMIN 160
     4,UT(9),UV(3),UW(3),WC,WOBS,WS(9),WV,WX,XYZA(3),XYZAS(3)            WMIN 165
     5,XYZDS(3),ZMC                                                      WMIN 170
C     /SNGL/ USED BY WMIN, WPRE, WCALC                                   WMIN 175
      REAL*4 CMBT,FM,FMC,FNS,GXT,GYT,GZT,HMT,HXNEG,HXT,HYNEG             WMIN 180
     1,HYT,HZNEG,HZT,REPT,RT,SMC,SRBT,STITLE,TITLE,VDWT                  WMIN 185
      COMMON/SNGL/FM,FNS,HXNEG,HYNEG,HZNEG,STITLE(17),TITLE(18)          WMIN 190
C     /MAX/ USED BY MAIN, WMIN, WDYN, WPRE, WCALC, AND GCWX              WMIN 195
      COMMON/MAX/NPCMAX,NAMAX,NKAMAX,NSMAX,NRBMAX,NPXMAX,NCTMAX,NBCMAX   WMIN 200
     1,MMAX,NFSMAX,NGSMAX,NPSMAX,NPMAX,NOSMAX,NOMAX,NVMAX,ND,NB,NSD,NSP  WMIN 205
C     /ITGR/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, IBYPAS, TIMOUT       WMIN 210
      COMMON/ITGR/IBK,ICCAX,ICENT,ICMB,IGEM,ILSQ,IMOL,INK,IPLM,IPRC      WMIN 215
     1,IPRT,IRBA,IREP,IRSC,ISB,ISW,IVDW,IWGT,IZAM,JC,KPW,KPWS,LTI(9)     WMIN 220
     2,MODE,NA,NAC,NAF,NBC,NCT,NKA,NDS,NP,NPC,NPR,NPS,NPX,NQ,ISETA       WMIN 225
     3,NR,NRB,NRP,NSYMT(9),NV,NVA,NVC,NVO,NVR,NVUS(9),NVX                WMIN 230
      DIMENSION DKT(9)                                                   WMIN 235
      DATA DKT/1.0D0,.6D0,.4D0,.2D0,.16D0,.1D0,.06D0,.04D0,.02D0/WMIN 240
      DATA NONE/4HNONE/                                                  WMIN 245
C                                                                        WMIN 250
C     THIS SUBPROGRAM IS CALLED FROM MAIN TO SET LOCATIONS OF ARRAYS     WMIN 255
C                                                                        WMIN 260
C     PROGRAM TO REPRESENT CRYSTALS OR MOLECULES BY A POTENTIAL-ENERGY   WMIN 265
C     MODEL, ADJUST PARAMETERS OF THE POTENTIAL, ADJUST THE STRUCTURE    WMIN 270
C     FOR MINIMUM ENERGY, OR CALCULATE ITS VIBRATIONAL FREQUENCIES.      WMIN 275
C                                                                        WMIN 280
      CALL IDAY(DATE)                                                    WMIN 285
C     READ OVERALL TITLE AND CONTROL CARD                                WMIN 290
      READ  5,TITLE                                                      WMIN 295
    5 FORMAT(18A4)                                                       WMIN 300
      PRINT  10,TITLE,DATE                                               WMIN 305
   10 FORMAT(1H1,18A4,8X,A8)                                             WMIN 310
      READ  15,MODE,NC,NPC,ILSQ,IWGT,IPLM,IPRT,NSTG,IBPC                 WMIN 315
     1,ARE,SLIM,CMPR,XDRD,EPSC                                           WMIN 320
   15 FORMAT(9I3,5E9.0)                                                  WMIN 325
      PRINT  20,MODE,NC,NPC,ILSQ,IWGT,IPLM,IPRT,NSTG,IBPC                WMIN 330
     1,ARE,SLIM,CMPR,XDRD,EPSC                                           WMIN 335
   20 FORMAT(10  MODE    NC    NPC   ILSQ  IWGT  IPLM  IPRT  NSTG  IBPC  WMIN 340
     1        ARE        SLIM       CMPR       XDRD       EPSC'          WMIN 345
     2/X,9I6,5E12.3)                                                     WMIN 350
      IF(NPC.LE.NPCMAX) GO TO 503                                        WMIN 355
      PRINT 22,NPCMAX                                                    WMIN 360
   22 FORMAT('0*** NUMBER OF COMMON PARAMETERS EXCEEDS PRESET LIMIT OF'  WMIN 365
     1,I3,' ***')                                                        WMIN 370
      CALL EXIT                                                          WMIN 375
  503 NP=NPC                                                             WMIN 380
      NVC=0                                                              WMIN 385
      NCY=NC+1                                                           WMIN 390
      IF(NPC)505,595,505                                                 WMIN 395
  505 IF(IBPC)515,510,515                                                WMIN 400
C     READ COMMON PARAMETER INFORMATION                                  WMIN 405
  510 READ  25,(NAMPC(I),I=1,NPC)                                        WMIN 410
   25 FORMAT(8(5X,A4))                                                   WMIN 415
  515 PRINT 30,(NAMPC(I),I=1,NPC)                                        WMIN 420
   30 FORMAT('0 NAMPC(I)'/(X,5(5X,A4)))                                  WMIN 425
      IF(IBPC)525,520,525                                                WMIN 430
  520 READ 35,(PC(I),I=1,NPC)                                            WMIN 435
   35 FORMAT(8F9.0)                                                      WMIN 440
  525 PRINT 40,(PC(I),I=1,NPC)                                           WMIN 445
   40 FORMAT('0   PC(I)'/(X,8F9.5))                                      WMIN 450
      IF(IBPC)535,530,535                                                WMIN 455
  530 READ 45,(DPC(I),I=1,NPC)                                           WMIN 460
   45 FORMAT(8F9.0)                                                      WMIN 465
  535 PRINT 50,(DPC(I),I=1,NPC)                                          WMIN 470
   50 FORMAT('0   DPC(I)'/(X,8F9.5))                                     WMIN 475
      IF(IPLM.NE.0) GO TO 539                                            WMIN 480
      DO 537 I=1,NPC                                                     WMIN 485
      PCMN(I)=0.0                                                        WMIN 490
      PCMX(I)=0.0                                                        WMIN 495
  537 CONTINUE                                                           WMIN 500
      GO TO 558                                                          WMIN 505
  539 IF(IBPC)545,540,545                                                WMIN 510
  540 READ 55,(PCMN(I),I=1,NPC)                                          WMIN 515
   55 FORMAT(8F9.0)                                                      WMIN 520
  545 PRINT 60,(PCMN(I),I=1,NPC)                                         WMIN 525
   60 FORMAT('0   PCMN(I)'/(X,8F9.5))                                    WMIN 530
      IF(IBPC)555,550,555                                                WMIN 535
  550 READ 65,(PCMX(I),I=1,NPC)                                          WMIN 540
   65 FORMAT(8F9.0)                                                      WMIN 545
  555 PRINT 70,(PCMX(I),I=1,NPC)                                         WMIN 550
   70 FORMAT('0   PCMX(I)'/(X,8F9.5))                                    WMIN 555
  558 IF(IBPC)565,560,565                                                WMIN 560
  560 READ 75,(KPC(I),I=1,NPC)                                           WMIN 565
   75 FORMAT(72I1)                                                       WMIN 570
  565 PRINT 80,(KPC(I),I=1,NPC)                                          WMIN 575
   80 FORMAT('0   KPC(I)'/(X,8I9))                                       WMIN 580
      READ 85,(KQC(I),I=1,NPC)                                           WMIN 585
   85 FORMAT(72I1)                                                       WMIN 590
C     MOVE COMMON PARAMETERS TO MAIN PARAMETER LIST                      WMIN 595
      DO 585 I=1,NPC                                                     WMIN 600
      NAMP(I)=NAMPC(I)                                                   WMIN 605
      P(I)=PC(I)                                                         WMIN 610
      DP(I)=DPC(I)                                                       WMIN 615
      PMN(I)=PCMN(I)                                                     WMIN 620
      PMX(I)=PCMX(I)                                                     WMIN 625
      KP(I)=0                                                            WMIN 630
      ISBP(I)=0                                                          WMIN 635
      SP(I)=0.0                                                          WMIN 640
C     SELECT VARIABLES ACCORDING TO MODE AND COUNT THEM                  WMIN 645
      IF(MODE)570,575,570                                                WMIN 650
  570 KQ(I)=0                                                            WMIN 655
      GO TO 585                                                          WMIN 660
  575 KQ(I)=KQC(I)                                                       WMIN 665
      IF(KQ(I))580,585,580                                               WMIN 670
  580 NVC=NVC+1                                                          WMIN 675
  585 CONTINUE                                                           WMIN 680
C     PREPARE TO USE AUXILIARY STORAGE IF COMMON PARAMETERS ARE VARIABLEWMIN 685
      IF(NVC)590,595,590                                                 WMIN 690
  590 REWIND ND                                                          WMIN 695
C     READ SUBSTANCE IDENTIFICATION CARD AND TEST FOR TERMINATION        WMIN 700
  595 READ 90,ISB,STITLE                                                 WMIN 705
   90 FORMAT(I3,17A4)                                                    WMIN 710
      IF(ISB)620,600,620                                                 WMIN 715
  600 IF(NVC)610,605,610                                                 WMIN 720
C     NO MORE SUBSTANCES. ADJUSTMENTS HAVE BEEN MADE. TERMINATE JOB      WMIN 725
  605 RETURN                                                             WMIN 730
C     NO MORE SUBSTANCES. PREPARE FOR OVERALL LEAST-SQUARES ADJUSTMENT   WMIN 735
  610 END FILE ND                                                        WMIN 740
      IF(IPRT-3)615,615,635                                              WMIN 745
  615 PRINT 95,TITLE,DATE                                                WMIN 750
   95 FORMAT(1H1,18A4,8X,A8)                                             WMIN 755
      GO TO 635                                                          WMIN 760
C     READ AND PRINT INPUT, MAKE PRELIM CALC FOR CURRENT SUBSTANCE       WMIN 765
  620 PRINT 100,TITLE,DATE,STITLE,ISB                                    WMIN 770
  100 FORMAT(1H1,18A4,8X,A8/X,17A4/'0   ISB*/X,I6)                       WMIN 775
      CALL WPRE                                                          WMIN 780
      IF(IPRT-5)625,630,625                                              WMIN 785
C     COMMON PARAMETERS TO BE VARIED, SAVE INPUT FROM CURRENT SUBSTANCE  WMIN 790
  625 WRITE(ND)          CK,CKKCAL,FM,FNS,HXNEG,HYNEG,HZNEG,ISENT,ISETA  WMIN 795
     1,ICMB,IGEM,IMOL,INK,ISB,IREP,IRSC,IVDW,IZAM,NPW,NA,NAC,NAF         WMIN 800
     2,NBC,NCT,NKA,NOS,NPX,NQ,NR,NRB,NRP,NS,NVA,NVR,NVX,PICK             WMIN 805
     3,PICKZ,PIDKSQ,PINHZ,QLIM,RLIM,RTPIZ,SIGWG,SOTPDK,SOTPIN            WMIN 810
     4,STITLE,WOBS,ZMC,(IKA(J),IRBI(J),NAME(J),(XYZI(I,J),I=1,3)         WMIN 815
     5,ZAM(J),J=1,NA),(FMC(J),IRBC(J),ISC(J),JAC(J),SMC(J),XC(J)         WMIN 820
     6,YC(J),ZC(J),J=1,NAC),(LBCI(J),LBCJ(J),J=1,NBC),(IACT(J)           WMIN 825
     7,(IAZ(I,J),I=1,6),(ICT(I,J),IDZ(I,J),ITBR(I,J),I=1,4)              WMIN 830
     8,J=1,NCT),(AMASS(J),AR(J),BR(J),NAMK(J),PL(J),Q(J),J=1,NKA)        WMIN 835
     9,(JOTS(J),NOSS(J),J=1,NOS),((ACZ(I,J),I=1,9),IU(J),IV(J)           WMIN 840
     A,IW(J),IZ(J),J=1,NRB),(NAMS(J),(SYM(I,J),I=1,12),J=1,NS)           WMIN 845
      GO TO 595                                                          WMIN 850
C     JUMP IF IN MAPPING MODE                                            WMIN 855
  630 IF(MODE)1710,635,635                                               WMIN 860
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C     PRINT OVERALL PARAMETER LIST                                      WMIN 865
  635 IF(IPRT-3)640,640,665                                             WMIN 870
  640 PRINT 105                                                         WMIN 875
  105 FORMAT('0   I   NAMP(I)        P(I)       DP(I)      PMN(I)      PMX(I) WMIN 880
     1 KP(I)  KQ(I)  DKT(KQ)       SP(I)   ISBP(I)')                   WMIN 885
      DO 660 I=1,NP                                                     WMIN 890
      KQI=KQ(I)                                                         WMIN 895
      IF(KQI)645,645,650                                                WMIN 900
  645 DKTKQI=0.0                                                        WMIN 905
      GO TO 655                                                         WMIN 910
  650 DKTKQI=DKT(KQI)                                                   WMIN 915
  655 PRINT 110,I,NAMP(I),P(I),DP(I),PMN(I),PMX(I),KP(I),KQ(I),DKTKQI   WMIN 920
     1,SP(I),ISBP(I)                                                    WMIN 925
  110 FORMAT(X,I3,5X,A4,4F11.6,2I7,F9.3,F11.6,I6)                       WMIN 930
  660 CONTINUE                                                          WMIN 935
C     COUNT OBSERVATIONS, VARIABLES, AND SET UP CERTAIN ARRAYS          WMIN 940
  665 NO=0                                                              WMIN 945
      NV=0                                                              WMIN 950
      NOV=0                                                             WMIN 955
      DO 695 I=1,NP                                                     WMIN 960
      IF(KP(I))670,680,670                                              WMIN 965
  670 NO=NO+1                                                           WMIN 970
      IF(NO.LE.NOMAX) GO TO 672                                         WMIN 975
      PRINT 112,NOMAX                                                   WMIN 980
  112 FORMAT('0*** NUMBER OF OBSERVATIONS EXCEEDS PRESET LIMIT OF',I4   WMIN 985
     1,' ***')                                                          WMIN 990
      CALL EXIT                                                         WMIN 995
  672 JOUT(NO)=I                                                        WMIN1000
      NOBS(NO)=NAMP(I)                                                  WMIN1005
      IF(KQ(I))675,690,675                                              WMIN1010
  675 NOV=NOV+1                                                         WMIN1015
      GO TO 685                                                         WMIN1020
  680 IF(KQ(I))685,690,685                                              WMIN1025
  685 NV=NV+1                                                           WMIN1030
      IF(NV.LE.NVMAX) GO TO 687                                         WMIN1035
      PRINT 113,NVMAX                                                   WMIN1040
  113 FORMAT('0*** NUMBER OF VARIABLES EXCEEDS PRESET LIMIT OF',I4      WMIN1045
     1,' ***')                                                          WMIN1050
      CALL EXIT                                                         WMIN1055
  687 IOUT(NV)=I                                                        WMIN1060
      NOUT(NV)=NAMP(I)                                                  WMIN1065
      PS(1,NV)=P(I)                                                     WMIN1070
  690 LI(I)=NV                                                          WMIN1075
  695 CONTINUE                                                          WMIN1080
      DGF=NO-NV                                                         WMIN1085
      IF(DGF)700,700,705                                                WMIN1090
  700 DGF=1.0                                                           WMIN1095
  705 NVV=NV*NV                                                         WMIN1100
C     SET LEAST-SQUARES AND WEIGHT INDICATORS                           WMIN1105
      IF(ILSQ)725,710,725                                               WMIN1110
  710 IF(NO-NV)725,715,725                                              WMIN1115
  715 IF(NO-NOV)725,720,725                                             WMIN1120
  720 LS=0                                                              WMIN1125
      IWT=0                                                             WMIN1130
      GO TO 730                                                         WMIN1135
  725 LS=1                                                              WMIN1140
      IWT=IWGT                                                          WMIN1145
  730 IF(IPRT-4)735,735,740                                             WMIN1150
  735 PRINT 115,NO,NV,NOV,LS,IWT                                        WMIN1155
  115 FORMAT('0     NO     NV    NOV     LS    IWT'/X,5I6)              WMIN1160
C     START FIRST CYCLE                                                 WMIN1165
  740 IC=1                                                              WMIN1170
      JC=1                                                              WMIN1175
      IPRC=IPRT-2                                                       WMIN1180
      GO TO 760                                                         WMIN1185
C     START SUBSEQUENT CYCLES                                           WMIN1190
  745 JC=IC                                                             WMIN1195
      IF(IC-NCY)755,750,755                                             WMIN1200
  750 IPRC=IPRT-1                                                       WMIN1205
      GO TO 760                                                         WMIN1210
  755 IPRC=IPRT                                                         WMIN1215
C     CLEAR MATRIX AND VECTOR                                           WMIN1220
  760 DO 765 I=1,NVV                                                    WMIN1225
  765 AN(I)=0.0                                                         WMIN1230
      DO 770 I=1,NV                                                     WMIN1235
  770 VN(I)=0.0                                                         WMIN1240
      SDWST=0.0                                                         WMIN1245
C     PREPARE TO READ AUXILIARY STORAGE IF COMMON PARAM ARE VARIABLES   WMIN1250
      IF(NVC)775,800,775                                                WMIN1255
  775 REWIND ND                                                         WMIN1260
      REWIND NB                                                         WMIN1265
C     BRING INFORMATION ON ONE SUBSTANCE FROM AUXILIARY STORAGE         WMIN1270
  780 READ(ND,END=785) CK,CKKCAL,FM,FNS,HXNEG,HYNEG,HZNEG,ICENT,ISETA   WMIN1275
     1,ICMB,IGEN,IMOL,INK,ISG,IREP,IRSC,IVDW,IZAM,KPW,NA,NAC,NAF        WMIN1280
     2,NBC,NCT,NKA,NOS,NPS,NPX,NQ,NR,NRB,NRP,NS,NVA,NVR,NVX,PICK        WMIN1285
     3,PICKZ,PIDKSQ,PINMZ,QLIM,RLIM,RTPIZ,SIGWO,SQTPDK,SQTPIK           WMIN1290
     4,STITLE,WOBS,ZMC,(IKA(J),IRB(J),NAME(J),(XYZ(I,J),I=1,3)          WMIN1295
     5,ZAM(J),J=1,NA),(FMC(J),IRBC(J),ISC(J),JAC(J),SMC(J),XC(J)        WMIN1300
     6,YC(J),ZC(J),J=1,NAC),(LBCI(J),LBCJ(J),J=1,NBC),(IACT(J)          WMIN1305
     7,(IAZ(I,J),I=1,6),(ICT(I,J),IDZ(I,J),ITBR(I,J),I=1,4)             WMIN1310
     8,J=1,NCT),(AMASS(J),ARK(J),BR(J),NAMK(J),PL(J),Q(J),J=1,NKA)      WMIN1315
     9,(JOTS(J),NOSS(J),J=1,NOS),(IACZ(I,J),I=1,9),IU(J),IV(J)          WMIN1320
     A,IW(J),IZ(J),J=1,NRB),(NAMS(J),(SYM(I,J),I=1,12),J=1,NS)          WMIN1325
      GO TO 800                                                         WMIN1330
C     TEST FOR LAST CYCLE                                               WMIN1335
  785 IF(IC-NCY)790,1600,790                                            WMIN1340
C     PRINT DISCREPANCY FACTORS EXCEPT ON LAST CYCLE                    WMIN1345
  790 PRINT 120,TITLE,DATE,IC                                           WMIN1350
  120 FORMAT(1H1,18A4,8X,A8/'0CYCLE',I3)                                WMIN1355
      RDWST=DSQRT(SDWST)                                                WMIN1360
      SIGMA=DSQRT(SDWST/DGF)                                            WMIN1365
      PRINT 125,RDWST,SDWST,SIGMA                                       WMIN1370
  125 FORMAT('0          RDWST              SDWST              SIGMA'/X,3E15.6) WMIN1375
C     SAVE DISCREPANCY FACTOR FOR OUTPUT IN SUMMARY                     WMIN1380
      IF(IC-9)795,795,1200                                              WMIN1385
  795 RDWSS(IC)=RDWST                                                   WMIN1390
      GO TO 1200                                                        WMIN1395
C     INITIALIZE COUNTERS AND TIMERS                                    WMIN1400
  800 DO 805 I=1,9                                                      WMIN1405
      NT(I)=0                                                           WMIN1410
      LT(I)=0                                                           WMIN1415
  805 CONTINUE                                                          WMIN1420
C     SET INDICATORS                                                    WMIN1425
      IBK=0                                                             WMIN1430
      ISW=1                                                             WMIN1435
C     DUMMY ENTRY TO INITIALIZE IBYPAS                                  WMIN1440
      IBY=IBYPAS(0,0,KPC)                                               WMIN1445
C     ENTER WCALC FOR FIRST ENERGY CALCULATION OF THIS CYCLE            WMIN1450
      W=WCALC(0)                                                        WMIN1455
      ISW=0                                                             WMIN1460
C     PRINT CALCULATED ENERGY                                           WMIN1465
      PRINT 130,TITLE,DATE,STITLE                                       WMIN1470
  130 FORMAT(1H0,18A4,8X,A8/X,17A4)                                     WMIN1475
      PRINT 135,IC,WOBS,W                                               WMIN1480
  135 FORMAT('0          WOBS       WCALC BEFORE CYCLE',I3/X,2F11.4)    WMIN1485
C     SAVE CALCULATED ENERGY FOR OUTPUT IN SUMMARY                      WMIN1490
      IF(IC-9)810,810,815                                               WMIN1495
  810 WS(IC)=W                                                          WMIN1500
C     JUMP IF ROSENBROCK SEARCH IS TO BE MADE FOR MINIMUM ENERGY        WMIN1505
  815 IF(MODE-3)820,2030,820                                            WMIN1510
C     START LOOP PRELIMINARY TO DERIVATIVE CALCULATION                  WMIN1515
  820 DO 860 I=1,NP                                                     WMIN1520
C     ARE DERIVATIVES TO BE CALCULATED WITH RESPECT TO THIS PARAMETER   WMIN1525
      IF(ISBP(I))825,830,825                                            WMIN1530
  825 IF(ISBP(I)-ISB)860,830,860                                        WMIN1535
  830 IF(KP(I))850,835,850                                              WMIN1540
  835 IF(KQ(I))840,860,840                                              WMIN1545
  840 IF(IC-NCY)845,860,845                                             WMIN1550
  845 IF(KPW)850,855,850                                                WMIN1555
C     DECREMENT PARAMETER AND RECALCULATE ENERGY                        WMIN1560
  850 PISAVE=P(I)                                                       WMIN1565
      P(I)=PISAVE-DP(I)                                                 WMIN1570
      WN(I)=WCALC(IBYPAS(I,0,KPC))                                      WMIN1575
      P(I)=PISAVE                                                       WMIN1580
C     INCREMENT PARAMETER AND RECALCULATE ENERGY                        WMIN1585
  855 PISAVE=P(I)                                                       WMIN1590
      P(I)=PISAVE+DP(I)                                                 WMIN1595
      WP(I)=WCALC(IBYPAS(I,0,KPC))                                      WMIN1600
      P(I)=PISAVE                                                       WMIN1605
  860 CONTINUE                                                          WMIN1610
C     START LOOPS TO STORE FIRST AND SECOND DERIVATIVES OF ENERGY       WMIN1615
      IY=0                                                              WMIN1620
      IM=0                                                              WMIN1625
      IN=0                                                              WMIN1630
      DO 1005 J=1,NP                                                    WMIN1635
C     DOES PARAMETER PERTAIN TO CURRENT SUBSTANCE                       WMIN1640
      IF(ISBP(J)-ISB)870,865,870                                        WMIN1645
C     IS PARAMETER USED AS AN OBSERVATION                               WMIN1650
  865 IF(KP(J))875,870,875                                              WMIN1655
C     NO. SET DERIVATIVE TO ZERO                                        WMIN1660
  870 DW(J)=0.0                                                         WMIN1665
      MJ(J)=IY                                                          WMIN1670
      GO TO 1005                                                        WMIN1675
C     YES. COMPUTE AND STORE DERIVATIVE                                 WMIN1680
  875 IY=IY+1                                                           WMIN1685
      MJ(J)=IY                                                          WMIN1690
      DW(J)=(WP(J)-WN(J))/(2.0*DP(J))                                   WMIN1695
      DYC(IY)=-DW(J)                                                    WMIN1700
      SPW(IY)=SP(J)                                                     WMIN1705
C     OMIT CALCULATION OF SECOND DERIVS FOR METHOD OF STEEPEST DESCENTS WMIN1710
      IF(MODE-2)880,1005,880                                            WMIN1715
C     OMIT SECOND DERIVS ON LAST CYCLE UNLESS FREQUENCIES ARE TO BE CALCWMIN1720
  880 IF(IC-NCY)890,885,890                                             WMIN1725
  885 IF(MODE-4)1005,890,1005                                           WMIN1730
C     START INNER LOOP TO STORE SECOND DERIVS IN BTR (AND UMAT IF IWT=1)WMIN1735
  890 DO 1000 I=1,NP                                                    WMIN1740
      IDD=0                                                             WMIN1745
C     IS PARAMETER A VARIABLE                                           WMIN1750
      IF(KQ(I))895,915,895                                              WMIN1755
  895 IM=IM+1                                                           WMIN1760
C     IS IT A COMMON PARAMETER                                          WMIN1765
      IF(ISBP(I))900,910,900                                            WMIN1770
C     DOES IT PERTAIN TO THIS SUBSTANCE                                 WMIN1775
  900 IF(ISBP(I)-ISB)905,910,905                                        WMIN1780
  905 BTR(IM)=0.0                                                       WMIN1785
      GO TO 1000                                                        WMIN1790
  910 IS=0                                                              WMIN1795
      GO TO 940                                                         WMIN1800
C     IS WEIGHT MATRIX TO BE USED AND IS PARAMETER AN OBSERVATION       WMIN1805
  915 IF(IWT)920,1000,920                                               WMIN1810
  920 IF(KP(I))925,1000,925                                             WMIN1815
  925 IF(ISBP(I)-ISB)1000,930,1000                                      WMIN1820
  930 IN=IN+1                                                           WMIN1825
C     IS DERIVATIVE FOR UMAT SAME AS THAT JUST STORED IN BTR            WMIN1830
      IF(IDD)995,935,995                                                WMIN1835
  935 IS=1                                                              WMIN1840
  940 IDD=1                                                             WMIN1845
      IF(I-J)945,980,975                                                WMIN1850
C     PICK UP DERIVATIVE IF IT HAS BEEN COMPUTED PREVIOUSLY             WMIN1855
  945 IF(ISBP(I)-ISB)975,950,975                                        WMIN1860
  950 IF(KP(I))955,975,955                                              WMIN1865
  955 IF(IWT)960,965,960                                                WMIN1870
  960 LM=(MJ(I)-1)*NOS+MJ(J)                                            WMIN1875
      DDWIJ=UMAT(LM)                                                    WMIN1880
      GO TO 985                                                         WMIN1885
  965 IF(KQ(J))970,975,970                                              WMIN1890
  970 LM=(MJ(I)-1)*NV+LI(J)                                             WMIN1895
      DDWIJ=BTR(LM)                                                     WMIN1900
      GO TO 985                                                         WMIN1905
C     CALCULATE SECOND DERIVATIVE FOR I NOT EQUAL TO J                  WMIN1910
  975 PISAVE=P(I)                                                       WMIN1915
      P(I)=PISAVE+DP(I)                                                 WMIN1920
      PJSAVE=P(J)                                                       WMIN1925
      P(J)=PJSAVE+DP(J)                                                 WMIN1930
      WPPIJ=WCALC(IBYPAS(I,J,KPC))                                      WMIN1935
      P(I)=PISAVE                                                       WMIN1940
      P(J)=PJSAVE                                                       WMIN1945
      DDWIJ=(WPPIJ+W -WP(I)-WP(J))/(DP(I)*DP(J))                        WMIN1950
      GO TO 985                                                         WMIN1955
C     CALCULATE SECOND DERIVATIVE FOR I EQUAL TO J                      WMIN1960
  980 DDWIJ=(WP(I)+WN(I)-2.0*W )/(DP(I)**2)                             WMIN1965
      GO TO 985                                                         WMIN1970
C     TEST SWITCH AND STORE IN BTR OR UMAT                              WMIN1975
  985 IF(IS)995,990,995                                                 WMIN1980
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  990 BTR(IM)=DDW(J                                                     WMIN1985
      GO TO 915                                                         WMIN1990
  995 UMAT(IN)=DDW(J                                                    WMIN1995
 1000 CONTINUE                                                          WMIN2000
 1005 CONTINUE                                                          WMIN2005
C     OMIT REFINEMENT ON FINAL CYCLE                                    WMIN2010
      IF(IC-NCY)1010,1505,1010                                          WMIN2015
C     COMPUTE OBS MINUS CALC ENERGY. IS IT TO BE USED AS AN OBSERVATION WMIN2020
 1010 WOWC=WOBS-W                                                       WMIN2025
      IF(KPW)1015,1080,1020                                             WMIN2030
 1015 IF(WOWC)1080,1080,1020                                            WMIN2035
C     YES. START LOOP TO COMPUTE FIRST DERIVS WITH RESPECT TO VARIABLES WMIN2040
 1020 J=0                                                               WMIN2045
      DO 1045 I=1,NP                                                    WMIN2050
      IF(KQ(I))1025,1045,1025                                           WMIN2055
 1025 J=J+1                                                             WMIN2060
      IF(ISBP(I))1030,1040,1030                                         WMIN2065
 1030 IF(ISBP(I)-ISB)1035,1040,1035                                     WMIN2070
 1035 DWDQ(J)=0.0                                                       WMIN2075
      GO TO 1045                                                        WMIN2080
 1040 DWDQ(J)=(WP(I)-WN(I))/(2.0*DP(I))                                 WMIN2085
 1045 CONTINUE                                                          WMIN2090
C     PRINT FIRST DERIVATIVES WITH RESPECT TO VARIABLES                 WMIN2095
      IF(IPRT-3)1050,1050,1055                                          WMIN2100
 1050 PRINT 140,IC,(IOUT(I),NOUT(I),I=1,NV)                             WMIN2105
  140 FORMAT('0CONTRIBUTION OF WOBS TO CYCLE',I3/24X,'DWDQ(I) FOR I='/ WMIN2110
     16X,'WOWC=WOBS-WCALC',9(I5,2X,A4)/(21X,9(I5,2X,A4)))               WMIN2115
      PRINT 145,WOWC,(DWDQ(I),I=1,NV)                                   WMIN2120
  145 FORMAT(10X,10F11.4/(21X,9F11.4))                                  WMIN2125
C     COMPUTE CONTRIBUTION OF OBS ENERGY TO MATRIX AND VECTOR           WMIN2130
 1055 CALL GMTRA(DWDQ,TMAT,NV,1)                                        WMIN2135
      IF(IWT)1065,1060,1065                                             WMIN2140
 1060 SOWST=SOWST+WOWC**2                                               WMIN2145
      GO TO 1075                                                        WMIN2150
 1065 WGT=1.0/SIGWO**2                                                  WMIN2155
      SOWST=SOWST+WGT*WOWC**2                                           WMIN2160
      DO 1070 I=1,NV                                                    WMIN2165
      DWDQ(I)=WGT*DWDQ(I)                                               WMIN2170
 1070 CONTINUE                                                          WMIN2175
 1075 CALL GMPRD(DWDQ,TMAT,AM,NV,1,NV)                                  WMIN2180
      CALL GMPRD(DWDQ,WOWC,VM,NV,1,1)                                   WMIN2185
      CALL GMADD(AM,AN,AN,NV,NV)                                        WMIN2190
      CALL GMADD(VM,VN,VN,NV,1)                                         WMIN2195
C     JUMP TO USE METHOD OF STEEPEST DESCENTS                           WMIN2200
 1080 IF(MODE-2)1085,1650,1085                                          WMIN2205
C     CALCULATE AND PRINT WEIGHT MATRIX IF IT IS TO BE USED             WMIN2210
 1085 IF(IWT)1090,1120,1090                                             WMIN2215
 1090 CALL MPRD(SPW,UMAT,TMAT,NOS,NOS,2,0,NOS)                          WMIN2220
      CALL GTPRD(TMAT,TMAT,WMAT,NOS,NOS,NOS)                            WMIN2225
      CALL MINV(WMAT,NOS,DET,TMAT,UMAT)                                 WMIN2230
      IF(DET)1095,1095,1100                                             WMIN2235
 1095 PRINT 150                                                         WMIN2240
  150 FORMAT('0VARIANCE-COVARIANCE MATRIX SINGULAR. WMAT NOT USED')     WMIN2245
      IWT=0                                                             WMIN2250
      GO TO 1120                                                        WMIN2255
 1100 IF(IPRC-1)1105,1105,1115                                          WMIN2260
 1105 PRINT 155,(JOTS(J),NOSS(J),J=1,NOS)                               WMIN2265
  155 FORMAT('0WMAT'/10X,10(I5,2X,A4)/(10X,10(I5,2X,A4)))               WMIN2270
      K2=0                                                              WMIN2275
      DO 1110 I=1,NOS                                                   WMIN2280
      K1=K2+1                                                           WMIN2285
      K2=K2+NOS                                                         WMIN2290
      PRINT 160,JOTS(I),NOSS(I),(WMAT(K),K=K1,K2)                       WMIN2295
  160 FORMAT(X,I3,2X,A4,10E11.3/(10X,10E11.3))                          WMIN2300
 1110 CONTINUE                                                          WMIN2305
C     COMPUTE WEIGHTED DISCREPANCY FACTOR                               WMIN2310
 1115 CALL GMPRD(WMAT,DYC,TMAT,NOS,NOS,1)                               WMIN2315
      CALL GTPRD(DYC,TMAT,SDWS,NOS,1,1)                                 WMIN2320
      GO TO 1125                                                        WMIN2325
C     COMPUTE UNWEIGHTED DISCREPANCY FACTOR                             WMIN2330
 1120 CALL GTPRD(DYC,DYC,SDWS,NOS,1,1)                                  WMIN2335
C     PRINT FIRST AND SECOND DERIVATIVES                                WMIN2340
 1125 IF((IPRT-3)1130,1130,1140                                         WMIN2345
 1130 PRINT 165,IC,(IOUT(I),NOUT(I),I=1,NV)                             WMIN2350
  165 FORMAT('0DERIVATIVES BEFORE CYCLE',I3/24X,'DDW/DP(I)DP(J) FOR I='WMIN2355
     1'    J   NAMP(J)   DYC(J)',9(I5,2X,A4)/(21X,9(I5,2X,A4)))         WMIN2360
      K2=0                                                              WMIN2365
      DO 1135 J=1,NOS                                                   WMIN2370
      K1=K2+1                                                           WMIN2375
      K2=K2+NV                                                          WMIN2380
      PRINT 170,JOTS(J),NOSS(J),DYC(J),(BTR(K),K=K1,K2)                 WMIN2385
  170 FORMAT(X,I3,2X,A4,10F11.4/(21X,9F11.4))                           WMIN2390
 1135 CONTINUE                                                          WMIN2395
C     CALCULATE AND PRINT DISCREPANCY FACTORS                           WMIN2400
 1140 SOWST=SOWST+SOWS                                                  WMIN2405
      ROWS=DSQRT(SDWS)                                                  WMIN2410
      SIGMA=DSQRT(SOWST/DSF)                                            WMIN2415
      IF(IPRT-4)1145,1145,1150                                          WMIN2420
 1145 PRINT 175,ROWS,SOWS                                               WMIN2425
  175 FORMAT('0                ROWS                SOWS'/X,2E15.6)      WMIN2430
C     ANALYZE AND PRINT TIMES FOR VARIOUS PARTS OF ENERGY CALCULATION   WMIN2435
 1150 IF((PRC-1)1156,1155,1160                                          WMIN2440
 1155 CALL TINOUT                                                       WMIN2445
C     SAVE DISCREPANCY FACTORS FOR OUTPUT IN SUMMARY                    WMIN2450
 1160 IF(IC-9)1165,1165,1170                                            WMIN2455
 1165 ROWSS(IC)=ROWS                                                    WMIN2460
C     TEST WHETHER LEAST-SQUARES IS TO BE USED                          WMIN2465
 1170 IF(LS)1180,1175,1180                                              WMIN2470
C     NO. COPY MATRIX AND VECTOR FOR EQUATIONS TO BE SOLVED             WMIN2475
 1175 CALL MCPY(BTR,AN,NV,NV,0)                                         WMIN2480
      CALL MCPY(DYC,VN,NV,1,0)                                          WMIN2485
      GO TO 1200                                                        WMIN2490
C     CALCULATE CONTRIB OF SUBSTANCE TO LEAST-SQUARES MATRIX AND VECTOR WMIN2495
 1180 CALL GMTRA(BTR,TMAT,NV,NOS)                                       WMIN2500
      IF(IWT)1185,1190,1185                                             WMIN2505
 1185 CALL GMPRD(BTR,WMAT,UMAT,NV,NOS,NOS)                              WMIN2510
      CALL MCPY(UMAT,BTR,NV,NOS,0)                                      WMIN2515
 1190 CALL GMPRD(BTR,TMAT,AM,NV,NOS,NV)                                 WMIN2520
      CALL GMPRD(BTR,DYC,VM,NV,NOS,1)                                   WMIN2525
      CALL GMADD(AM,AN,AN,NV,NV)                                        WMIN2530
      CALL GMADD(VM,VN,VN,NV,1)                                         WMIN2535
C     IF NO COMMON PARAMETERS VARIABLE SUBSTANCES TREATED SEPARATELY    WMIN2540
      IF(NVC)1195,1200,1195                                             WMIN2545
C     SAVE DATA FOR THIS SUBSTANCE AND PROCEED TO NEXT SUBSTANCE        WMIN2550
 1195 NVOS=NV*NOS                                                       WMIN2555
      WRITE(NB)          KPW,NOS,NVOS,WOWC,(BTR(I),I=1,NVOS)            WMIN2560
     1,(DWDQ(I),I=1,NV),(DYC(I),I=1,NO)                                 WMIN2565
      GO TO 780                                                         WMIN2570
C     PREPARE TO INVERT MATRIX BY DETERMINING PRINCIPAL COMPONENTS      WMIN2575
C     DETERMINE SCALE FACTORS FROM DIAGONAL ELEMENTS                    WMIN2580
 1200 IM=1                                                              WMIN2585
      DO 1220 I=1,NV                                                    WMIN2590
      IF(SLIM)1202,1203,1203                                            WMIN2595
 1202 SAN(I)=1.0                                                        WMIN2600
      GO TO 1215                                                        WMIN2605
 1203 DGAN=AN(IM)                                                       WMIN2610
      IF(DGAN-SLIM)1205,1205,1210                                       WMIN2615
 1205 SAN(I)=0.0                                                        WMIN2620
      GO TO 1215                                                        WMIN2625
 1210 SAN(I)=1.0/DSQRT(DGAN)                                            WMIN2630
 1215 IM=IM+NV+1                                                        WMIN2635
 1220 CONTINUE                                                          WMIN2640
      IF(IPRC)1225,1225,1230                                            WMIN2645
 1225 PRINT 180,(IOUT(I),NOUT(I),I=1,NV)                                WMIN2650
  180 FORMAT('0',17X,'SAN(I)'/(15X,9(I5,2X,A4)))                        WMIN2655
      PRINT 185,(SAN(I),I=1,NV)                                         WMIN2660
  185 FORMAT(15X,9F11.6)                                                WMIN2665
C     SCALE MATRIX AND VECTOR                                           WMIN2670
 1230 IM=0                                                              WMIN2675
      DO 1240 I=1,NV                                                    WMIN2680
      VN(I)=VN(I)*SAN(I)                                                WMIN2685
      DO 1235 J=1,NV                                                    WMIN2690
      IM=IM+1                                                           WMIN2695
      AN(IM)=AN(IM)*SAN(I)*SAN(J)                                       WMIN2700
 1235 CONTINUE                                                          WMIN2705
 1240 CONTINUE                                                          WMIN2710
C     ADD CONSTANT TO (UNIT) DIAGONAL ELEMENTS FOR MARQUARDTS COMPROMISEWMIN2715
      IM=1                                                              WMIN2720
      DO 1245 I=1,NV                                                    WMIN2725
      AN(IM)=AN(IM)+CMPR                                                WMIN2730
      IM=IM+NV+1                                                        WMIN2735
 1245 CONTINUE                                                          WMIN2740
C     DETERMINE EIGENVALUES AND EIGENVECTORS OF MATRIX AND PRINT THEM   WMIN2745
      DO 1250 I=1,NVV                                                   WMIN2750
 1250 EVEC(I)=AN(I)                                                     WMIN2755
      IF(NV-1)1260,1255,1260                                            WMIN2760
 1255 EVAL(1)=AN(1)                                                     WMIN2765
      EVEC(1)=1.0                                                       WMIN2770
      GO TO 1270                                                        WMIN2775
 1260 CALL HOUSEH(EVEC,NV,NV,EVAL,TQ)                                   WMIN2780
      CALL VALVEC(EVAL,TQ,EVEC,NE,NV,NV)                                WMIN2785
      IF(NE)1265,1270,1265                                              WMIN2790
 1265 PRINT 190                                                         WMIN2795
  190 FORMAT('0*** VALVEC FAILS ***')                                   WMIN2800
 1270 IF(IPRC-1)1275,1275,1285                                          WMIN2805
 1275 PRINT 195,(IOUT(I),NOUT(I),I=1,NV)                                WMIN2810
  195 FORMAT('0',16X,'EVEC(I,J)'/'    J     EVAL(J)',9(I5,2X,A4)        WMIN2815
     1/(15X,9(I5,2X,A4)))                                               WMIN2820
      K2=0                                                              WMIN2825
      DO 1280 J=1,NV                                                    WMIN2830
      K1=K2+1                                                           WMIN2835
      K2=K2+NV                                                          WMIN2840
      PRINT 200,J,EVAL(J),(EVEC(K),K=K1,K2)                             WMIN2845
  200 FORMAT(X,I3,E11.3,9F11.6/(15X,9F11.6))                            WMIN2850
 1280 CONTINUE                                                          WMIN2855
C     PRINT RESCALED EIGENVECTORS                                       WMIN2860
 1285 CALL MPRD( SAN,EVEC,TMAT,NV,NV,2,0,NV)                            WMIN2865
      IF(IPRC)1290,1290,1330                                            WMIN2870
 1290 PRINT 205,(IOUT(I),NOUT(I),I=1,NV)                                WMIN2875
  205 FORMAT('0',16X,'SAN(I)*EVEC(I,J)'/'    J     EVAL(J)',9(I5,2X,A4) WMIN2880
     1/(15X,9(I5,2X,A4)))                                               WMIN2885
      K2=0                                                              WMIN2890
      DO 1295 J=1,NV                                                    WMIN2895
      K1=K2+1                                                           WMIN2900
      K2=K2+NV                                                          WMIN2905
      PRINT 210,J,EVAL(J),(TMAT(K),K=K1,K2)                             WMIN2910
  210 FORMAT(X,I3,E11.3,9F11.6/(15X,9F11.6))                            WMIN2915
 1295 CONTINUE                                                          WMIN2920
C     PREPARE TO PRINT CORRELATION OF OBSERVATIONS WITH EIGENVECTORS    WMIN2925
      J=0                                                               WMIN2930
      PRINT 215,(I,I=1,NV)                                              WMIN2935
  215 FORMAT('0',23X,'WMAT*SMAT*SAN*EVEC'/'    J   NAMP(J)   DYC(J)'    WMIN2940
     1,9(I1/(21X,9I1)))                                                 WMIN2945
C     BRING INFORMATION FOR EACH SUBSTANCE FROM AUX STORAGE IF USED     WMIN2950
      IF(NVC)1300,1310,1300                                             WMIN2955
 1300 END FILE NB                                                       WMIN2960
      REWIND NB                                                         WMIN2965
 1305 READ(NB,END=1330) KPW,NOS,NVOS,WOWC,(BTR(I),I=1,NVOS)             WMIN2970
     1,(DWDQ(I),I=1,NV),(DYC(I),I=1,NO)                                 WMIN2975
C     PRINT TERMS IN OBSERVED ENERGY IF USED AS OBSERVATION             WMIN2980
 1310 IF(KPW)1315,1320,1315                                             WMIN2985
 1315 CALL GTPRD(TMAT,DWDQ,UMAT,NV,NV,1)                                WMIN2990
      PRINT 220,WOWC,(UMAT(I),I=1,NV)                                   WMIN2995
  220 FORMAT(6X,'WOBS',10F11.4/(21X,9F11.4))                            WMIN3000
C     PRINT TERMS IN OTHER OBSERVATIONS FOR ONE SUBSTANCE               WMIN3005
 1320 CALL GTPRD(TMAT,BTR,UMAT,NV,NV,NOS)                               WMIN3010
      K2=0                                                              WMIN3015
      DO 1325 I=1,NOS                                                   WMIN3020
      J=J+1                                                             WMIN3025
      K1=K2+1                                                           WMIN3030
      K2=K2+NV                                                          WMIN3035
      PRINT 225,JOUT(J),NOBS(J),DYC(I),(UMAT(K),K=K1,K2)                WMIN3040
  225 FORMAT(X,I3,2X,A4,10F11.4/(21X,9F11.4))                           WMIN3045
 1325 CONTINUE                                                          WMIN3050
C     JUMP BACK TO PRINT TERMS FOR NEXT SUBSTANCE                       WMIN3055
      IF(NVC)1305,1330,1305                                             WMIN3060
C     INVERT EIGENVALUES AND COUNT EIGENVECTORS TO BE USED IN REFINEMENTWMIN3065
 1330 ELIM=EVAL(1)*ARE                                                  WMIN3070
      NVU=0                                                             WMIN3075
      DO 1340 K=1,NV                                                    WMIN3080
      IF(EVAL(K)-ELIM)1345,1345,1335                                    WMIN3085
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 1335 EVAL(K)=1.0/EVAL(K)
      NVU=NVU+1
 1340 CONTINUE
      GO TO 1350
 1345 PRINT 230,NVU
  230 FORMAT('0ONLY FIRST',I3,' VARIED')
C     SAVE NUMBER USED FOR FINAL SUMMARY
 1350 IF(IC-8)1355,1355,1360
 1355 NVUS(IC+1)=NVU
C     GENERATE INVERSE MATRIX INCLUDING ONLY NVU EIGENVECTORS
 1360 IJ=0
      DO 1390 J=1,NV
      JI=J
      DO 1385 I=1,NV
      IF(I-J)1365,1370,1370
 1365 ANIJ=AN(JI)
      GO TO 1380
 1370 IK=I
      JK=J
      ANIJ=0.0
      DO 1375 K=1,NVU
      ANIJ=ANIJ+EVAL(K)*EVEC(IK)*EVEC(JK)
      IK=IK+NV
      JK=JK+NV
 1375 CONTINUE
 1380 IJ=IJ+1
      AN(IJ)=ANIJ
      JI=JI+NV
 1385 CONTINUE
 1390 CONTINUE
C     CALCULATE PARAMETER CHANGES AND THEIR ERRORS
      IM=0
      DO 1415 J=1,NV
      PDJ=0.0
      DO 1410 I=1,NV
      IM=IM+1
      PDJ=PDJ+VN(I)*AN(IM)
      IF(I-J)1410,1395,1410
 1395 DIAG=AN(IM)
      IF(LS)1405,1400,1405
 1400 ERR(J)=DIAG*SAN(J)**2*SIGMA
      GO TO 1410
 1405 ERR(J)=DSQRT(DIAG)*SAN(J)*SIGMA
 1410 CONTINUE
      PD(J)=PDJ*SAN(J)
 1415 CONTINUE
C     ADJUST PARAMETERS AND PRINT
      IF(IPRT-2)1420,1420,1425
 1420 PRINT 235,IC
  235 FORMAT('0PARAMETERS AFTER CYCLE',I3/'   I      NAMP       OLD P
     1CHANGE       NEW P        ERR')
 1425 ID=0
      IB=0
      DO 1475 I=1,NP
      PSV(I)=P(I)
      IF(KQ(I))1430,1475,1430
 1430 ID=ID+1
      KQI=KQ(I)
      PDK=PD(ID)*DKT(KQI)
      P(I)=P(I)+PDK
C     SAVE PARAMETERS FOR SUMMARY OUTPUT
      IF(IC-8)1435,1435,1440
 1435 PS(IC+1,ID)=P(I)
 1440 IF(IPRT-2)1445,1445,1450
 1445 PRINT 240,I,NAMP(I),PSV(I),PDK,P(I),ERR(ID)
  240 FORMAT(X,I3,5X,A4,4F11.6)
C     TEST PARAMETER AGAINST UPPER AND LOWER LIMITS
 1450 IF(P(I)-PMN(I))1460,1455,1455
 1455 IF(P(I)-PMX(I))1475,1475,1460
 1460 IB=1
 1475 CONTINUE
C     TEST INDICATORS AND IF NECESSARY REDUCE NUMBER OF VARIABLES
      IF(IPLM)1480,1500,1480
 1480 IF(IB)1485,1500,1485
 1485 NVU=NVU-1
      PRINT 250,NVU
  250 FORMAT('0NUMBER OF VARIABLES REDUCED TO',I3)
      DO 1490 I=1,NP
      P(I)=PSV(I)
 1490 CONTINUE
      IF(NVU)1495,1495,1350
 1495 NCS=IC-1
      GO TO 1610
C     JUMP BACK FOR NEXT CYCLE
 1500 IC=IC+1
      GO TO 745
C     PRINT DERIVATIVES ON LAST CYCLE UNLESS NUMBER OF CYCLES IS ZERO
 1505 IF(MODE-4)1510,1515,1510
 1510 IF(NC)1515,1525,1515
 1515 IF(IPRT-3)1520,1520,1525
 1520 PRINT 255,IC
  255 FORMAT('0DERIVATIVES BEFORE CYCLE' I3/'   J  NAMP(J)  DYC(J)')
      PRINT 260,(JOTS(J),NOSS(J),DYC(J),J=1,NOS)
  260 FORMAT(X,I3,2X,A4,F11.4)
C     ANALYZE AND PRINT TIMES FOR VARIOUS PARTS OF ENERGY CALCULATION
 1525 IF(IPRC-1)1530,1530,1535
 1530 CALL TIMOUT
C     CALL SUBROUTINE TO CALCULATE AND PRINT VIBRATIONS IF SPECIFIED
 1535 IF(MODE-4)1545,1540,1545
 1540 CALL WDYN
C     MAKE FINAL ENTRY TO WCALC AND PRINT REVISED ATOM COORDINATES
 1545 IF(NC)1550,1585,1550
 1550 IRK=1
      W=WCALC(0)
      PRINT 265,(J,NAME(J),IKA(J),IRB(J),(XYZR(I,J),I=1,3),J=1,NA)
  265 FORMAT('0  J  NAME   IKA   IRB          X          Y          Z'
     1/(X,I3,2X,A4,2I6,2X,3F9.5))
C     PUNCH LATTICE PARAMETERS IF ADJUSTED
      IF(NVA)1555,1560,1555
 1555 PUNCH 270,A
  270 FORMAT(6F9.5)
C     PUNCH ATOM COORDINATES IF ALTERED
 1560 IF(NVR)1565,1575,1565
 1565 DO 1570 J=1,NA
      PUNCH 275,NAME(J),IKA(J),(XYZR(I,J),I=1,3)
  275 FORMAT(A4,I5,I8X,3F9.5)
 1570 CONTINUE
C     PUNCH EXTRA PARAMETERS IF ADJUSTED
 1575 IF(NVX)1580,1585,1580
 1580 PUNCH 280,(PX(I),I=1,NPX)
  280 FORMAT(8F9.5)
C     PUNCH VIBRATIONAL FREQUENCIES IF CALCULATED
 1585 IF(MODE-4)1595,1590,1595
 1590 PUNCH 285,(FREQ(I),I=1,NVD)
  285 FORMAT(8F9.2)
C     PUNCH COMMON PARAMETERS IF ADJUSTED
 1595 IF(NC)1597,1605,1597
 1597 IF(NVC)780,1605,780
 1600 PUNCH 290,(PC(I),I=1,NPC)
  290 FORMAT(8F9.5)
C     PREPARE TO PRINT SUMMARY, ONCE ON EACH OF TWO OUTPUT STREAMS
 1605 NCS=NC
 1610 IF(NCS-8)1620,1620,1615
 1615 NCS=8
 1620 NCYS=NCS+1
      NSO=NSP
      NSU=1
      IF(IPRT-4)1625,1625,1630
 1625 NSU=2
 1630 DO 1695 N=1,NSU
      WRITE(NSO,295)
  295 FORMAT('1*****************************************************')
      WRITE(NSO,300) TITLE,DATE
  300 FORMAT(1H0,18A4,8X,A8)
      IF(NVC)1640,1635,1640
 1635 WRITE(NSO,305) STITLE
  305 FORMAT(X,17A4)
 1640 WRITE(NSO,310) MODE,NC,NPC,ILSQ,IWGT,IPLM,IPRT,NSTG,IBPC
     1,ARE,SLIM,CMPR,XDRD,EPSC
  310 FORMAT('0  MODE    NC    NPC   ILSQ  IWGT  IPLM  IPRT  NSTG  IBPC
     1       ARE          SLIM         CMPR         XDRD         EPSC'
     2/X,9I6,5E12.3)
      IF(NPC)1643,1644,1643
 1643 WRITE(NSO,311) (NAMPC(I),I=1,NPC)
  311 FORMAT(/(X,8(5X,A4)))
      WRITE(NSO,312) (PC(I),I=1,NPC)
  312 FORMAT(X,8F9.5)
 1644 IF(NVC)1650,1645,1650
 1645 WRITE(NSO,315) NA,NKA,NS,ICENT,HXNEG,HYNEG,HZNEG,NRB,NPX,NRP
     1,ICMB,IVDW,IREP,IMOL,NCT,IRSC,IZAM,IGEM,IRBA,ISETA
  315 FORMAT('0    NA    NKA    NS ICENT HXNEG HYNEG HZNEG   NRB   NPX
     1NRP  ICMB  IVDW  IREP  IMOL   NCT  IRSC  IZAM  IGEM  IRBA ISETA'
     2/X,4I6,3F6.1,13I6)
 1650 IF(NC)1652,1680,1652
 1652 WRITE(NSO,320) NO,NV,NOV,LS,IWT
  320 FORMAT('0    NO    NV   NOV    LS   IWT'/X,5I6)
      WRITE(NSO,325) (I,I=1,NCS)
  325 FORMAT('0',20X,'PARAMETERS AFTER EACH CYCLE'/
     1'  J   NAMP    DKT       INITIAL',I7,7I11)
      DO 1655 I=1,NV
      J=IOUT(I)
      KQI=KQ(J)
      DKTKQI=DKT(KQI)
      WRITE(NSO,330) J,NOUT(I),DKTKQI,(PS(K,I),K=1,NCYS)
  330 FORMAT(X,I3,2X,A4,F7.3,9F11.6)
 1655 CONTINUE
      IF(MODE-4)1660,1665,1660
 1660 IF(MODE-2)1665,1670,1675
 1665 WRITE(NSO,335) (NVUS(I),I=2,NCYS)
  335 FORMAT(1H0,12X,'NVU',12X,8I11)
 1670 WRITE(NSO,340) (RDWSS(I),I=1,NCS)
  340 FORMAT(1H0,12X,'RDWS',9F11.4)
      IF(NVC)1680,1675,1680
 1675 WRITE(NSO,345) (WS(I),I=1,NCYS)
  345 FORMAT(1H0,12X,'W    ',9F11.4)
 1680 IF(MODE-4)1690,1685,1690
 1685 WRITE(NSO,350) (FREQ(I),I=1,NVD)
  350 FORMAT('0FREQ(I)'/('0',8F10.2))
 1690 WRITE(NSO,355)
  355 FORMAT('0*****************************************************')
      NSO=NSP
 1695 CONTINUE
C     BACK FOR NEXT SUBSTANCE IF TREATED SEPARATELY. OTHERWISE NEXT JOB
 1700 IF(NVC)1705,595,1705
 1705 RETURN
C     ENERGY MAPPING MODE
C     SET UP PARAM AND NAME FOR OUTPUT IF LESS THAN THREE ARE STEPPED
 1710 P(NPMAX)=0.0
      NAMP(NPMAX)=NONE
C     READ DATA FOR OUTER LOOP
 1715 READ 360,KPI,MPI,PINI,PDLI,PLMI
  360 FORMAT(2I3,3X,3F9.0)
C     SET PARAMETER NUMBER FOR OUTER LOOP. TERMINATE MAPPING ON BLANK
      IF(KPI)1730,1720,1735
 1720 IF(MPI)1725,595,1725
 1725 LPI=MPI
      GO TO 1740
 1730 LPI=NPMAX
      GO TO 1740
 1735 LPI=MPI+NPC
C     PRINT TITLES AND OUTER LOOP INPUT
 1740 PRINT 365,TITLE,DATE,STITLE
  365 FORMAT(1H1,18A4,8X,A8/X,17A4)
      PRINT 370,KPI,MPI,LPI,PINI,PDLI,PLMI
  370 FORMAT('0   KPI    MPI    LPI      PINI       PDLI       PLMI'
     1/X,3I6,3F9.5)
C     READ DATA FOR MIDDLE LOOP
      READ 375,KPJ,MPJ,PINJ,PDLJ,PLMJ
  375 FORMAT(2I3,3X,3F9.0)
C     SET PARAMETER NUMBER FOR MIDDLE LOOP
      IF(KPJ)1745,1750,1755
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 1745 LPJ=NPMAX                                                         WMIN4195
      GO TO 1760                                                        WMIN4200
 1750 LPJ=MPJ                                                           WMIN4205
      GO TO 1760                                                        WMIN4210
 1755 LPJ=MPJ+NPC                                                       WMIN4215
C     PRINT MIDDLE LOOP INPUT                                           WMIN4220
 1760 PRINT 380,KPJ,MPJ,LPJ,PINJ,PDLJ,PLMJ                              WMIN4225
  380 FORMAT('0   KPJ    MPJ    LPJ      PINJ      PDLJ      PLMJ'      WMIN4230
     1/X,3I6,3F9.5)                                                     WMIN4235
C     READ DATA FOR INNER LOOP                                          WMIN4240
      READ 385,KPK,MPK,PINK,PDLK,PLMK                                   WMIN4245
  385 FORMAT(2I3,3X,3F9.0)                                              WMIN4250
C     SET PARAMETER NUMBER FOR INNER LOOP                               WMIN4255
      IF(KPK)1765,1770,1775                                             WMIN4260
 1765 LPK=NPMAX                                                         WMIN4265
      GO TO 1780                                                        WMIN4270
 1770 LPK=MPK                                                           WMIN4275
      GO TO 1780                                                        WMIN4280
 1775 LPK=MPK+NPC                                                       WMIN4285
C     PRINT INNER LOOP INPUT                                            WMIN4290
 1780 PRINT 390,KPK,MPK,LPK,PINK,PDLK,PLMK                              WMIN4295
  390 FORMAT('0   KPK    MPK    LPK      PINK      PDLK      PLMK'      WMIN4300
     1/X,3I6,3F9.5)                                                     WMIN4305
C     INITIALIZE COUNTERS AND TIMERS                                    WMIN4310
      DO 1785 I=1,9                                                     WMIN4315
      NT(I)=0                                                           WMIN4320
      LT(I)=0                                                           WMIN4325
 1785 CONTINUE                                                          WMIN4330
C     CALL ENERGY SUBROUTINE TWICE SO THAT ALL ITS PRINTING IS FINISHED WMIN4335
      JC=0                                                              WMIN4340
      IPRC=IPRT-2                                                       WMIN4345
      ISW=0                                                             WMIN4350
      ISW=1                                                             WMIN4355
      WT=WCALC(0)                                                       WMIN4360
      ISW=0                                                             WMIN4365
      WT=WCALC(0)                                                       WMIN4370
C     PRINT CAPTION                                                     WMIN4375
      PRINT 395,LPI,NAMP(LPI),LPJ,NAMP(LPJ),LPK,NAMP(LPK)               WMIN4380
  395 FORMAT(1H0,I5,2X,A4,I5,2X,A4,I5,2X,A4,'          WC          WV   WMIN4385
     1    WR          WX          WT')                                 WMIN4390
C     SAVE VARIABLE PARAMETERS                                          WMIN4395
      PSVI=P(LPI)                                                       WMIN4400
      PSVJ=P(LPJ)                                                       WMIN4405
      PSVK=P(LPK)                                                       WMIN4410
C     START OUTER LOOP IF USED                                          WMIN4415
      IF(KPI)1795,1790,1790                                             WMIN4420
 1790 P(LPI)=PINI                                                       WMIN4425
      PRINT 400                                                         WMIN4430
  400 FORMAT(X)                                                         WMIN4435
C     START MIDDLE LOOP IF USED                                         WMIN4440
 1795 IF(KPJ)1805,1800,1800                                             WMIN4445
 1800 P(LPJ)=PINJ                                                       WMIN4450
      PRINT 405                                                         WMIN4455
  405 FORMAT(X)                                                         WMIN4460
C     START INNER LOOP IF USED                                          WMIN4465
 1805 IF(KPK)1815,1810,1810                                             WMIN4470
 1810 P(LPK)=PINK                                                       WMIN4475
      PRINT 410                                                         WMIN4480
  410 FORMAT(X)                                                         WMIN4485
C     CALCULATE ENERGY AND PRINT IT WITH PARAMETER VALUES               WMIN4490
 1815 WT=WCALC(0)                                                       WMIN4495
      PRINT 415,P(LPI),P(LPJ),P(LPK),WC,WV,WR,WX,WT                     WMIN4500
  415 FORMAT(X,3F11.5,5F11.3)                                           WMIN4505
C     ADVANCE AND TEST LOOPS                                            WMIN4510
      IF(KPK)1825,1820,1820                                             WMIN4515
 1820 P(LPK)=P(LPK)+PDLK                                                WMIN4520
      IF(P(LPK)-PLMK)1815,1815,1825                                     WMIN4525
 1825 IF(KPJ)1835,1830,1830                                             WMIN4530
 1830 P(LPJ)=P(LPJ)+PDLJ                                                WMIN4535
      IF(P(LPJ)-PLMJ)1805,1805,1835                                     WMIN4540
 1835 IF(KPI)1845,1840,1840                                             WMIN4545
 1840 P(LPI)=P(LPI)+PDLI                                                WMIN4550
      IF(P(LPI)-PLMI)1795,1795,1845                                     WMIN4555
C     RESTORE ORIGINAL VALUES TO PARAMETERS                             WMIN4560
 1845 P(LPI)=PSVI                                                       WMIN4565
      P(LPJ)=PSVJ                                                       WMIN4570
      P(LPK)=PSVK                                                       WMIN4575
C     ANALYZE AND PRINT TIMES FOR VARIOUS PARTS OF ENERGY CALCULATION   WMIN4580
      CALL TIMOUT                                                       WMIN4585
C     JUMP BACK TO READ FURTHER MAPPING INSTRUCTIONS                    WMIN4590
      GO TO 1715                                                        WMIN4595
C     METHOD OF STEEPEST DESCENTS                                       WMIN4600
C     PRINT FIRST DERIVATIVES AND ACCUMULATE DISCREPANCY FACTOR         WMIN4605
 1850 SDWS=0.0                                                          WMIN4610
      PRINT 420,IC                                                      WMIN4615
  420 FORMAT('0DERIVATIVES BEFORE STEEPEST DESCENT CYCLE',I3            WMIN4620
     1/'   I  NAMP(I)  -DW(I)')                                         WMIN4625
      DO 1860 I=1,NP                                                    WMIN4630
      IF(KG(I))1855,1860,1855                                           WMIN4635
 1855 DWMI=-DW(I)                                                       WMIN4640
      SDWS=SDWS+DWMI**2                                                 WMIN4645
      PRINT 425,I,NAMP(I),DWMI                                          WMIN4650
  425 FORMAT(X,I3,2X,A4,F11.4)                                          WMIN4655
 1860 CONTINUE                                                          WMIN4660
C     PRINT DISCREPANCY FACTORS                                         WMIN4665
      RDWS=DSQRT(SDWS)                                                  WMIN4670
      PRINT 430,RDWS,SDWS                                               WMIN4675
  430 FORMAT('0          RDWS              SDWS'/X,2E15.6)              WMIN4680
C     SAVE DISCREPANCY FACTOR FOR SUMMARY                               WMIN4685
      IF(IC-9)1865,1865,1870                                            WMIN4690
 1865 RDWSS(IC)=RDWS                                                    WMIN4695
C     SET INITIAL STEP SIZE FROM INPUT ON OVERALL CONTROL CARD          WMIN4700
 1870 XD=XDRG                                                           WMIN4705
C     SET MINIMUM STEP SIZE                                             WMIN4710
      XDMN=0.1*DABS(XD)                                                 WMIN4715
C     PRINT CAPTION                                                     WMIN4720
      IF(IPRC)1875,1875,1880                                            WMIN4725
 1875 PRINT 435                                                         WMIN4730
  435 FORMAT('0          WXN          WXL          XN          XL          XD  WMIN4735
     1IFST ISTP IRGT')                                                  WMIN4740
C     INITIALIZE SEARCH FOR ENERGY MINIMUM ALONG STEEPEST DESCENT VECTORWMIN4745
 1880 XL=0.0                                                            WMIN4750
      WXL=W                                                             WMIN4755
C     SAVE PARAMETERS                                                   WMIN4760
      DO 1885 I=1,NP                                                    WMIN4765
 1885 PSV(I)=P(I)                                                       WMIN4770
C     SET INDICATORS                                                    WMIN4775
      ISTP=1                                                            WMIN4780
      IFST=1                                                            WMIN4785
 1890 IRGT=1                                                            WMIN4790
C     MAKE A STEP. CALCULATE AND PRINT ENERGY                           WMIN4795
 1895 XN=XL+XD                                                          WMIN4800
      DO 1900 I=1,NP                                                    WMIN4805
 1900 P(I)=PSV(I)-XN*DW(I)                                              WMIN4810
      WXN=WCALC(0)                                                      WMIN4815
      IF(IPRC)1905,1905,1910                                            WMIN4820
 1905 PRINT 440,WXN,WXL,XN,XL,XD,IFST,ISTP,IRGT                         WMIN4825
  440 FORMAT(X,2F11.4,3F11.8,3I5)                                       WMIN4830
 1910 IF(WXN-WXL)1915,1920,1920                                         WMIN4835
C     SUCCESSFUL.                                                       WMIN4840
 1915 IFST=0                                                            WMIN4845
      XL=XN                                                             WMIN4850
      WXL=WXN                                                           WMIN4855
C     KEEP STEPPING IF MINIMUM HAS NOT BEEN FOUND                       WMIN4860
      IF(ISTP)1890,1950,1890                                            WMIN4865
 1920 IF(IFST)1925,1930,1925                                            WMIN4870
C     ENERGY INCREASES ON FIRST STEP. REVERSE DIRECTION                 WMIN4875
 1925 IFST=0                                                            WMIN4880
      XD=-XD                                                            WMIN4885
      GO TO 1890                                                        WMIN4890
 1930 IF(ISTP)1935,1940,1935                                            WMIN4895
C     ENERGY INCREASES AFTER AN EARLIER DECREASE.                       WMIN4900
 1935 ISTP=0                                                            WMIN4905
      GO TO 1950                                                        WMIN4910
C     FAILURE AFTER PASSING MINIMUM. TRY OTHER DIRECTION ONCE.          WMIN4915
 1940 IF(IRGT)1945,1950,1945                                            WMIN4920
 1945 IRGT=0                                                            WMIN4925
      XD=-XD                                                            WMIN4930
      GO TO 1895                                                        WMIN4935
C     TEST SIZE OF STEP AND HALVE IT OR END SEARCH                      WMIN4940
 1950 IF(DABS(XD)-XDM)1960,1960,1955                                    WMIN4945
 1955 XD=0.5*XD                                                         WMIN4950
      GO TO 1890                                                        WMIN4955
C     PRINT PARAMETER CHANGES FOR STEEPEST DESCENTS OR ROSENBROCK SEARCHWMIN4960
 1960 IF(IPRT-2)1965,1965,1970                                          WMIN4965
 1965 PRINT 445,IC                                                      WMIN4970
  445 FORMAT('0PARAMETERS AFTER CYCLE',I3                               WMIN4975
     1/'   I      NAMP       OLD P      CHANGE      NEW P')             WMIN4980
 1970 ID=0                                                              WMIN4985
      DO 2020 I=1,NP                                                    WMIN4990
      IF(KG(I))1975,2020,1975                                           WMIN4995
 1975 IF(MODE-2)1985,1985,1980                                          WMIN5000
 1980 PDK=P(I)-PSV(I)                                                   WMIN5005
      GO TO 1990                                                        WMIN5010
 1985 PDK=-XL*DW(I)                                                     WMIN5015
      P(I)=PSV(I)+PDK                                                   WMIN5020
 1990 IF(IPRT-2)1995,1995,2000                                          WMIN5025
 1995 PRINT 450,I,NAMP(I),PSV(I),PDK,P(I)                               WMIN5030
  450 FORMAT(X,I3,5X,A4,3F11.6)                                         WMIN5035
 2000 ID=ID+1                                                           WMIN5040
C     SAVE VARIABLE PARAMETERS FOR OUTPUT IN SUMMARY                    WMIN5045
      IF(IC-6)2005,2005,2020                                            WMIN5050
 2005 PS(IC+1,ID)=P(I)                                                  WMIN5055
 2020 CONTINUE                                                          WMIN5060
C     ANALYZE AND PRINT TIMES FOR VARIOUS PARTS OF ENERGY CALCULATION   WMIN5065
      IF(IPRC-1)2025,2025,1500                                          WMIN5070
 2025 CALL TIMOUT                                                       WMIN5075
C     JUMP BACK TO START NEXT CYCLE                                     WMIN5080
      GO TO 1500                                                        WMIN5085
C     ROSENBROCK SEARCH FOR ENERGY MINIMUM. OMIT FINAL CYCLE.           WMIN5090
 2030 IF(IC-NCY)2040,2035,2040                                          WMIN5095
 2035 IF(IC)1650,1700,1550                                              WMIN5100
C     INITIALIZE. CALCULATE ENERGY. SAVE PARAMETERS. PRINT CAPTION      WMIN5105
 2040 ISTG=1                                                            WMIN5110
      WCUR=WCALC(0)                                                     WMIN5115
      DO 2045 I=1,NP                                                    WMIN5120
 2045 PSV(I)=P(I)                                                       WMIN5125
      IF(IPRC)2050,2050,2055                                            WMIN5130
 2050 PRINT 460                                                         WMIN5135
  460 FORMAT('0SEARCH FOR MINIMUM ENERGY'                               WMIN5140
     1/'   I          EPS(I)              P(I)              WYR')       WMIN5145
C     ON FIRST CYCLE START WITH EXPLORATORY SEARCH. LAYER CYCLES. VECTORWMIN5150
 2055 IF(IC-1)2135,2060,2135                                            WMIN5155
C     INITIALIZE INCREMENTS. SAVE INITIAL PARAMETERS OF FIRST STAGE     WMIN5160
 2060 DO 2065 I=1,NP                                                    WMIN5165
      EPS(I)=EPSC*DP(I)                                                 WMIN5170
      PBASE(I)=P(I)                                                     WMIN5175
 2065 CONTINUE                                                          WMIN5180
C     EXPLORATORY SEARCH. EACH PARAMETER ADJUSTED FOR AT LEAST ONE      WMIN5185
C        SUCCESS AND AT LEAST ONE FAILURE                               WMIN5190
 2070 DO 2125 I=1,NP                                                    WMIN5195
      IF(KG(I))2075,2125,2075                                           WMIN5200
 2075 ISU=0                                                             WMIN5205
      IFL=0                                                             WMIN5210
C     INCREMENT PARAMETER AND CALCULATE TRIAL ENERGY. PRINT OUTPUT      WMIN5215
 2080 PSAVE=P(I)                                                        WMIN5220
      P(I)=P(I)+EPS(I)                                                  WMIN5225
      WTR=WCALC(0)                                                      WMIN5230
      IF(IPRC)2085,2085,2090                                            WMIN5235
 2085 PRINT 465,I,EPS(I),P(I),WTR                                       WMIN5240
  465 FORMAT(X,I6,D16.6,2F16.8)                                         WMIN5245
 2090 IF(WTR-WCUR)2095,2095,2105                                        WMIN5250
C     SUCCESS. IF NO FAILURE YET INCREASE INCREMENT AND REPEAT          WMIN5255
 2095 WCUR=WTR                                                          WMIN5260
      IF(IFL)2125,2100,2125                                             WMIN5265
 2100 EPS(I)=3.0*EPS(I)                                                 WMIN5270
      ISU=1                                                             WMIN5275
      GO TO 2080                                                        WMIN5280
C     FAILURE. IF NO SUCCESS YET REDUCE INCREMENT AND CHANGE ITS SIGN   WMIN5285
 2105 P(I)=PSAVE                                                        WMIN5290
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      IF(WTR-WCUR-1.0D-6)2125,2125,2110
 2110 IF(ISU)2120,2115,2120
 2115 EPS(I)=-0.5*EPS(I)
      IFL=1
      GO TO 2080
 2120 EPS(I)=EPS(I)/3.0
 2125 CONTINUE
C     EXPLORATORY SEARCH FINISHED. COMPUTE VECTOR OF PARAMETER CHANGES
      VBSQ=0.0
      DO 2130 I=1,NP
      VBEST(I)=P(I)-PBASE(I)
      VBSQ=VBSQ+VBEST(I)**2
      PBASE(I)=P(I)
 2130 CONTINUE
C     TEST FOR END OF CYCLE
      ISTG=ISTG+1
      IF(ISTG-NSTG)2135,2135,1960
C     TEST FOR NULL VECTOR OF PARAMETER CHANGES
 2135 IF(VBSQ-1.0D-15)2140,2140,2145
 2140 PRINT 470
  470 FORMAT('0***SEARCH TERMINATED BECAUSE VBEST HAS BECOME NULL')
      GO TO 1960
C     VECTOR SEARCH. PARAMETERS ADJUSTED TOGETHER UNTIL AT LEAST ONE
C        SUCCESS AND AT LEAST ONE FAILURE HAS OCCURRED
 2145 ISU=0
      IFL=0
      EPSL=0.25
C     INCREMENT PARAMETERS AND CALCULATE ENERGY. PRINT OUTPUT
 2150 DO 2155 I=1,NP
 2155 P(I)=P(I)+EPSL*VBEST(I)
      WTR=WCALC(0)
      IF(IPRC)2160,2160,2165
 2160 PRINT 475,EPSL,WTR
  475 FORMAT(6X,'*',D16.6,16X,F16.6)
 2165 IF(WTR-WCUR)2190,2190,2170
C     FAILURE. IF NO SUCCESS YET REDUCE INCREMENTS AND CHANGE SIGN
 2170 DO 2175 I=1,NP
 2175 P(I)=P(I)-EPSL*VBEST(I)
      IF(WTR-WCUR-1.0D-6)2070,2070,2180
 2180 IF(ISU)2070,2185,2070
 2185 EPSL=-0.5*EPSL
      IFL=1
      GO TO 2150
C     SUCCESS. IF NO FAILURE YET INCREASE INCREMENTS AND REPEAT
 2190 WCUR=WTR
      IF(IFL)2070,2195,2070
 2195 EPSL=3.0*EPSL
      ISU=1
      GO TO 2150
      END


      SUBROUTINE WDYNI (AKE,AMASS,BTR,CHAR,DP,DXQ
     1,DYQ,DZQ,EVAL,FREQ,IKA,IOUT,KQ
     2,NAME,NAMS,NOUT,P,SYM,TQ,VN
     3,XYZ,XYZC,XYZD,XYZN,ZAM)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION AKE(1),AMASS(1),BTR(1),CHAR(1),DP(1),DXQ(NVMAX,1)
     1,DYQ(NVMAX,1),DZQ(NVMAX,1),EVAL(1),FREQ(1),IKA(1),IOUT(1),KQ(1)
     2,NAME(1),NAMS(1),NOUT(1),P(1),SYM(12,1),TQ(1),VN(1)
     3,XYZ(3,1),XYZC(3,1),XYZD(3,1),XYZN(3,1),ZAM(1)
C     /DUBL/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, TIMOUT
      COMMON/DUBL/A(6),AC(9),ACB(9),ASV(5),CA(9),CAB(9),CK
     1,CKKCAL,CRA(9),DAA,DATE,FKCAL,WR,PI,PICK,PICKZ,PIOKSQ
     2,PINHZ,QLIM(5),QMAX,RDWSS(9),RLIM(5),RM(9),RMAX,RTPIZ
     3,SA(6),SIGWO,SQTPDK,SQTPI,SQTPIK,TM(9),TPI,TRT(3),TV(3)
     4,UT(5),UV(3),UW(3),WC,WCBS,WS(9),WV,WX,XYZA(3),XYZAS(3)
     5,XYZDS(3),ZMC
C     /MAXX/ USED BY MAIN, WMIN, WDYN, WPRE, WCALC, AND GCWX
      COMMON/MAX/NPCMAX,NAMAX,NKAMAX,NSMAX,NRBMAX,NPXMAX,NCTMAX,NBCMAX
     1,MMAX,NFSMAX,NGSMAX,NPSMAX,NPMAX,NOSMAX,NOMAX,NVMAX,ND,NB,NSD,NSP
C     /ITGR/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, IBYPAS, TIMOUT
      COMMON/ITGR/IBK,ICCAX,ICENT,ICMB,IGEM,ILSQ,IMOL,INK,IPLM,IPRC
     1,IPRT,IRBA,IREP,IRSC,ISB,ISW,IVDW,IWGT,IZAM,JC,KPW,KPWS,LT(9)
     2,MODE,NA,NAC,NAF,NBC,NCT,NKA,NOS,NP,NPC,NPR,NPS,NPX,NQ,ISETA
     3,NR,NRB,NRP,NS,NT(9),NV,NVA,NVC,NVD,NVR,NVUS(9),NVX
      REAL*4 XXD,YYD,ZZD
      RETURN
C
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS
C
C     CALCULATE FREQUENCIES AND NORMAL MODES
C
      ENTRY WDYN
C     SET INDICATOR TO STOP ENERGY CALCULATION AFTER COORDS ARE OBTAINED
      IBK=1
      II=0
C     CALCULATE DERIVATIVES OF ATOM COORDS WITH RESPECT TO VARIABLES
      NPCA=NPC+7
      DO 520 I=NPCA,NP
      IF(KQ(I))500,520,500
  500 II=II+1
      PISAVE=P(I)
      P(I)=PISAVE-DP(I)
      W=WCALC(0)
      DO 510 K=1,NA
      DO 505 L=1,3
C     SAVE CARTESIAN COORDS GENERATED IN ENERGY SUBROUTINE
      XYZN(L,K)=XYZC(L,K)
  505 CONTINUE
  510 CONTINUE
      P(I)=PISAVE+DP(I)
      W=WCALC(0)
      P(I)=PISAVE
      DO 515 K=1,NA
      DXQ(II,K)=(XYZC(1,K)-XYZN(1,K))/(2.0*DP(I))
      DYQ(II,K)=(XYZC(2,K)-XYZN(2,K))/(2.0*DP(I))
      DZQ(II,K)=(XYZC(3,K)-XYZN(3,K))/(2.0*DP(I))
  515 CONTINUE
  520 CONTINUE
      IBK=0
C     GET NUMBER OF DYNAMIC VARIABLES. EXCLUDES LATTICE PARAMETERS
      NVD=NV-NVA
C     PRINT DERIVATIVES
      IF(IPRT-2)525,525,535
  525 DO 530 I=1,NVD
      PRINT 5,I,(K,NAME(K),DXQ(I,K),DYQ(I,K),DZQ(I,K),K=1,NA)
    5 FORMAT('0DDYNAMIC VARIABLE',I4
     1/16X,'ATOM      DXQ          DYQ          DZQ'
     2/(11X,I3,2X,A4,3F11.6))
  530 CONTINUE
C     SET UP KINETIC ENERGY MATRIX (INVERSE OF USUAL G MATRIX)
  535 DO 550 I=1,NVD
      DO 545 J=1,NVD
      AKEIJ=0.0
      DO 540 K=1,NA
      L=IKA(K)
      IF(L)540,540,538
  538 AKEIJ=AKEIJ+ZAM(K)*AMASS(L)*(DXQ(I,K)*DXQ(J,K)+DYQ(I,K)*DYQ(J,K)
     1+DZQ(I,K)*DZQ(J,K))
  540 CONTINUE
      IJ=I+NVD*(J-1)
      JI=J+NVD*(I-1)
      AKE(IJ)=AKEIJ
      AKE(JI)=AKEIJ
  545 CONTINUE
  550 CONTINUE
C     REMOVE TERMS IN LATTICE PARAMETERS FROM POTENTIAL ENERGY MATRIX
  555 IF(NVA)560,575,560
  560 IJ=0
      KL=NV*NVA
      DO 570 J=1,NVD
      KL=KL+NVA
      DO 565 I=1,NVD
      IJ=IJ+1
      KL=KL+1
      BTR(IJ)=BTR(KL)
  565 CONTINUE
  570 CONTINUE
C     PRINT POTENTIAL ENERGY MATRIX
  575 NVAP=NVA+1
      IF(IPRT-1)580,580,590
  580 PRINT 10,(IOUT(I),NOUT(I),I=NVAP,NV)
   10 FORMAT('0',14X,'BTR'/(15X,9(I5,2X,A4)))
      K2=0
      DO 585 J=1,NVD
      K1=K2+1
      K2=K2+NVD
      JVD=J+NVA
      PRINT 15,IOUT(JVD),NOUT(JVD),(BTR(K),K=K1,K2)
   15 FORMAT(X,I5,2X,A4,3X,9F11.4/(15X,9F11.4))
  585 CONTINUE
C     PRINT KINETIC ENERGY MATRIX
  590 IF(IPRT-1)595,595,605
  595 PRINT 20,(IOUT(I),NOUT(I),I=NVAP,NV)
   20 FORMAT('0',14X,'AKE'/(15X,9(I5,2X,A4)))
      K2=0
      DO 600 J=1,NVD
      K1=K2+1
      K2=K2+NVD
      JVD=J+NVA
      PRINT 25,IOUT(JVD),NOUT(JVD),(AKE(K),K=K1,K2)
   25 FORMAT(X,I5,2X,A4,3X,9F11.4/(15X,9F11.4))
  600 CONTINUE
C     TREAT SPECIAL CASE OF ONLY ONE VARIABLE
  605 IF(NVD-1)620,610,620
  610 IF(AKE(1))625,625,615
  615 EVAL(1)=BTR(1)/AKE(1)
      BTR(1)=1.0/DSQRT(AKE(1))
      GO TO 645
C     SOLVE EIGENVALUE PROBLEM
  620 CALL AXELBX(NVD,BTR,AKE,NVD,TQ,NE)
      IF(NE)625,630,625
  625 PRINT 30
   30 FORMAT('0*** AXELBX FAILS ***')
      GO TO 725
  630 CALL HOUSEH(BTR,NVD,NVD,EVAL,VN)
      CALL VALVEC(EVAL,VN,BTR,NE,NVD,NVD)
      IF(NE)635,640,635
  635 PRINT 35
   35 FORMAT('0*** VALVEC FAILS ***')
      GO TO 725
  640 CALL TRANSF(BTR,AKE,TQ,NVD,NVD,NVD)
C     CALCULATE FREQUENCIES IN WAVE NUMBERS
  645 DO 650 I=1,NVD
      FREQ(I)=DSIGN(DSQRT(DABS(EVAL(I))),EVAL(I))*108.594100
  650 CONTINUE
C     PRINT EIGENVALUES AND EIGENVECTORS
      IF(IPRT-1)655,655,665
  655 PRINT 40,(IOUT(I),NOUT(I),I=NVAP,NV)
   40 FORMAT('0',14X,'EVEC'
     1/'  J   EVAL(J) ',9(I5,2X,A4)/(15X,9(I5,2X,A4)))
      K2=0
      DO 660 J=1,NVD
      K1=K2+1
      K2=K2+NVD
      PRINT 45,J,EVAL(J),(BTR(K),K=K1,K2)
   45 FORMAT(X,I3,E11.3,9F11.6/(15X,9F11.6))
  660 CONTINUE
C     COMPUTE MATRIX FOR TRANSFORMING NORMAL COORDS TO CRYSTAL SYSTEM
  665 IF(IPRT.GT.4) GO TO 725
      CALL INVRS(ACB,D,CAB)
C     START LOOP THROUGH THE NORMAL MODES OF VIBRATION
      DO 720 J=1,NVD
C     GENERATE CARTESIAN VECTORS FOR EACH ATOM FOR THIS MODE
      DO 675 K=1,NA
      XYZD(1,K)=0.0
      XYZD(2,K)=0.0
      XYZD(3,K)=0.0
      IJ=NVD*(J-1)
      DO 670 I=1,NVD
      IJ=IJ+1
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      XYZD(1,K)=XYZD(1,K)+DXG(I,K)*BTR(IJ)                              WDYN 855
      XYZD(2,K)=XYZD(2,K)+DYG(I,K)*BTR(IJ)                              WDYN 860
      XYZD(3,K)=XYZD(3,K)+DZG(I,K)*BTR(IJ)                              WDYN 865
  670 CONTINUE                                                          WDYN 870
  675 CONTINUE                                                          WDYN 875
C     PRINT RESULTS FOR ONE VIBRATIONAL MODE                            WDYN 880
      PRINT 50,J,FREQ(J),(K,NAME(K),(XYZD(L,K),L=1,3),K=1,NA)           WDYN 885
   50 FORMAT('0FREQ(',I3,')      CARTESIAN NORMAL COORDINATE'           WDYN 890
     1/X,F9.2,6X,'ATOM       DX          DY          DZ'                WDYN 895
     2(11X,I3,2X,A4,3F11.6))                                            WDYN 900
C     DETERMINE SYMMETRY OF THIS VIBRATIONAL MODE                       WDYN 905
C     ACCUMULATE SUM OF SQUARES OF DISPLACEMENTS                        WDYN 910
      UU=0.0                                                            WDYN 915
      DO 685 K=1,NA                                                     WDYN 920
C     OMIT EXTRA ATOMS                                                  WDYN 925
      IF(IKA(K))678,685,678                                             WDYN 930
  678 DO 680 L=1,3                                                      WDYN 935
      UU=UU+XYZD(L,K)**2                                                WDYN 940
  680 CONTINUE                                                          WDYN 945
  685 CONTINUE                                                          WDYN 950
C     START LOOP THROUGH SYMMETRY OPERATIONS TO GET CHARACTERS OF MODE  WDYN 955
      DO 715 I=1,NS                                                     WDYN 960
C     START LOOP THROUGH ATOMS TO ACCUMULATE INNER PRODUCT              WDYN 965
      US=0.0                                                            WDYN 970
      DO 714 L=1,NA                                                     WDYN 975
C     OMIT EXTRA ATOMS                                                  WDYN 980
      IF(IKA(L))686,714,686                                             WDYN 985
C     TRANSFORM ATOM DISPLACEMENTS TO CRYSTAL COORDINATES               WDYN 990
  686 CALL MV(CAB,XYZD(1,L),XYZA)                                       WDYN 995
C     TRANSFORM ATOM DISPLACEMENTS ACCORDING TO SYMMETRY                WDYN1000
      XYZAS(1)=SYM( 2,I)*XYZA(1)+SYM( 3,I)*XYZA(2)+SYM( 4,I)*XYZA(3)    WDYN1005
      XYZAS(2)=SYM( 6,I)*XYZA(1)+SYM( 7,I)*XYZA(2)+SYM( 8,I)*XYZA(3)    WDYN1010
      XYZAS(3)=SYM(10,I)*XYZA(1)+SYM(11,I)*XYZA(2)+SYM(12,I)*XYZA(3)    WDYN1015
C     CONVERT TRANSFORMED DISPLACEMENT BACK TO CARTESIAN SYSTEM         WDYN1020
      CALL MV(ACB,XYZAS,XYZDS)                                          WDYN1025
C     TRANSFORM ATOM COORDINATES ACCORDING TO SYMMETRY                  WDYN1030
      XXC=SYM(1,I)+SYM( 2,I)*XYZ(1,L)+SYM( 3,I)*XYZ(2,L)                WDYN1035
     1+SYM( 4,I)*XYZ(3,L)                                               WDYN1040
      YYC=SYM(5,I)+SYM( 6,I)*XYZ(1,L)+SYM( 7,I)*XYZ(2,L)                WDYN1045
     1+SYM( 8,I)*XYZ(3,L)                                               WDYN1050
      ZZC=SYM(9,I)+SYM(10,I)*XYZ(1,L)+SYM(11,I)*XYZ(2,L)                WDYN1055
     1+SYM(12,I)*XYZ(3,L)                                               WDYN1060
C     LOOP TO FIND SYMMETRY EQUIVALENT ATOM OF SAME KIND                WDYN1065
      DO 705 K=1,NA                                                     WDYN1070
      IF(IKA(K)-IKA(L))705,689,705                                      WDYN1075
  689 XXD=XXC-XYZ(1,K)+10.001                                           WDYN1080
      IF(AMOD(XXD,1.0)-0.002)690,690,705                                WDYN1085
  690 YYD=YYC-XYZ(2,K)+10.001                                           WDYN1090
      IF(AMOD(YYD,1.0)-0.002)695,695,705                                WDYN1095
  695 ZZD=ZZC-XYZ(3,K)+10.001                                           WDYN1100
      IF(AMOD(ZZD,1.0)-0.002)700,700,705                                WDYN1105
  700 KA=K                                                              WDYN1110
      GO TO 710                                                         WDYN1115
  705 CONTINUE                                                          WDYN1120
C     ERRGR. NO EQUIVALENT ATOM FOUND                                   WDYN1125
      CHAR(I)=10000.0                                                   WDYN1130
      GO TO 715                                                         WDYN1135
C     ADD CONTRIBUTION OF ATOM TO INNER PRODUCT                         WDYN1140
  710 DO 712 N=1,3                                                      WDYN1145
      US=US+XYZD(N,KA)*XYZDS(N)                                         WDYN1150
  712 CONTINUE                                                          WDYN1155
  714 CONTINUE                                                          WDYN1160
C     COMPUTE CHARACTER WITH RESPECT TO SYMMETRY OPERATION I            WDYN1165
      CHAR(I)=US/UU                                                     WDYN1170
  715 CONTINUE                                                          WDYN1175
      PRINT 55,(I,I=1,NS)                                               WDYN1180
   55 FORMAT('0CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION WDYN1185
     1 I(I4,'      ',10(I8/19X,10(I8)))                                 WDYN1190
      PRINT 57,(NAMS(I),I=1,NS)                                         WDYN1195
   57 FORMAT(' NAMS(I) ',10(4X,A4)/(9X,10(4X,A4)))                      WDYN1200
      PRINT 60,(CHAR(I),I=1,NS)                                         WDYN1205
   60 FORMAT(' CHAR(I) ',10F8.4/(9X,10F8.4))                            WDYN1210
      PRINT 65                                                          WDYN1215
   65 FORMAT('0-----------------------------------------------------')  WDYN1220
  720 CONTINUE                                                          WDYN1225
  725 RETURN                                                            WDYN1230
      END                                                               WDYN1235
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      SUBROUTINE WPRE1 (ACZ,AMASS,AR,BR,OP,DPX                          WPRE   5
     1,FMC,IACT,IAZ,ICT,IDZ,IKA,IRB                                     WPRE  10
     2,IRSC,ISBP,ISC,ITBP,IU,IV,IW                                      WPRE  15
     3,IZ,JAC,JOTS,KPS,KG,KQS,LBCI                                      WPRE  20
     4,LBCJ,NAME,NAMK,NAMP,NAMPX,NAMS,NOSS                              WPRE  25
     5,PI,PL,PMN,PMX,PX,PXMN,PXMX                                       WPRE  30
     6,Q,SMC,SP,SSR,STR,SXR                                             WPRE  35
     7,SYM,SYR,SYF,YR,XC,XYZ                                            WPRE  40
     8,YC,ZAM,ZC,KP)                                                    WPRE  45
      IMPLICIT REAL*8(A-H,O-Z)                                          WPRE  50
      DIMENSION ACZ(9,1),AMASS(1),AR(1),BR(1),OP(1),DPX(1)              WPRE  55
     1,FMC(1),IACT(1),IAZ(6,1),ICT(4,1),IDZ(4,1),IKA(1),IRB(1)          WPRE  60
     2,IRBC(1),ISBP(1),ISC(1),ITBR(4,1),IU(1),IV(1),IW(1)               WPRE  65
     3,IZ(1),JAC(1),JOTS(1),KPS(1),KQ(1),KQS(1),LBCI(1)                 WPRE  70
     4,LBCJ(1),NAME(1),NAMK(1),NAMP(1),NAMPX(1),NAMS(1),NOSS(1)         WPRE  75
     5,P(1),PL(1),PMN(1),PMX(1),PX(1),PXMN(1),PXMX(1)                   WPRE  80
     6,Q(1),SMC(1),SP(1),SSR(1),STR(1),SXR(1)                           WPRE  85
     7,SYM(12,1),SYR(12,12R(1),TR(3,1),XC(1),XYZ(3,1)                   WPRE  90
     8,YC(1),ZAM(1),ZC(1),KP(1)                                         WPRE  95
C     /DUBL/ USED BY WMIN, WDYN, WPRE, WCALC, GCMX, TIMOUT              WPRE 100
      COMMON/DUBL/A(6),AC(9),ACB(9),ASY(6),CA(9),CAB(9),CK              WPRE 105
     1,KKKCAL,CRA(9),DAA,DATE,FKCAL,WR,PI,PICK,PICKZ,PIDKSQ             WPRE 110
     2,PIMHZ,QLIM(5),QMAX,RDKSS(9),RLIM(5),RM(9),RMAX,RTPIZ             WPRE 115
     3,SA(6),SIGNQ,SQTPDK,SQTPI,SQTPIK,TM(9),TPI,TR(3),TY(3)            WPRE 120
     4,UTR(9),UV(3),UW(3),XC,WOBS,WS(9),WV,WX,XYZA(3),XYZAS(3)          WPRE 125
     5,XYZDS(3),ZMC                                                     WPRE 130
C     /SNGL/ USED BY WMIN, WPRE, WCALC                                  WPRE 135
      REAL*4 CMBT,FD,FMC,FNS,GXT,GYT,GZT,HMT,HXNEG,HXT,HYNEG            WPRE 140
     1,HTT,HZNEG,HZT,REPT,RT,SMC,SRBT,STITLE,TITLE,VDWT                 WPRE 145
      COMMON/SNGL/FD,FNS,HXNEG,HYNEG,HZNEG,STITLE(7),TITLE(18)          WPRE 150
C     /MAX/ USED BY MAIN, WMIN, WDYN, WPRE, WCALC, AND GCMX             WPRE 155
      COMMON/MAX/NPCMAX,NAMAX,NKAMAX,NGMAX,NRBMAX,NPXMAX,NCTMAX,NBCMAX  WPRE 160
     1,MMAX,NPSMAX,NGSMAX,NPSMAX,NPMAX,NOSMAX,NOMAX,NVMAX,ND,NB,NSD,NSP WPRE 165
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C     /ITGR/ USED BY WMIN, WDYN, WPRE, WCALC, GCMX, ISYPAS, TIMOUT      WPRE 170
      COMMON/ITGR/IBK,ICCAX,ICENT,ICMB,IGEM,ILSG,IMOL,INK,IPLM,IPRC     WPRE 175
     1,IPRT,IRBA,IREP,IRSC,ISB,ISN,IVDW,IWGT,IZAM,JC,KPW,KPWS,LT(9)     WPRE 180
     2,MODE,M,NAC,NAF,NEC,NCT,NKA,NOS,NP,NPC,NPR,NPS,NPX,NQ,ISETA       WPRE 185
     3,NR,NRB,NRP,NS,NT(5),NV,NVA,NVC,NVD,NVP,NVUS(9),NVX               WPRE 190
C     /AB/ USED BY WPRE, WCALC, AVV, CONF, DST, NORM, JNIT              WPRE 195
      COMMON/AB/AA(9),A11,A22,A33,A12,A13,A23,BB(9),B11,B22,B33,B12,B13 WPRE 200
     1,B23,VA                                                           WPRE 205
      DIMENSION UX(3),UY(3)                                             WPRE 210
      DATA UX/1.0D0,0.0D0,0.0D0/,UY/0.0D0,1.0D0,0.0D0/                  WPRE 215
      DIMENSION NAMA(6),NAMR(3),NAMT(3)                                 WPRE 220
      DATA NAMA/1HA,1HB,1HC,4HCOSA,4HCOSB,4HCOSG/                       WPRE 225
     1,NAMR/2HRX,2HRY,2HRZ/,NAMT/2HTX,2HTY,2HTZ/                        WPRE 230
      REAL*4 XXD,YYD,ZZD                                                WPRE 235
      RETURN                                                            WPRE 240
C                                                                       WPRE 245
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS     WPRE 250
C                                                                       WPRE 255
C     READ INPUT AND MAKE PRELIMINARY CALCULATIONS FOR ONE SUBSTANCE    WPRE 260
C                                                                       WPRE 265
      ENTRY WPRE                                                        WPRE 270
C     READ AND PRINT CONTROL CARD                                       WPRE 275
      READ 5,NA,NKA,NS,ICENT,HXNEG,HYNEG,HZNEG,NRB,NPX,NRP              WPRE 280
     1,ICMB,IVDW,IREP,IMOL,NCT,IRSC,IZAM,IGEM,IRBA,ISETA                WPRE 285
    5 FORMAT(4I3,3F3.0,13I3)                                            WPRE 290
      PRINT 10,NA,NKA,NS,ICENT,HXNEG,HYNEG,HZNEG,NRB,NPX,NRP            WPRE 295
     1,ICMB,IVDW,IREP,IMOL,NCT,IRSC,IZAM,IGEM,IRBA,ISETA                WPRE 300
   10 FORMAT('0    NA   NKA    NS ICENT HXNEG HYNEG HZNEG   NRB   NPX  WPRE 305
     1NRP   ICMB   IVDW   IREP   IMOL    NCT   IRSC   IZAM   IGEM   IRBA ISETA'  WPRE 310
     2/X,4I6,3F6.1,13I6)                                                WPRE 315
      IF(NA.LE.NAMAX.AND.NKA.LE.NKAMAX.AND.NS.LE.NSMAX.AND.             WPRE 320
     1NRB.LE.NRBMAX.AND.NPX.LE.NPXMAX.AND.NCT.LE.NCTMAX) GO TO 495      WPRE 325
      PRINT 12                                                          WPRE 330
   12 FORMAT('0*** INPUT VALUE OF NA, NKA, NS, NRB, NPX, OR NCT EXCEEDS WPRE 335
     1PRESET LIMIT ***')                                                WPRE 340
      CALL EXIT                                                         WPRE 345
C     READ AND PRINT EWALD CONSTANT AND LIMITS FOR RECIP AND DIRECT SUMS WPRE 350
  495 READ 15,CK,NQ,NR                                                  WPRE 355
   15 FORMAT(F9.0,2I3)                                                  WPRE 360
C     OMIT RECIPROCAL SUM IF ICMB AND IVDW ARE ZERO OR IMOL IS NON-ZERO WPRE 365
      IF(ICMB)505,500,505                                               WPRE 370
  500 IF(IVDW)505,510,505                                               WPRE 375
  505 IF(IMOL)510,515,510                                               WPRE 380
  510 CK=0.0                                                            WPRE 385
  515 PRINT 20,CK,NQ,NR                                                 WPRE 390
   20 FORMAT('0        CK      NQ      NR'/X,F9.5,2I6)                  WPRE 395
      IF(NQ.LE.5.AND.NR.LE.5) GO TO 516                                 WPRE 400
      PRINT 22                                                          WPRE 405
   22 FORMAT('0*** INPUT VALUE OF NQ OR NR EXCEEDS LIMIT OF 5 ***')     WPRE 410
      CALL EXIT                                                         WPRE 415
  516 READ 25,(QLIM(I),I=1,NQ)                                          WPRE 420
   25 FORMAT(8F9.0)                                                     WPRE 425
      PRINT 30,(QLIM(I),I=1,NQ)                                         WPRE 430
   30 FORMAT('0  QLIM(I)'/(X,8F9.5))                                    WPRE 435
      READ 35,(RLIM(I),I=1,NR)                                          WPRE 440
   35 FORMAT(8F9.0)                                                     WPRE 445
      PRINT 40,(RLIM(I),I=1,NR)                                         WPRE 450
   40 FORMAT('0  RLIM(I)'/(X,8F9.5))                                    WPRE 455
C     READ AND PRINT LATTICE PARAMETERS                                 WPRE 460
      READ 45,A                                                         WPRE 465
   45 FORMAT(6F9.0)                                                     WPRE 470
      PRINT 50,A                                                        WPRE 475
   50 FORMAT('0      A(I)'/X,6F9.5)                                     WPRE 480
      IF(IWGT.NE.0) GO TO 518                                           WPRE 485
C     LATTICE PARAMETER ERRORS NOT USED. SET TO ZERO                    WPRE 490
      DO 517 I=1,6                                                      WPRE 495
      SA(I)=0.0                                                         WPRE 500
  517 CONTINUE                                                          WPRE 505
      GO TO 519                                                         WPRE 510
C     READ AND PRINT LATTICE PARAMETER ERRORS                           WPRE 515
  518 READ 55,SA                                                        WPRE 520
   55 FORMAT(6F9.0)                                                     WPRE 525
      PRINT 60,SA                                                       WPRE 530
   60 FORMAT('0     SA(I)'/X,6F9.5)                                     WPRE 535
C     READ AND PRINT SYMMETRY TRANSFORMATIONS                           WPRE 540
  519 READ 65,(NAMS(J),(SYM(I,J),I=1,12),J=1,NS)                        WPRE 545
   65 FORMAT(A4,F11.0,3F3.0,F15.0,3F3.0,F15.0,3F3.0)                    WPRE 550
      PRINT 70                                                          WPRE 555
   70 FORMAT('0NAMS',10X,'TRANSFORMED X',20X,'TRANSFORMED Y',20X        WPRE 560
     1,'TRANSFORMED Z'/X)                                               WPRE 565
      PRINT 75,(NAMS(J),(SYM(I,J),I=1,12),J=1,NS)                       WPRE 570
   75 FORMAT((X,A4,3(5X,F7.4,F5.1,2H*X,F5.1,2H*Y,F5.1,2H*Z)))           WPRE 575
C     READ AND PRINT LIST OF KINDS OF ATOMS                             WPRE 580
      READ 80,(NAMK(K),Q(K),PL(K),AR(K),BR(K),AMASS(K),K=1,NKA)         WPRE 585
   80 FORMAT(A4,5X,5F9.0)                                               WPRE 590
      PRINT 85,(K,NAMK(K),Q(K),PL(K),AR(K),BR(K),AMASS(K),K=1,NKA)      WPRE 595
   85 FORMAT('0  K  NAMK          Q          PL          AR          BR      AMASS'WPRE 600
     1/(X,I3,2X,A4,2X,5F9.5))                                           WPRE 605
C     READ ATOM COORDINATES                                             WPRE 610
      READ 90,(NAME(J),IKA(J),(XYZ(I,J),I=1,3),J=1,NA)                  WPRE 615
   90 FORMAT(A4,I2,10X,3F6.0)                                           WPRE 620
C     TEST WHETHER ATOM LIST WILL BE EXPANDED                           WPRE 625
      IF(IRSC-1)530,530,520                                             WPRE 630
C     YES. TEMPORARILY CLEAR ASSIGNMENT OF ATOMS TO RIGID BODIES        WPRE 635
  520 DO 525 J=1,NA                                                     WPRE 640
      IRB(J)=0                                                          WPRE 645
  525 CONTINUE                                                          WPRE 650
      GO TO 535                                                         WPRE 655
C     NO. READ ASSIGNMENT OF ATOMS TO RIGID BODIES                      WPRE 660
  530 READ 95,(IRB(J),J=1,NA)                                           WPRE 665
   95 FORMAT(24I3)                                                      WPRE 670
C     PRINT ATOM COORDINATES AND ASSIGNMENT TO RIGID BODIES             WPRE 675
  535 PRINT 100,(J,NAME(J),IKA(J),IRB(J),(XYZ(I,J),I=1,3),J=1,NA)       WPRE 680
  100 FORMAT('0  J   NAME   IKA   IRB              X           Y           Z'WPRE 685
     1/(X,I3,2X,A4,2I6,2X,3F9.5))                                       WPRE 690
C     INITIALIZE SWITCH TO PERMIT RELAXATION OF SYMMETRY CONSTRAINTS    WPRE 695
      KRSC=1                                                            WPRE 700
C     COMPUTE NUMBER OF EQUIVALENT POSITIONS USED FOR STRUCTURE FACTORS WPRE 705
      NSF=NS/(3-ICENT)                                                  WPRE 710
  540 K=6                                                               WPRE 715
      NAF=0                                                             WPRE 720
C     START LOOPS TO GENERATE ALL ATOMS IN UNIT CELL                    WPRE 725
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      DO 595 I=1,NS                                                     WPRE 730
      DO 585 J=1,NA                                                     WPRE 735
C     GENERATE POSITION                                                 WPRE 740
      XXC=SYM(1,I)+SYM( 2,I)*XYZ(1,J)+SYM( 3,I)*XYZ(2,J)                WPRE 745
     1+SYM( 4,I)*XYZ(3,J)                                               WPRE 750
      YYC=SYM(5,I)+SYM( 6,I)*XYZ(1,J)+SYM( 7,I)*XYZ(2,J)                WPRE 755
     1+SYM( 8,I)*XYZ(3,J)                                               WPRE 760
      ZZC=SYM(9,I)+SYM(10,I)*XYZ(1,J)+SYM(11,I)*XYZ(2,J)                WPRE 765
     1+SYM(12,I)*XYZ(3,J)                                               WPRE 770
      IF(K)550,580,550                                                  WPRE 775
C     COMPARE NEW POSITION WITH ALL ATOMS ALREADY STORED                WPRE 780
  550 DO 575 L=1,K                                                      WPRE 785
      IF(IKA(J)-IKA(JAC(L)))575,553,575                                 WPRE 790
  553 IF(IMOL)561,554,561                                               WPRE 795
C     COMPARE COORDINATES MOD 1.0 FOR CRYSTAL                           WPRE 800
  554 XXD=XXC-XC(L)+10.001                                              WPRE 805
      IF(AMOD(XXD,1.0)-0.002)555,555,575                                WPRE 810
  555 YYD=YYC-YC(L)+10.001                                              WPRE 815
      IF(AMOD(YYD,1.0)-0.002)560,560,575                                WPRE 820
  560 ZZD=ZZC-ZC(L)+10.001                                              WPRE 825
      IF(AMOD(ZZD,1.0)-0.002)565,565,575                                WPRE 830
C     COMPARE COORDINATES FOR ISOLATED MOLECULE                         WPRE 835
  561 IF(DABS(XXC-XC(L))-0.001)562,562,575                              WPRE 840
  562 IF(DABS(YYC-YC(L))-0.001)563,563,575                              WPRE 845
  563 IF(DABS(ZZC-ZC(L))-0.001)565,565,575                              WPRE 850
C     DUPLICATES PREVIOUS POSITION. ACCUMULATE MULTIPLICITY OF PREV POS WPRE 855
  565 SMC(L)=SMC(L)+1.0                                                 WPRE 860
C     CHANGE MULTYPLICITY OF SPECIAL POSIT FOR STR FAC CALC IF REQUIRED WPRE 865
      IF(L-NAF)570,570,585                                              WPRE 870
  570 FMC(L)=0.5                                                        WPRE 875
      GO TO 585                                                         WPRE 880
  575 CONTINUE                                                          WPRE 885
C     POSITION IS UNIQUE. STORE IT                                      WPRE 890
  580 K=K+1                                                             WPRE 895
      XC(K)=XXC                                                         WPRE 900
      YC(K)=YYC                                                         WPRE 905
      ZC(K)=ZZC                                                         WPRE 910
      JAC(K)=J                                                          WPRE 915
      ISC(K)=I                                                          WPRE 920
      SMC(K)=1.0                                                        WPRE 925
      FMC(K)=1.0                                                        WPRE 930
      IRBC(K)=(I-1)*NRB+IRB(J)                                          WPRE 935
  585 CONTINUE                                                          WPRE 940
C     SET NUMBER OF ATOMS NEEDED FOR STRUCTURE FACTOR CALCULATION       WPRE 945
      IF(I-NSF)595,590,595                                              WPRE 950
  590 NAF=K                                                             WPRE 955
  595 CONTINUE                                                          WPRE 960
C     SET NUMBER OF ATOMS IN CELL                                       WPRE 965
      NAC=K                                                             WPRE 970
C     PRINT LIST OF ATOMS IN CELL                                       WPRE 975
      IF(IPRT-4)600,600,615                                             WPRE 980
  600 PRINT 105                                                         WPRE 985
  105 FORMAT('0  I  NAME   ISC   JAC   SMC   FMC  IRBC        XC        YCWPRE 990
     1        ZC')                                                      WPRE 995
      DO 610 I=1,NAC                                                    WPRE1000
      J=JAC(I)                                                          WPRE1005
      PRINT 110,I,NAME(J),ISC(I),JAC(I),SMC(I),FMC(I),IRBC(I),XC(I)     WPRE1010
     1,YC(I),ZC(I)                                                      WPRE1015
  110 FORMAT(X,I3,2X,A4,2I6,F6.0,F6.1,I6,3F9.5)                         WPRE1020
      IF(I-NAF)610,605,610                                              WPRE1025
  605 PRINT 115                                                         WPRE1030
  115 FORMAT(' ABOVE ATOMS USED TO COMPUTE STRUCTURE FACTORS')          WPRE1035
  610 CONTINUE                                                          WPRE1040
C     TEST WHETHER SYMMETRY CONSTRAINTS ARE TO BE RELAXED               WPRE1045
  615 IF(KRSC)620,655,620                                               WPRE1050
  620 IF(IRSC-1)655,655,625                                             WPRE1055
C     YES. PREPARE TO MAKE INVERSE OF FIRST SYMMETRY TRANSFORMATION     WPRE1060
  625 TM(1)=SYM( 2,1)                                                   WPRE1065
      TM(2)=SYM( 6,1)                                                   WPRE1070
      TM(3)=SYM(10,1)                                                   WPRE1075
      TM(4)=SYM( 3,1)                                                   WPRE1080
      TM(5)=SYM( 7,1)                                                   WPRE1085
      TM(6)=SYM(11,1)                                                   WPRE1090
      TM(7)=SYM( 4,1)                                                   WPRE1095
      TM(8)=SYM( 8,1)                                                   WPRE1100
      TM(9)=SYM(12,1)                                                   WPRE1105
      CALL INVRS(TM,D,TM)                                               WPRE1110
C     TEST FOR SINGULARITY                                              WPRE1115
      IF(D)635,630,635                                                  WPRE1120
  630 PRINT 120                                                         WPRE1125
  120 FORMAT('0*** FIRST SYMMETRY OPERATION IS SINGULAR. PROGRAM ASSUMESWPRE1130
     1 X,Y,Z ***')                                                      WPRE1135
      TM(1)=1.0                                                         WPRE1140
      TM(2)=0.0                                                         WPRE1145
      TM(3)=0.0                                                         WPRE1150
      TM(4)=0.0                                                         WPRE1155
      TM(5)=1.0                                                         WPRE1160
      TM(6)=0.0                                                         WPRE1165
      TM(7)=0.0                                                         WPRE1170
      TM(8)=0.0                                                         WPRE1175
      TM(9)=1.0                                                         WPRE1180
C     STORE EXPANDED LIST OF ATOMS                                      WPRE1185
  635 DO 645 K=1,NAC                                                    WPRE1190
      IF(ISC(K)-IRSC)640,640,650                                        WPRE1195
  640 TV(1)=XC(K)-SYM(1,1)                                              WPRE1200
      TV(2)=YC(K)-SYM(5,1)                                              WPRE1205
      TV(3)=ZC(K)-SYM(9,1)                                              WPRE1210
      CALL MV(TM,TV,XYZ(1,K))                                           WPRE1215
      J=JAC(K)                                                          WPRE1220
      NAME(K)=NAME(J)                                                   WPRE1225
      IKA(K)=IKA(J)                                                     WPRE1230
      NA=K                                                              WPRE1235
      IF(NA.LE.NAMAX) GO TO 645                                         WPRE1240
      PRINT 123,NAMAX                                                   WPRE1245
  123 FORMAT('0*** EXPANDED NUMBER OF ATOMS PRODUCED BY RELAXING SYMMETRWPRE1250
     1Y CONSTRAINTS EXCEEDS PRESET LIMIT OF',I3,' ***')                 WPRE1255
      CALL EXIT                                                         WPRE1260
  645 CONTINUE                                                          WPRE1265
C     READ ASSIGNMENT OF ATOMS TO RIGID BODIES                          WPRE1270
  650 READ 125,(IRB(J),J=1,NA)                                          WPRE1275
  125 FORMAT(24I3)                                                      WPRE1280
C     PRINT EXPANDED ATOM LIST                                          WPRE1285
      PRINT 130,(J,NAME(J),IKA(J),IRB(J),(XYZ(I,J),I=1,3),J=1,NA)       WPRE1290
  130 FORMAT('OREVISED ATOM LIST AFTER RELAXING SYMMETRY CONSTRAINTS'   WPRE1295
     1/'  J   NAME   IKA   IRB        X         Y         Z'           WPRE1300
     2/(X,I3,2X,A4,2I6,2X,3F9.5))                                       WPRE1305
C     SET SWITCH AND JUMP BACK TO RECALCULATE ATOMS IN CELL             WPRE1310
      KRSC=0                                                            WPRE1315
      GO TO 540                                                         WPRE1320
C     TEST WHETHER IZAM DEFINES SIZE OF FORMULA UNIT                    WPRE1325
  655 IF(IZAM)665,665,660                                               WPRE1330
C     YES. SET SMCMX ACCORDINGLY                                        WPRE1335
  660 SMCMX=SMC(1)*DFLOAT(IZAM)                                         WPRE1340
      GO TO 680                                                         WPRE1345
C     NO. FIND MAXIMUM NUMBER OF ATOMS FALLING ON ONE SPECIAL POSITION  WPRE1350
  665 SMCMX=0.0                                                         WPRE1355
      DO 675 I=1,NA                                                     WPRE1360
  670 SMCMX=SMC(I)                                                      WPRE1365
  675 CONTINUE                                                          WPRE1370
C     COMPUTE NUMBER OF MOLECULES OR FORMULA UNITS IN CELL              WPRE1375
  680 FNS=NS                                                            WPRE1380
      ZMC=FNS/SMCMX                                                     WPRE1385
C     COMPUTE NUMBER OF ATOMS OF EACH KIND IN MOLECULE OR FORMULA UNIT  WPRE1390
      DO 685 I=1,NA                                                     WPRE1395
      ZAM(I)=SMCMX/SMC(I)                                               WPRE1400
  685 CONTINUE                                                          WPRE1405
C     PRINT THESE RESULTS                                               WPRE1410
      IF(IPRT-4)690,690,695                                             WPRE1415
  690 PRINT 135,ZMC,(I,NAME(I),ZAM(I),I=1,NA)                           WPRE1420
  135 FORMAT('0   ZMC=',X,F6.1/'0  I   NAME(I)    ZAM(I)'               WPRE1425
     1/(X,I3,4X,A4,F9.1))                                               WPRE1430
C     READ AND PRINT DEFINITIONS OF RIGID BODY COORDINATE SYSTEMS       WPRE1435
  695 READ 140,(IZ(J),IU(J),IV(J),IW(J),SSR(J),STR(J)                   WPRE1440
     1,SXR(J),SYR(J),SZR(J),(TR(I,J),I=1,3),J=1,NRB)                    WPRE1445
  140 FORMAT(4I3,6X,2F9.0,6F6.0)                                        WPRE1450
      PRINT 145,(J,IZ(J),IU(J),IV(J),IW(J),SSR(J),STR(J)                WPRE1455
     1,SXR(J),SYR(J),SZR(J),(TR(I,J),I=1,3),J=1,NRB)                    WPRE1460
  145 FORMAT('0   J  IZ(J)  IU(J)  IV(J)  IW(J)    SSR(J)    STR(J)    SXR(J)  WPRE1465
     1SYR(J)    SZR(J)   TR(1,J)  TR(2,J)  TR(3,J)'                     WPRE1470
     2/(X,I3,4I6,8F9.5))                                                WPRE1475
C     READ AND PRINT ATOM CONNECTION TABLE                              WPRE1480
      NBC=0                                                             WPRE1485
      IF(NCT)698,725,698                                                WPRE1490
  698 READ 150, ((IACT(J),(ICT(I,J),I=1,4),(IDZ(I,J),I=1,4)             WPRE1495
     1,((IAZ(I,J),I=1,6),(ITBR(I,J),I=1,4),J=1,NCT)                     WPRE1500
  150 FORMAT(I3,3X,4I3,3X,4I3,3X,6I3,3X,4I3)                            WPRE1505
      PRINT 155,(IACT(J),(ICT(I,J),I=1,4),(IDZ(I,J),I=1,4)              WPRE1510
     1,(IAZ(I,J),I=1,6),(ITBR(I,J),I=1,4),J=1,NCT)                      WPRE1515
  155 FORMAT('0IACT    ICT',16X,'IDZ',16X,'IAZ',23X,'ITBR'              WPRE1520
     1/(X,I4,3X,4I4,3X,4I4,3X,6I4,3X,4I4))                              WPRE1525
C     STORE LIST OF BONDED CONTACTS TO BE OMITTED FROM NON-BONDED ENERGYWPRE1530
      DO 715 I=1,NCT                                                    WPRE1535
      IA=IACT(I)                                                        WPRE1540
      DO 710 J=1,4                                                      WPRE1545
      JA=ICT(J,I)                                                       WPRE1550
      IF(JA.EQ.0) GO TO 710                                             WPRE1555
      IF(JA.GT.IA) GO TO 701                                            WPRE1560
C     TEST WHETHER JA IS BACKBONE ATOM                                  WPRE1565
      DO 700 L=1,NCT                                                    WPRE1570
      IF(JA.EQ.IACT(L)) GO TO 705                                       WPRE1575
  700 CONTINUE                                                          WPRE1580
      IF(NBC.GE.NBCMAX) GO TO 702                                       WPRE1585
      NBC=NBC+1                                                         WPRE1590
      LBCI(NBC)=JA                                                      WPRE1595
      LBCJ(NBC)=IA                                                      WPRE1600
      GO TO 705                                                         WPRE1605
  701 IF(NBC.LT.NBCMAX) GO TO 704                                       WPRE1610
  702 PRINT 157,NBCMAX                                                  WPRE1615
  157 FORMAT('0*** NUMBER OF BONDED CONTACTS GENERATED EXCEEDS PRESET LIWPRE1620
     1MIT OF ',I3,' ***')                                               WPRE1625
      CALL EXIT                                                         WPRE1630
  704 NBC=NBC+1                                                         WPRE1635
      LBCI(NBC)=IA                                                      WPRE1640
      LBCJ(NBC)=JA                                                      WPRE1645
C     ADD PAIRS OF GEMINAL ATOMS TO LIST IF IGEM.NE.0                   WPRE1650
  705 IF(IGEM.EQ.0.OR.J.EQ.4) GO TO 710                                 WPRE1655
      JP=J+1                                                            WPRE1660
      DO 708 K=JP,4                                                     WPRE1665
      KA=ICT(K,1)                                                       WPRE1670
      IF(KA.EQ.0) GO TO 708                                             WPRE1675
      IF(NBC.GE.NBCMAX) GO TO 702                                       WPRE1680
      NBC=NBC+1                                                         WPRE1685
      IF(KA.LT.JA) GO TO 706                                            WPRE1690
      LBCI(NBC)=JA                                                      WPRE1695
      LBCJ(NBC)=KA                                                      WPRE1700
      GO TO 708                                                         WPRE1705
  706 LBCI(NBC)=KA                                                      WPRE1710
      LBCJ(NBC)=JA                                                      WPRE1715
  708 CONTINUE                                                          WPRE1720
  710 CONTINUE                                                          WPRE1725
  715 CONTINUE                                                          WPRE1730
      IF(IPRT-4)720,720,725                                             WPRE1735
  720 PRINT 160,(LBCI(K),LBCJ(K),K=1,NBC)                               WPRE1740
  160 FORMAT('0LBCI LBCJ'/(X,12(2I4,2X)))                               WPRE1745
C     READ AND PRINT EXTRA PARAMETER INFORMATION                        WPRE1750
  725 IF(NPX)730,735,730                                                WPRE1755
  730 READ 165,(NAMPX(I),I=1,NPX)                                       WPRE1760
  165 FORMAT(8(5X,A4))                                                  WPRE1765
      PRINT 170,(NAMPX(I),I=1,NPX)                                      WPRE1770
  170 FORMAT('0 NAMPX(I)'/(X,8(5X,A4)))                                 WPRE1775
      READ 175,(PX(I),I=1,NPX)                                          WPRE1780
  175 FORMAT(8F9.0)                                                     WPRE1785
      PRINT 180,(PX(I),I=1,NPX)                                         WPRE1790
  180 FORMAT('0    PX(I)'/(X,8F9.5))                                    WPRE1795
      READ 185,(DPX(I),I=1,NPX)                                         WPRE1800
  185 FORMAT(8F9.0)                                                     WPRE1805
      PRINT 190,(DPX(I),I=1,NPX)                                        WPRE1810
  190 FORMAT('0   DPX(I)'/(X,8F9.5))                                    WPRE1815
      IF(IPLM.NE.0) GO TO 733                                           WPRE1820
      DO 732 I=1,NPX                                                    WPRE1825
      PXMN(I)=0.0                                                       WPRE1830
                                                                        WPRE1835
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      PXMX(I)=0.0                                                       WPRE1840
  732 CONTINUE                                                          WPRE1845
      GO TO 735                                                         WPRE1850
  733 READ 195,(PXMN(I),I=1,NPX)                                        WPRE1855
  195 FORMAT(8F9.0)                                                     WPRE1860
      PRINT 200,(PXMN(I),I=1,NPX)                                       WPRE1865
  200 FORMAT('0  PXMN(I)'/(X,8F9.5))                                    WPRE1870
      READ 205,(PXMX(I),I=1,NPX)                                        WPRE1875
  205 FORMAT(8F9.0)                                                     WPRE1880
      PRINT 210,(PXMX(I),I=1,NPX)                                       WPRE1885
  210 FORMAT('0  PXMX(I)'/(X,8F9.5))                                    WPRE1890
C     SET MULTIPLIER NEEDED FOR STRUCTURE FACTORS                       WPRE1895
  735 FM=3-ICENT                                                        WPRE1900
C     FACTOR TO CONVERT ELECTRONS**2/ANGSTROM TO KILOCALORIES/MOLE      WPRE1905
      FKCAL=232.17                                                      WPRE1910
C     SET VARIOUS CONSTANTS NEEDED FOR LATTICE SUMS                     WPRE1915
      PI=3.14159265358979300                                            WPRE1920
      TPI=2.0*PI                                                        WPRE1925
      SQTPI=DSQRT(PI)                                                   WPRE1930
      SQTPIK=SQTPI*CK                                                   WPRE1935
      IF(CK)740,745,740                                                 WPRE1940
  740 SQTPDK=SQTPI/CK                                                   WPRE1945
      PIDKSQ=PI/(CK*CK)                                                 WPRE1950
  745 RTPIZ=FKCAL/(TPI*ZMC)                                             WPRE1955
      PINHZ=-((PI**2)**2)*SQTPI/(3.0*ZMC)                               WPRE1960
      PICKZ=-((PI*CK)**3)*ZMC/6.0                                       WPRE1965
      PICK=((PI*CK*CK)**3)/12.0                                         WPRE1970
      CKKCAL=-FKCAL*CK                                                  WPRE1975
C     LOOP TO STORE PARAMETERS FOR THIS SUBSTANCE IN OVERALL PARAM LIST WPRE1980
      IF(NVC)750,755,750                                                WPRE1985
C     ALL SUBSTANCES TO BE COMBINED. START AT END OF LIST ALREADY STORED WPRE1990
  750 K=NP                                                              WPRE1995
      GO TO 760                                                         WPRE2000
C     SUBSTANCES TREATED SEPARATELY. START AT END OF COMMON PARAMETERS  WPRE2005
  755 K=NPC                                                             WPRE2010
C     SAVE STARTING POINT FOR THIS SUBSTANCE                            WPRE2015
  760 INK=K                                                             WPRE2020
      IF(INK+6+(6-3*IRBA)*NRB+NPX.LE.NPMAX) GO TO 762                   WPRE2025
      PRINT 212,NPMAX                                                   WPRE2030
  212 FORMAT('0*** NUMBER OF PARAMETERS EXCEEDS PRESET LIMIT OF',I4     WPRE2035
     1,' ***')                                                          WPRE2040
      CALL EXIT                                                         WPRE2045
C     STORE LATTICE PARAMETERS                                          WPRE2050
  762 DO 765 I=1,3                                                      WPRE2055
      K=K+1                                                             WPRE2060
      P(K)=A(I)                                                         WPRE2065
      DP(K)=0.00001                                                     WPRE2070
      PMN(K)=A(I)-1.0                                                   WPRE2075
      PMX(K)=A(I)+1.0                                                   WPRE2080
      NAMP(K)=NAMA(I)                                                   WPRE2085
      SP(K)=SA(I)                                                       WPRE2090
  765 CONTINUE                                                          WPRE2095
      DO 770 I=4,6                                                      WPRE2100
      K=K+1                                                             WPRE2105
      P(K)=A(I)                                                         WPRE2110
      DP(K)=0.00001                                                     WPRE2115
      PMN(K)=A(I)-0.2                                                   WPRE2120
      PMX(K)=A(I)+0.2                                                   WPRE2125
      NAMP(K)=NAMA(I)                                                   WPRE2130
      SP(K)=SA(I)                                                       WPRE2135
  770 CONTINUE                                                          WPRE2140
C     STORE RIGID BODY ROTATIONS AND TRANSLATIONS                       WPRE2145
      DO 785 J=1,NRB                                                    WPRE2150
      IF(IRBA.NE.0) GO TO 777                                           WPRE2155
      P(K+1)=SXR(J)                                                     WPRE2160
      P(K+2)=SYR(J)                                                     WPRE2165
      P(K+3)=SZR(J)                                                     WPRE2170
      DO 775 I=1,3                                                      WPRE2175
      K=K+1                                                             WPRE2180
      DP(K)=0.00001                                                     WPRE2185
      PMN(K)=P(K)-0.2                                                   WPRE2190
      PMX(K)=P(K)+0.2                                                   WPRE2195
      NAMP(K)=NAMR(I)                                                   WPRE2200
      SP(K)=SSR(J)                                                      WPRE2205
  775 CONTINUE                                                          WPRE2210
  777 DO 780 I=1,3                                                      WPRE2215
      K=K+1                                                             WPRE2220
      P(K)=TR(I,J)                                                      WPRE2225
      DP(K)=0.00001                                                     WPRE2230
      PMN(K)=P(K)-0.5                                                   WPRE2235
      PMX(K)=P(K)+0.5                                                   WPRE2240
      NAMP(K)=NAMT(I)                                                   WPRE2245
      SP(K)=STR(J)                                                      WPRE2250
  780 CONTINUE                                                          WPRE2255
  785 CONTINUE                                                          WPRE2260
C     STORE EXTRA PARAMETERS                                            WPRE2265
      IF(NPX)790,800,790                                                WPRE2270
  790 DO 795 I=1,NPX                                                    WPRE2275
      K=K+1                                                             WPRE2280
      P(K)=PX(I)                                                        WPRE2285
      DP(K)=DPX(I)                                                      WPRE2290
      PMN(K)=PXMN(I)                                                    WPRE2295
      PMX(K)=PXMX(I)                                                    WPRE2300
      NAMP(K)=NAMPX(I)                                                  WPRE2305
      SP(K)=DPX(I)                                                      WPRE2310
  795 CONTINUE                                                          WPRE2315
C     SAVE TOTAL NUMBER OF PARAMETERS AND NUMBER FOR THIS SUBSTANCE     WPRE2320
  800 NP=K                                                              WPRE2325
      NPS=NP-INK                                                        WPRE2330
      IF(NPS.LE.NPSMAX) GO TO 802                                       WPRE2335
      PRINT 213,NPSMAX                                                  WPRE2340
  213 FORMAT('0*** NUMBER OF PARAMETERS FOR ONE SUBSTANCE EXCEEDS PRESET WPRE2345
     1 LIMIT OF',I4,' ***')                                             WPRE2350
      CALL EXIT                                                         WPRE2355
C     READ AND PRINT OBSERVED ENERGY. SET INDICATOR FOR USING IT        WPRE2360
  802 READ 215,KPWS,WOBS,SIGWO                                          WPRE2365
  215 FORMAT(I3,6X,2F9.0)                                               WPRE2370
      IF(MODE)810,805,810                                               WPRE2375
  805 KPW=KPWS                                                          WPRE2380
      GO TO 815                                                         WPRE2385
  810 KPW=0                                                             WPRE2390
  815 PRINT 220,KPWS,KPW,WOBS,SIGWO                                     WPRE2395
  220 FORMAT('0  KPWS   KPW     WOBS     SIGWO'/X,2I6,2F9.3)            WPRE2400
C     READ OBSERVATION SELECTION AND VARIABLE SELECTION INTEGERS        WPRE2405
      READ 225,(KQS(I),I=1,NPS)                                         WPRE2410
  225 FORMAT(72I1)                                                      WPRE2415
      READ 230,(KQS(I),I=1,NPS)                                         WPRE2420
  230 FORMAT(72I1)                                                      WPRE2425
C     LOOP TO STORE OVERALL SELECTION INTEGERS ACCORDING TO MODE        WPRE2430
      NOS=0                                                             WPRE2435
      K=INK                                                             WPRE2440
      DO 840 I=1,NPS                                                    WPRE2445
      K=K+1                                                             WPRE2450
      KP(K)=KPS(I)                                                      WPRE2455
      ISDP(K)=ISB                                                       WPRE2460
      IF(KPS(I))820,825,820                                             WPRE2465
C     COUNT OBSERVATIONS FOR SUBSTANCE AND STORE ARRAYS NEEDED LATER    WPRE2470
  820 NOS=NOS+1                                                         WPRE2475
      IF(NOS.LE.NOSMAX) GO TO 822                                       WPRE2480
      PRINT 235,NOSMAX                                                  WPRE2485
  235 FORMAT('0***A NUMBER OF OBSERVATIONS FOR ONE SUBSTANCE EXCEEDS PRESWPRE2490
     1ET LIMIT OF',I4,' ***')                                           WPRE2495
      CALL EXIT                                                         WPRE2500
  822 JOYS(NOS)=K                                                       WPRE2505
      NOSS(NOS)=NAMP(K)                                                 WPRE2510
  825 IF(MODE)835,830,835                                               WPRE2515
  830 KQ(K)=KQS(I)                                                      WPRE2520
      GO TO 840                                                         WPRE2525
  835 KQ(K)=KPS(I)                                                      WPRE2530
  840 CONTINUE                                                          WPRE2535
C     LOOP TO COUNT LATTICE, RIGID BODY, AND EXTRA PARAM VARIABLES      WPRE2540
      NPR=(6-3*IRBA)*NRB                                                WPRE2545
      K=INK                                                             WPRE2550
      NVA=0                                                             WPRE2555
      NVR=0                                                             WPRE2560
      NVX=0                                                             WPRE2565
      DO 850 I=1,6                                                      WPRE2570
      K=K+1                                                             WPRE2575
      IF(KQ(K))845,850,845                                              WPRE2580
  845 NVA=NVA+1                                                         WPRE2585
  850 CONTINUE                                                          WPRE2590
      DO 860 I=1,NPR                                                    WPRE2595
      K=K+1                                                             WPRE2600
      IF(KQ(K))855,860,855                                              WPRE2605
  855 NVR=NVR+1                                                         WPRE2610
  860 CONTINUE                                                          WPRE2615
      IF(NPX)865,880,865                                                WPRE2620
  865 DO 875 I=1,NPX                                                    WPRE2625
      K=K+1                                                             WPRE2630
      IF(KQ(K))870,875,870                                              WPRE2635
  870 NVX=NVX+1                                                         WPRE2640
  875 CONTINUE                                                          WPRE2645
C     SET LATTICE PARAMETERS ACCORDING TO SYMMETRY                      WPRE2650
  880 CALL SETA(ISETA,A)                                                WPRE2655
C     CALCULATE DIRECT AND RECIPROCAL LATTICE COEFFICIENTS              WPRE2660
      AA(1)=A(1)**2                                                     WPRE2665
      AA(2)=A(1)*A(2)*A(6)                                              WPRE2670
      AA(3)=A(1)*A(3)*A(5)                                              WPRE2675
      AA(4)=AA(2)                                                       WPRE2680
      AA(5)=A(2)**2                                                     WPRE2685
      AA(6)=A(2)*A(3)*A(4)                                              WPRE2690
      AA(7)=AA(3)                                                       WPRE2695
      AA(8)=AA(6)                                                       WPRE2700
      AA(9)=A(3)**2                                                     WPRE2705
      CALL INVRS(AA,DAA,BB)                                             WPRE2710
      A11=AA(1)                                                         WPRE2715
      A22=AA(5)                                                         WPRE2720
      A33=AA(9)                                                         WPRE2725
      A12=2.0*AA(2)                                                     WPRE2730
      A13=2.0*AA(3)                                                     WPRE2735
      A23=2.0*AA(6)                                                     WPRE2740
      B11=BB(1)                                                         WPRE2745
      B22=BB(5)                                                         WPRE2750
      B33=BB(9)                                                         WPRE2755
      B12=2.0*BB(2)                                                     WPRE2760
      B13=2.0*BB(3)                                                     WPRE2765
      B23=2.0*BB(6)                                                     WPRE2770
C     ENTER USERS SUBROUTINE TO SET CONSTRAINTS                         WPRE2775
      CALL CNSTRN                                                       WPRE2780
C     FOR EACH RIGID BODY, GET CARTESIAN TRANSFORMATION MATRIX ACZ BASEDWPRE2785
C        ON ORIGINAL LATTICE PARAMETERS                                 WPRE2790
      DO 900 J=1,NRB                                                    WPRE2795
      IUJ=IU(J)                                                         WPRE2800
      IF(IUJ)890,885,890                                                WPRE2805
  885 CALL AXES(UX,UY,UT)                                               WPRE2810
      GO TO 895                                                         WPRE2815
  890 IVJ=IV(J)                                                         WPRE2820
      IWJ=IW(J)                                                         WPRE2825
      CALL DIFV(XYZ(1,IVJ),XYZ(1,IUJ),UV)                               WPRE2830
      IF(IWJ.EQ.0) GO TO 893                                            WPRE2835
      CALL DIFV(XYZ(1,IWJ),XYZ(1,IUJ),UW)                               WPRE2840
      CALL AXES(UV,UW,UT)                                               WPRE2845
      GO TO 895                                                         WPRE2850
  893 CALL AXES(UV,UX,UT)                                               WPRE2855
  895 CALL MM(AA,UT,AC)                                                 WPRE2860
      CALL XFRAN(AC,ACZ(1,J))                                           WPRE2865
  900 CONTINUE                                                          WPRE2870
      RETURN                                                            WPRE2875
      END                                                               WPRE2880


      FUNCTION XCALCI (ACZ,AR,BR,CMBT,CSV,FMC                           WCAL   5
     1,GMT,GXT,GYT,GZT,HMT,HXT,HYT                                      WCAL  10
     2,HZT,IAT,ICC,IKA,IRB,IRBC,ISC                                     WCAL  15
     3,IU,IV,IW,IZ,JAC,JAT,LBCI                                         WCAL  20
     4,LBCJ,NAME,P,PC,PCSV,PL,PX                                        WCAL  25
     5,PXSV,Q,REPT,RSV,RT,SRBT,SXR                                      WCAL  30
     6,SYM,SYR,SZR,TR,VOMT,VSV                                          WCAL  35
     7,XC,XYZ,XYZC,XYZR,YC,ZAM                                          WCAL  40
     8,ZC)                                                              WCAL  45
      IMPLICIT REAL*8(A-H,O-Z)                                          WCAL  50
      DIMENSION ACZ(9,1),AR(1),BR(1),CMBT(1),CSV(1),FMC(1)              WCAL  55
     1,GMT(1),GXT(1),GYT(1),GZT(1),HMT(1),HXT(1),HYT(1)                 WCAL  60
     2,HZT(1),IAT(1),ICC(1),IKA(1),IRB(1),IRBC(1),ISC(1)                WCAL  65
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      3,IU(1),IV(1),IW(1),IZ(1),JAC(1),JAT(1),LBCI(1)
      4,LBCJ(1),NAME(1),P(1),PC(1),PCSV(1),PL(1),PX(1)
      5,PXSV(1),Q(1),REPT(1),RSV(1),RT(1),SRBT(1),SXR(1)
      6,SYM(12,1),SYR(1),SZR(1),TR(3,1),VDWT(1),VSV(1)
      7,XC(1),XYZ(3,1),XYZC(3,1),XYZR(3,1),YC(1),ZAM(1)
      8,ZC(1)
C     /DUBL/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, TIMOUT
      COMMON/DUBL/A(6),AC(9),ACB(9),ASV(6),CA(9),CAB(9),CK
      1,CKKCAL,CRA(9),DAA,DATE,FKCAL,WR,PI,PICK,PICKZ,PIDKSQ
      2,PINHZ,QLIM(5),QMAX,RDWSS(9),RLIM(5),RM(9),RMAX,RTPIZ
      3,SA(6),SIGWO,SQTPDK,SQTPI,SQTPIK,TM(9),TPI,TRT(3),TV(3)
      4,UT(9),UV(3),UW(3),WC,WGBS,WS(9),WV,WX,XYZA(3),XYZAS(3)
      5,XYZDS(3),ZMC
C     /SNGL/ USED BY WMIN, WPRE, WCALC
      REAL*4 CHBT,FM,FMC,FNS,GXT,GYT,GZT,HMT,HXNEG,HXT,HYNEG
      1,HYT,HZNEG,HZT,REPT,RT,SMC,SRBT,STITLE,TITLE,VDWT
      COMMON/SNGL/FM,FNS,HXNEG,HYNEG,HZNEG,STITLE(17),TITLE(18)
C     /MAX/ USED BY MAIN, WMIN, WDYN, WPRE, WCALC, AND GCWX
      COMMON/MAX/NPCMAX,NAMAX,NKAMAX,NSMAX,NRBMAX,NPXMAX,NCTMAX,NBCMAX
      1,MMAX,NFSMAX,NGSMAX,NPSMAX,NPMAX,NDSMAX,NDMAX,NVMAX,ND,NS,NSD,NSP
C     /ITGR/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, IBYPAS, TIMOUT
      COMMON/ITGR/IBK,ICCAX,ICENT,ICMB,IGEM,ILSQ,IMOL,INK,IPLM,IPRC
      1,IPRT,IRBA,IREP,IRSC,ISB,ISW,IVDW,IWGT,IZAM,JC,KPW,KPWS,LT(9)
      2,MODE,NA,NAC,NAF,NBC,NCT,NKA,NOS,NP,NPC,NPR,NPS,NPX,NQ,ISETA
      3,NR,NRB,NRP,NS,NT(9),NV,NVA,NVC,NVD,NVR,NVUS(9),NVX
C     /AB/ USED BY WPRE, WCALC, AVV, CONF, DST, NORM, UNIT
      COMMON/AB/AA(9),A11,A22,A33,A12,A13,A23,BB(9),B11,B22,B33,B12,B13
      1,B23,VA
      DIMENSION UX(3),UY(3)
      DATA UX/1.0D0,0.0D0,0.0D0/,UY/0.0D0,1.0D0,0.0D0/
      REAL*4 HXMAX,HXMIN,HYMAX,HYMIN,HZMAX,HZMIN,HX,HY,HZ,HXM,HYM,HM
      1,GXMAX,GXMIN,GYMAX,GYMIN,GZMAX,GZMIN,GX,GY,GZ,SRB
      RETURN
C
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS
C
C     CALCULATE THE ENERGY OF ONE CRYSTAL OR MOLECULE
C     THREE PRESET INDICATORS CONTROL THE FLOW OF THIS CALCULATION
C        ISW=1 ON FIRST ENTRY OF EACH CYCLE. SETS UP TABLES USED LATER
C        ISW=0 ON SUBSEQUENT ENTRIES, USES TABLES TO SPEED CALCULATION
C        IBY=0 FORCES ALL OF ENERGY TO BE CALCULATED
C        IBY=1 TO 7 BYPASSES RECALCULATION OF UNCHANGED TERMS
C        IBK=0 NORMALLY
C        IBK=1 CAUSES ROUTINE TO TERMINATE AFTER SETTING ATOM COORDS
C     FURTHER BYPASSING CONTROLLED BY INTERNAL INDICATORS ICCAX AND ICC
C
      ENTRY WCALC(IBY)
C     READ INITIAL TIME
      LTI=ICLOCK(0)
C     PICK UP PARAMETERS FROM OVERALL PARAMETER LIST
      IF(NPC)500,510,500
  500 DO 505 I=1,NPC
      PCSV(I)=PC(I)
      PC(I)=P(I)
  505 CONTINUE
  510 K=INK
      DO 515 I=1,6
      K=K+1
      ASV(I)=A(I)
      A(I)=P(K)
  515 CONTINUE
      DO 525 J=1,NRB
      IF(IRBA.NE.0) GO TO 518
      SXR(J)=P(K+1)
      SYR(J)=P(K+2)
      SZR(J)=P(K+3)
      K=K+3
  518 DO 520 I=1,3
      K=K+1
      TR(I,J)=P(K)
  520 CONTINUE
  525 CONTINUE
      IF(NPX)530,540,530
  530 DO 535 I=1,NPX
      K=K+1
      PXSV(I)=PX(I)
      PX(I)=P(K)
  535 CONTINUE
C     ENTER ROUTINE TO CONSTRAIN LATTICE SYMMETRY
  540 CALL SETA(ISETA,A)
C     TEST FOR CHANGE IN LATTICE PARAMETERS AND SET INDICATOR
      ICA=1
      IF(ISW)555,545,555
  545 DO 550 I=1,6
      IF(A(I)-ASV(I))555,550,555
  550 CONTINUE
C     NO CHANGE. BYPASS CALCULATIONS BASED ON LATTICE PARAMETERS
      ICA=0
      GO TO 560
C     SET COEFFICIENTS INVOLVING LATTICE PARAMETERS
  555 AA(1)=A(1)**2
      AA(2)=A(1)*A(2)*A(6)
      AA(3)=A(1)*A(3)*A(5)
      AA(4)=AA(2)
      AA(5)=A(2)**2
      AA(6)=A(2)*A(3)*A(4)
      AA(7)=AA(3)
      AA(8)=AA(6)
      AA(9)=A(3)**2
      CALL INVRS(AA,DAA,BB)
      A11=AA(1)
      A22=AA(5)
      A33=AA(9)
      A12=2.0*AA(2)
      A13=2.0*AA(3)
      A23=2.0*AA(6)
      B11=BB(1)
      B22=BB(5)
      B33=BB(9)
      B12=2.0*BB(2)
      B13=2.0*BB(3)
      B23=2.0*BB(6)
      B1=DSQRT(B11)
      B2=DSQRT(B22)
      B3=DSQRT(B33)
      VA=DSQRT(DAA)
      RTPIZV=RTPIZ/VA
      PINHZV=PINHZ/VA
      PICKZV=PICKZ/VA
C     ENTER USER ROUTINE TO SET OTHER CONSTRAINTS
  560 CALL CNSTRN
C     TEST FOR CHANGE IN COMMON PARAMETERS AND SET INDICATOR
      ICPC=1
      IF(NPC)565,575,565
  565 DO 570 I=1,NPC
      IF(PC(I)-PCSV(I))580,570,580
  570 CONTINUE
  575 ICPC=0
C     TEST FOR CHANGE IN EXTRA PARAMETERS AND SET INDICATOR
  580 ICPX=1
      IF(NPX)585,595,585
  585 DO 590 I=1,NPX
      IF(PX(I)-PXSV(I))600,590,600
  590 CONTINUE
  595 ICPX=0
C     SET OVERALL INDICATOR FOR CHANGE IN COMMON, LATTICE, OR EXTRA PAR
  600 ICCAX=ICPC+ICA+ICPX
C     COUNT AND TIME PASSES THROUGH INITIAL CALCULATIONS
      NT(1)=NT(1)+1
      LTF=ICLOCK(0)
      LT(1)=LT(1)+LTF-LTI
      LTI=LTF
C     TO RECIPROCAL AND DIRECT SUMS, DIRECT SUM ONLY, OR BYPASS BOTH
      IBYP=IBY+1
      GO TO (605,605,605,605,1390,1390,1495,1495),IBYP
C     SET UP ATOM COORDINATES FROM RIGID BODY ROTATIONS AND TRANSLATIONS
C     TEMPORARILY SET COORDINATES FROM INPUT VALUES
  605 DO 615 J=1,NA
      DO 610 I=1,3
      XYZR(I,J)=XYZ(I,J)
  610 CONTINUE
  615 CONTINUE
C     START LOOP THROUGH RIGID BODIES
      DO 660 J=1,NRB
      IUJ=IU(J)
      IZJ=IZ(J)
      IF(IUJ)625,620,625
C     SET UP AXES BASED ON LATTICE COORDINATES
  620 CALL AXES(UX,UY,UT)
      GO TO 630
C     SET UP AXES BASED ON SPECIFIED ATOMS
  625 IVJ=IV(J)
      IWJ=IW(J)
      CALL DIFV(XYZR(1,IVJ),XYZR(1,IUJ),UV)
      IF(IWJ.EQ.0) GO TO 628
      CALL DIFV(XYZR(1,IWJ),XYZR(1,IUJ),UW)
      CALL AXES(UV,UW,UT)
      GO TO 630
C     SET UP AXES FOR SPECIAL CASE OF LINEAR MOLECULE
  628 CALL AXES(UV,UX,UT)
C     GENERATE MATRIX FOR CARTESIAN TO CRYSTAL TRANSFORMATION
  630 CALL MM(AA,UT,AC)
      CALL TRANS(AC,CA)
      CALL INVRS(CA,D,CA)
C     SAVE ONE CRYSTAL TO CARTESIAN MATRIX FOR CALC OF NORMAL VIBRATIONS
      IF(J.EQ.1) CALL TRANS(AC,ACB)
      IF(IRBA.EQ.0) GO TO 640
C     OMIT ROTATION MATRIX
      CALL MM(CA,ACZ(1,J),CRA)
      GO TO 643
C     SET UP ROTATION MATRIX
  640 SX=DSIN(SXR(J))
      SY=DSIN(SYR(J))
      SZ=DSIN(SZR(J))
      CX=DCOS(SXR(J))
      CY=DCOS(SYR(J))
      CZ=DCOS(SZR(J))
      RM(1)=CZ*CY
      RM(2)=-SZ*CY
      RM(3)=SY
      RM(4)=CZ*SY*SX+SZ*CX
      RM(5)=-SZ*SY*SX+CZ*CX
      RM(6)=-CY*SX
      RM(7)=-CZ*SY*CX+SZ*SX
      RM(8)=SZ*SY*CX+CZ*SX
      RM(9)=CY*CX
C     SET UP MATRIX CRA AND VECTOR TRT. MATRICES ACZ WERE SAVED BY WPRE
      CALL MM(RM,ACZ(1,J),TM)
      CALL MM(CA,TM,CRA)
  643 CALL MV(CA,TR(1,J),TPT)
      CALL SUMV(XYZR(1,IZJ),TRT,TRT)
      CALL MV(CRA,XYZ(1,IZJ),TV)
      CALL DIFV(TRT,TV,TRT)
C     GENERATE COORDINATES FOR EACH ATOM IN THIS RIGID BODY
      DO 655 I=1,NA
      IF(J-IRB(I))655,645,655
  645 CALL MV(CRA,XYZ(1,I),XYZR(1,I))
      CALL SUMV(TRT,XYZR(1,I),XYZR(1,I))
C     SAVE CARTESIAN COORDINATES IF REQUIRED FOR CALC OF NORM VIBRATIONS
      IF(IBK)650,655,650
  650 CALL MV(ACB,XYZR(1,I),XYZC(1,I))
  655 CONTINUE
  660 CONTINUE
C     TERMINATE ROUTINE IF ONLY COORDINATES ARE NEEDED
      IF(IBK)1525,665,1525
C     GENERATE COORDINATES FOR ALL ATOMS IN UNIT CELL
  665 DO 685 K=1,NAC
      I=ISC(K)
      J=JAC(K)
C     SAVE COORDINATES USED PREVIOUSLY
      XCSV=XC(K)
      YCSV=YC(K)
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      ZCSV=ZC(K)
C     GENERATE COORDINATES FROM SYMMETRY INFORMATION
      XC(K)=SYM(1,I)+SYM( 2,I)*XYZR(1,J)+SYM( 3,I)*XYZR(2,J)
     1+SYM( 4,I)*XYZR(3,J)
      YC(K)=SYM(5,I)+SYM( 6,I)*XYZR(1,J)+SYM( 7,I)*XYZR(2,J)
     1+SYM( 8,I)*XYZR(3,J)
      ZC(K)=SYM(9,I)+SYM(10,I)*XYZR(1,J)+SYM(11,I)*XYZR(2,J)
     1+SYM(12,I)*XYZR(3,J)
C     TEST FOR CHANGE IN COORDINATES AND SET INDICATOR
      ICC(K)=1
      IF(DABS(XC(K)-XCSV)-1.0D-10)670,670,685
  670 IF(DABS(YC(K)-YCSV)-1.0D-10)675,675,685
  675 IF(DABS(ZC(K)-ZCSV)-1.0D-10)680,680,685
  680 ICC(K)=0
  685 CONTINUE
C     COUNT AND TIME PASSES THROUGH COORDINATE CALCULATIONS
      NT(2)=NT(2)+1
      LTF=ICLOCK(0)
      LT(2)=LT(2)+LTF-LTI
      LTI=LTF
C     PREPARE FOR SUM OVER RECIPROCAL LATTICE
      SF=0.0
      SFV=0.0
      IF(ISW)700,690,700
  690 IF(CK)780,695,780
C     NOT FIRST ENTRY AND EWALD CONSTANT IS ZERO. OMIT RECIPROCAL SUM
  695 SQK=0.0
      SPLK=0.0
      SPPK=0.0
      GO TO 1390
C     FIRST ENTRY OF CYCLE. PRINT CAPTION
  700 IF(IPRC-2)705,705,710
  705 PRINT 5,TITLE,DATE,STITLE
    5 FORMAT(1H1,18A4,8X,A8/X,17A4)
      PRINT 10,JC
   10 FORMAT('0CYCLE',I3)
  710 NF=0
      NFS=0
      IF(CK)720,715,720
C     EWALD CONSTANT IS ZERO. OMIT RECIPROCAL LATTICE SUM
  715 CSF=0.0
      VSF=0.0
      SQK=0.0
      SPLK=0.0
      SPPK=0.0
      GO TO 940
C     RECIPROCAL LATTICE SUM FOR FIRST ENTRY OF EACH CYCLE
  720 IF(IPRC-1)725,725,730
  725 PRINT 15
   15 FORMAT('0              CSF              VSF              QMAX
     1 NF')
C     START LOOP OVER SHELLS IN RECIPROCAL LATTICE
  730 QQMAX=0.0
      IQ=1
C     INITIAL CALCULATIONS FOR A GIVEN SHELL
  735 QQMIN=QQMAX
      QMAX=QLIM(IQ)
      QQMAX=QMAX**2
      HXMAX=A(1)*QMAX
      HYMAX=A(2)*QMAX
      HZMAX=A(3)*QMAX
      HXMAX=AINT(HXMAX)
      HYMAX=AINT(HYMAX)
      HZMAX=AINT(HZMAX)
      HXMIN=-HXMAX*HXNEG
      HYMIN=-HYMAX*HYNEG
      HZMIN=-HZMAX*HZNEG
C     START LOOP OVER INDICES
      HX=HXMIN
  740 HXM=1.0+AMIN1(HX,1.0)*(1.0-HXNEG)
      QQX=HX*HX*B11
      HBXY=HX*B12
      HBXZ=HX*B13
      HY=HYMIN
  745 HYM=HXM*(1.0+AMIN1(HY,1.0)*(1.0-HYNEG))
      QQY=QQX+HY*(HY*B22+HBXY)
      HBYZ=HY*B23+HBXZ
      HZ=HZMIN
  750 QQ=QQY+HZ*(HZ*B33+HBYZ)
      IF(QQ-QQMIN)835,835,755
  755 IF(QQ-QQMAX)760,760,835
C     ENTER USERS ROUTINE TO TEST FOR SPACE-GROUP ABSENCES
  760 IREJ=0
      CALL REJECT(ISG,HX,HY,HZ,IREJ)
      IF(IREJ)835,765,835
C     COMPUTE MULTIPLICITY FACTOR
  765 HM=HYM*(1.0+AMIN1(HZ,1.0)*(1.0-HZNEG))
C     STORE INDICES AND MULTIPLICITY FOR USE ON LATER ENTRIES
      IF(NFS-NFSMAX)770,775,775
  770 NFS=NFS+1
  775 NF=NF+1
      HXT(NFS)=HX
      HYT(NFS)=HY
      HZT(NFS)=HZ
      HMT(NFS)=HM
C     JUMP TO STRUCTURE FACTOR CALCULATION
      GO TO 800
C     FAST RECIPROCAL LATTICE SUM USED ON ENTRIES OTHER THAN FIRST
C     BYPASS IF NO RECIPROCAL LATTICE POINTS WERE FOUND WITHIN RANGE
  780 IF(NFS)790,785,790
  785 VSF=0.0
      CSF=0.0
      GO TO 890
C     START FAST RECIPROCAL LATTICE SUM
  790 IH=1
C     PICK UP INDICES AND MULTIPLICITY STORED ON FIRST ENTRY
  795 HX=HXT(IH)
      HY=HYT(IH)
      HZ=HZT(IH)
      HM=HMT(IH)
      QQ=HX*HX*B11+HY*(HY*B22+HX*B12)+HZ*(HZ*B33+HY*B23+HX*B13)
C     STRUCTURE FACTOR CALCULATION USED FOR BOTH SLOW AND FAST SUMS
  800 AF=0.0
      BF=0.0
      AFV=0.0
      BFV=0.0
C     SUM OVER ALL OR HALF ATOMS IN UNIT CELL. NAF WAS SET IN WPRE
      DO 810 J=1,NAF
      JA=IKA1J4C(J)
      IF(JA)810,810,802
  802 ARG=TPI*(HX*XC(J)+HY*YC(J)+HZ*ZC(J))
      QJA=Q1JA)
      PLJA=PL(JA)
      COSARG=DCOS(ARG)
      AF=AF+FMC(J)*QJA*COSARG
      AFV=AFV+FMC(J)*PLJA*COSARG
C     OMIT SINE TERMS IF CENTROSYMMETRIC
      IF(ICENT-1)810,810,805
  805 SINARG=DSIN(ARG)
      BF=BF+QJA*SINARG
      BFV=BFV+PLJA*SINARG
  810 CONTINUE
C     COMPUTE MODIFICATION FUNCTION FOR EWALD-BERTAUT-WILLIAMS METHOD
      YYM=PIOKSQ*QQ
      EXPYYM=DEXP(-YYM)
C     CALCULATE EWALD MODIFIED COULOMB TERM AND ADD TO SUM
      IF(ICMB)815,820,815
  815 FSQ=(FM*AF)**2+BF**2
      SF=SF+FSQ*HM*EXPYYM/QQ
C     CALCULATE WILLIAMS MODIFIED VAN DER WAALS TERM AND ADD TO SUM
  820 IF(IVDW)825,830,825
  825 FSQV=(FM*AFV)**2+BFV**2
      QH=DSQRT(QQ)
      YM=SQTPOK*QH
      SFV=SFV+FSQV*HM*QQ*QH*((10.5/YYM-1.0)/YM)*EXPYYM*SQTPI*DERFC(YM))
C     BRANCH DEPENDING ON WHETHER THIS FIRST OR SUBSEQUENT ENTRY
  830 IF(ISW)835,880,835
C     FIRST ENTRY. ADVANCE INDICES AND TEST FOR END OF THIS SHELL
  835 HZ=HZ+1.0
      IF(HZ-HZMAX)750,750,840
  840 HY=HY+1.0
      IF(HY-HYMAX)745,745,845
  845 HX=HX+1.0
      IF(HX-HXMAX)740,740,850
  850 CSF=RTPIZV*SF
      VSF=01NHZV*SFV
C     PRINT OUTPUT FOR ONE SHELL
      IF(IPRC-1)855,855,860
  855 PRINT 20,CSF,VSF,QMAX,NF
   20 FORMAT(X,3F15.6,I5)
C     TEST FOR END OF LOOP THROUGH SHELLS
  860 IF(IQ-NQ)865,870,870
  865 IQ=IQ+1
      GO TO 735
C     COUNT AND TIME PASSES THROUGH SLOW RECIPROCAL-LATTICE SUM
  870 NT(3)=NT(3)+1
      LTF=ICLOCK(0)
      LT(3)=LT(3)+LTF-LTI
      LTI=LTF
C     TEST FOR OVERFLOW OF STORAGE ARRAYS AND PROCEED TO UNIT CELL SUMS
      IF(NF-NFS)875,890,875
  875 PRINT 25,NF,NFS
   25 FORMAT('0***NUMBER OF RECIPROCAL LATTICE POINTS GENERATED IS'
     1,I6,'. THIS EXCEEDS THE PRESET LIMIT OF',I6/8X,'THE INITIAL ENERGY
     2 CALCULATION IS CORRECT BUT DERIVATIVES, ETC. ARE NOT. ***')
      GO TO 890
C     TEST FOR END OF FAST RECIPROCAL LATTICE SUMS
  880 IH=IH+1
      IF(IH-NFS)795,795,885
  885 CSF=RTPIZV*SF
      VSF=PINHZV*SFV
C     COUNT AND TIME PASSES THROUGH FAST RECIPROCAL-LATTICE SUM
      NT(4)=NT(4)+1
      LTF=ICLOCK(0)
      LT(4)=LT(4)+LTF-LTI
      LTI=LTF
C     UNIT CELL SUMS ARE A PART OF THE RECIPROCAL LATTICE SUMMATION
C          THEY ARE BYPASSED IF EWALD CONSTANT IS ZERO
C     BYPASS IF NO PARAMETER HAS CHANGED. CANNOT OCCUR ON FIRST ENTRY
  890 IF(ICCAX)895,1390,895
  895 SQ=0.0
      SPL=0.0
      SPP=0.0
      DO 900 I=1,NA
      K=KA(I)
      IF(K)900,900,897
  897 SQ=SQ+ZAM(I)*Q(K)**2
      SPL=SPL+ZAM(I)*PL(K)
      SPP=SPP+ZAM(I)*PL(K)**2
  900 CONTINUE
      SQK=0.0
      SPLK=0.0
      SPPK=0.0
      IF(ICMB)905,910,905
  905 SQK=CKKCAL*SQ
  910 IF(IVDW)915,920,915
  915 SPLK=PICKZV*SPL**2
      SPPK=PICK*SPP
C     COUNT AND TIME PASSES THROUGH UNIT CELL SUM
  920 NT(5)=NT(5)+1
      LTF=ICLOCK(0)
      LT(5)=LT(5)+LTF-LTI
      LTI=LTF
C     ON FIRST ENTRY PRINT CELL SUMS. OTHERWISE JUMP TO FAST DIRECT SUM
      IF(ISW)930,1390,930
  930 IF(IPRC-1)935,935,940
  935 PRINT 30,SQK,SPLK,SPPK
   30 FORMAT('0              SQK              SPLK              SPPK'/X,3F15.6)
C     START DIRECT LATTICE SUM FOR FIRST ENTRY
  940 IF(IPRC-1)945,945,950
  945 PRINT 35
   35 FORMAT('0              SQX              SVDW              WR
     1MAX              NG              NSRB')
  950 SQ=0.0
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      WR=0.0                                                            WCAL2300
      SVDW=0.0                                                          WCAL2305
      REP=0.0                                                           WCAL2310
      VDW=0.0                                                           WCAL2315
      CMB=0.0                                                           WCAL2320
      RTM=0.0                                                           WCAL2325
      VTM=0.0                                                           WCAL2330
      CTM=0.0                                                           WCAL2335
      NG=0                                                              WCAL2340
      NGS=0                                                             WCAL2345
C     IF EWALD CONSTANT IS ZERO BYPASS CALCULATION OF INTRABODY TERMS   WCAL2350
      IF(CK)955,1045,955                                                WCAL2355
C     TREAT ALL INTRABODY AND BONDED CONTACTS SPECIALLY. THEY MUST BE   WCAL2360
C        SUBTRACTED OUT SINCE THEY ARE ALREADY IN RECIPROCAL LATTICE SUMWCAL2365
  955 DO 1040 I=1,NA                                                    WCAL2370
      IA=JAC(I)                                                         WCAL2375
      IK=IKA(IA)                                                        WCAL2380
      IF(IK)1040,1040,957                                               WCAL2385
  957 GMI=ZAM(I)                                                        WCAL2390
      IP=I+1                                                            WCAL2395
      IF(IP-NAC)958,958,1040                                            WCAL2400
  958 DO 1035 J=IP,NAC                                                  WCAL2405
      JA=JAC(J)                                                         WCAL2410
      JK=IKA(JA)                                                        WCAL2415
      IF(JK)1035,1035,959                                               WCAL2420
C     OMIT TERM OR SET MULTIPLICITY DEPENDING ON ATOM NUMBERS           WCAL2425
  959 IF(JA-IA)1035,960,965                                             WCAL2430
  960 GM=0.5*GMI                                                        WCAL2435
      GO TO 970                                                         WCAL2440
  965 GM=GMI                                                            WCAL2445
C     TEST FOR PAIRS IN SAME RIGID BODY                                 WCAL2450
  970 IF(IRBC(I)-IRBC(J))975,995,975                                    WCAL2455
C     TEST FOR PAIRS IN LIST OF BONDS                                   WCAL2460
  975 IF(NBC)980,1035,980                                               WCAL2465
  980 DO 990 K=1,NBC                                                    WCAL2470
      IF(I-LBCI(K))990,985,990                                          WCAL2475
  985 IF(J-LBCJ(K))990,995,990                                          WCAL2480
  990 CONTINUE                                                          WCAL2485
      GO TO 1035                                                        WCAL2490
C     COMPUTE VAN DER WAALS AND COULOMB TERMS. REPULSION TERM IS ZERO   WCAL2495
  995 DX=X(J)-X(I)                                                      WCAL2500
      DY=Y(J)-Y(I)                                                      WCAL2505
      DZ=Z(J)-Z(I)                                                      WCAL2510
      RR=DX*DX*A11+DY*(DY*A22+DX*A12)+DZ*(DZ*A33+DY*A23+DX*A13)         WCAL2515
      R=DSQRT(RR)                                                       WCAL2520
      IF(RR-1.0D-20)996,996,1000                                        WCAL2525
C     TREAT SPECIAL CASE OF ZERO R                                      WCAL2530
C     COMPUTE LIMITING VALUE OF WILLIAMS MODIFIED VAN DER WAALS TERM    WCAL2535
  996 IF(IVDW)997,998,997                                               WCAL2540
  997 VDW=0.0                                                           WCAL2545
      VTM=2.0*PICK*GM*PL(IK)*PL(JK)                                     WCAL2550
      SVDW=SVDW+VTM                                                     WCAL2555
C     COMPUTE LIMITING VALUE OF EWALD MODIFIED COULOMB TERM             WCAL2560
  998 IF(ICMB)999,1020,999                                              WCAL2565
  999 CMB=0.0                                                           WCAL2570
      CTM=-2.0*CK*GM*Q(IK)*Q(JK)                                        WCAL2575
      SG=SG+CTM                                                         WCAL2580
      GO TO 1020                                                        WCAL2585
C     TREAT USUAL CASE OF NON-ZERO R                                    WCAL2590
 1000 XM=SQTPIK*R                                                       WCAL2595
C     CALCULATE WILLIAMS MODIFIED VAN DER WAALS TERM LESS UNMODIFIED    WCAL2600
      IF(IVDW)1005,1010,1005                                            WCAL2605
 1005 VDW=-PL(IK)*PL(JK)/(RR*RR*RR)                                     WCAL2610
      XXM=XM*XM                                                         WCAL2615
      VTM=GM*VDW*((0.5*XXM*XXM+XXM+1.0)*DEXP(-XXM)-1.0)                 WCAL2620
      SVDW=SVDW+VTM                                                     WCAL2625
C     CALCULATE EWALD MODIFIED COULOMB TERM LESS UNMODIFIED             WCAL2630
 1010 IF(ICMB)1015,1020,1015                                            WCAL2635
 1015 CMB=Q(IK)*Q(JK)/R                                                 WCAL2640
      CTM=CMB*GM*(DERFC(XM)-1.0)                                        WCAL2645
      SG=SG+CTM                                                         WCAL2650
C     STORE QUANTITIES NEEDED FOR FAST SUM ON LATER ENTRIES             WCAL2655
 1020 IF(NGS-NGSMAX)1025,1030,1030                                      WCAL2660
 1025 NGS=NGS+1                                                         WCAL2665
 1030 NG=NG+1                                                           WCAL2670
      GXT(NGS)=0.0                                                      WCAL2675
      GYT(NGS)=0.0                                                      WCAL2680
      GZT(NGS)=0.0                                                      WCAL2685
      IAT(NGS)=I                                                        WCAL2690
      JAT(NGS)=J                                                        WCAL2695
      SRBT(NGS)=1.0                                                     WCAL2700
      GMT(NGS)=GM                                                       WCAL2705
      RT(NGS)=R                                                         WCAL2710
      REPT(NGS)=0.0                                                     WCAL2715
      VDWT(NGS)=VDW                                                     WCAL2720
      CMBT(NGS)=CMB*FKCAL                                               WCAL2725
      RSV(NGS)=0.0                                                      WCAL2730
      VSV(NGS)=VTM                                                      WCAL2735
      CSV(NGS)=CTM                                                      WCAL2740
 1035 CONTINUE                                                          WCAL2745
 1040 CONTINUE                                                          WCAL2750
C     SAVE NUMBER OF TERMS IN SAME RIGID BODY OR BONDED                 WCAL2755
 1045 NSRB=NG                                                           WCAL2760
C     PREPARE FOR SUM OVER DIRECT LATTICE VECTORS ON FIRST ENTRY        WCAL2765
C     FIND MAXIMUM AND MINIMUM VALUES OF COORDINATES IN UNIT CELL       WCAL2770
      CXMIN=100.                                                        WCAL2775
      CYMIN=100.                                                        WCAL2780
      CZMIN=100.                                                        WCAL2785
      CXMAX=-100.                                                       WCAL2790
      CYMAX=-100.                                                       WCAL2795
      CZMAX=-100.                                                       WCAL2800
      DO 1115 I=1,NAC                                                   WCAL2805
      IF(XC(I)-CXMIN)1050,1055,1055                                     WCAL2810
 1050 CXMIN=XC(I)                                                       WCAL2815
 1055 IF(XC(I)-CXMAX)1065,1065,1060                                     WCAL2820
 1060 CXMAX=XC(I)                                                       WCAL2825
 1065 IF(YC(I)-CYMIN)1070,1075,1075                                     WCAL2830
 1070 CYMIN=YC(I)                                                       WCAL2835
 1075 IF(YC(I)-CYMAX)1085,1085,1080                                     WCAL2840
 1080 CYMAX=YC(I)                                                       WCAL2845
 1085 IF(ZC(I)-CZMIN)1090,1095,1095                                     WCAL2850
 1090 CZMIN=ZC(I)                                                       WCAL2855
 1095 IF(ZC(I)-CZMAX)1105,1105,1100                                     WCAL2860
 1100 CZMAX=ZC(I)                                                       WCAL2865
C     ALSO GET MAX AND MIN COORDINATES IN BASIC ASYMMETRIC UNIT         WCAL2870
 1105 IF(I-NA)1115,1110,1115                                            WCAL2875
 1110 BXMIN=CXMIN                                                       WCAL2880
      BYMIN=CYMIN                                                       WCAL2885
      BZMIN=CZMIN                                                       WCAL2890
      BXMAX=CXMAX                                                       WCAL2895
      BYMAX=CYMAX                                                       WCAL2900
      BZMAX=CZMAX                                                       WCAL2905
 1115 CONTINUE                                                          WCAL2910
C     INITIALIZE LOOP OVER SHELLS IN DIRECT SPACE                       WCAL2915
      RRMAX=0.000001                                                    WCAL2920
      IR=1                                                              WCAL2925
C     START CALCULATIONS FOR ONE SHELL                                  WCAL2930
 1120 RRMIN=RRMAX                                                       WCAL2935
      RMAX=RLIM(IR)                                                     WCAL2940
      RRMAX=RMAX**2                                                     WCAL2945
C     ELIMINATE LATTICE TRANSLATIONS FOR CASE OF ISOLATED MOLECULE      WCAL2950
      IF(IMOL)1125,1130,1125                                            WCAL2955
 1125 GXMIN=0.0                                                         WCAL2960
      GYMIN=0.0                                                         WCAL2965
      GZMIN=0.0                                                         WCAL2970
      GXMAX=0.0                                                         WCAL2975
      GYMAX=0.0                                                         WCAL2980
      GZMAX=0.0                                                         WCAL2985
      GO TO 1135                                                        WCAL2990
C     COMPUTE LIMITS FOR LATTICE TRANSLATIONS IN CRYSTAL                WCAL2995
 1130 GXMIN=B1*RMAX+CXMAX-BXMIN                                         WCAL3000
      GYMIN=B2*RMAX+CYMAX-BYMIN                                         WCAL3005
      GZMIN=B3*RMAX+CZMAX-BZMIN                                         WCAL3010
      GXMIN=-AINT(GXMIN)                                                WCAL3015
      GYMIN=-AINT(GYMIN)                                                WCAL3020
      GZMIN=-AINT(GZMIN)                                                WCAL3025
      GXMAX=B1*RMAX+BXMAX-CXMIN                                         WCAL3030
      GYMAX=B2*RMAX+BYMAX-CYMIN                                         WCAL3035
      GZMAX=B3*RMAX+BZMAX-CZMIN                                         WCAL3040
      GXMAX=AINT(GXMAX)                                                 WCAL3045
      GYMAX=AINT(GYMAX)                                                 WCAL3050
      GZMAX=AINT(GZMAX)                                                 WCAL3055
C     START LOOPS OVER LATTICE TRANSLATIONS                             WCAL3060
 1135 GX=GXMIN                                                          WCAL3065
 1140 GY=GYMIN                                                          WCAL3070
 1145 GZ=GZMIN                                                          WCAL3075
C     START OUTER LOOP OVER ONE ASYMMETRIC UNIT                         WCAL3080
 1150 DO 1275 I=1,NA                                                    WCAL3085
      IA=JAC(I)                                                         WCAL3090
      IK=IKA(IA)                                                        WCAL3095
      IF(IK)1275,1275,1152                                              WCAL3100
 1152 DXI=GX-XC(I)                                                      WCAL3105
      DYI=GY-YC(I)                                                      WCAL3110
      DZI=GZ-ZC(I)                                                      WCAL3115
      GMI=ZAM(I)                                                        WCAL3120
C     START INNER LOOP OVER ONE UNIT CELL                               WCAL3125
      DO 1270 J=1,NAC                                                   WCAL3130
      JA=JAC(J)                                                         WCAL3135
      JK=IKA(JA)                                                        WCAL3140
      IF(JK)1270,1270,1153                                              WCAL3145
C     OMIT TERM OR SET MULTIPLICITY DEPENDING ON ATOM NUMBERS           WCAL3150
 1153 IF(JA-IA)1270,1155,1160                                           WCAL3155
 1155 GM=0.5*GMI                                                        WCAL3160
      GO TO 1165                                                        WCAL3165
 1160 GM=GMI                                                            WCAL3170
C     COMPUTE DISTANCE SQUARED AND TEST WHETHER IT FALLS IN SHELL       WCAL3175
 1165 DX=DXI+XC(J)                                                      WCAL3180
      DY=DYI+YC(J)                                                      WCAL3185
      DZ=DZI+ZC(J)                                                      WCAL3190
      RR=DX*DX*A11+DY*(DY*A22+DX*A12)+DZ*(DZ*A33+DY*A23+DX*A13)         WCAL3195
      IF(RR-RRMIN)1270,1270,1170                                        WCAL3200
 1170 IF(RR-RRMAX)1175,1175,1270                                        WCAL3205
C     IN SHELL. COMPUTE DISTANCE                                        WCAL3210
 1175 R=DSQRT(RR)                                                       WCAL3215
      XM=SQTPIK*R                                                       WCAL3220
C     OMIT PAIR IF IN SAME RIGID BODY OR BONDED. TERM ALREADY INCLUDED  WCAL3225
      IF(GX)1215,1180,1215                                              WCAL3230
 1180 IF(GY)1215,1185,1215                                              WCAL3235
 1185 IF(GZ)1215,1190,1215                                              WCAL3240
 1190 IF(IRBC(I)-IRBC(J))1195,1270,1195                                 WCAL3245
 1195 IF(NBC)1200,1215,1200                                             WCAL3250
 1200 DO 1210 K=1,NBC                                                   WCAL3255
      IF(I-LBCI(K))1210,1205,1210                                       WCAL3260
 1205 IF(J-LBCJ(K))1210,1270,1210                                       WCAL3265
 1210 CONTINUE                                                          WCAL3270
C     CALCULATE REPULSION TERM                                          WCAL3275
 1215 IF(IREP.EQ.0) GO TO 1235                                          WCAL3280
      REP=0.0                                                           WCAL3285
      GO TO (1225,1220,1220,1218,1218,1218,1218),IREP                   WCAL3290
 1218 REP=GPOT(ISB,I,J,IA,JA,IK,JK,GX,GY,GZ,DX,DY,DZ,R)                 WCAL3295
      GO TO (1225,1220,1220,1230,1225,1220,1220),IREP                   WCAL3300
 1220 REP=REP+REPL(ISB,IK,JK,R)                                         WCAL3305
      GO TO (1225,1230,1225,1230,1225,1230,1225),IREP                   WCAL3310
 1225 BRIJ=BR(IK)+BR(JK)                                                WCAL3315
      REP=REP+BRIJ*DEXP((AR(IK)+AR(JK)-R)/BRIJ)                         WCAL3320
 1230 RTM=GM*REP                                                        WCAL3325
      WR=WR+RTM                                                         WCAL3330
C     CALCULATE VAN DER WAALS TERM MODIFIED FOR WILLIAMS METHOD         WCAL3335
 1235 IF(IVDW)1240,1245,1240                                            WCAL3340
 1240 VDW=-PL(IK)*PL(JK)/(RR*RR*RR)                                     WCAL3345
      XXM=XM*XM                                                         WCAL3350
      VTM=GM*VDW*(0.5*XXM*XXM+XXM+1.0)*DEXP(-XXM)                       WCAL3355
      SVDW=SVDW+VTM                                                     WCAL3360
C     CALCULATE COULOMB TERM MODIFIED FOR EWALD METHOD                  WCAL3365
 1245 IF(ICMB)1250,1255,1250                                            WCAL3370
 1250 CMB=Q(IK)*Q(JK)/R                                                 WCAL3375
      CTM=CMB*GM*DERFC(XM)                                              WCAL3380
      SG=SG+CTM                                                         WCAL3385
C     STORE QUANTITIES NEEDED FOR FAST SUM ON LATER ENTRIES             WCAL3390
 1255 IF(NGS-NGSMAX)1260,1265,1265                                      WCAL3395
 1260 NGS=NGS+1                                                         WCAL3400
 1265 NG=NG+1                                                           WCAL3405
      GXT(NGS)=GX                                                       WCAL3410
      GYT(NGS)=GY                                                       WCAL3415
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      GZT(NGS)=GZ                                                       WCAL3420
      IAT(NGS)=I                                                        WCAL3425
      JAT(NGS)=J                                                        WCAL3430
      SRBT(NGS)=0.0                                                     WCAL3435
      GMT(NGS)=GM                                                       WCAL3440
      RT(NGS)=R                                                         WCAL3445
      REPT(NGS)=REP                                                     WCAL3450
      VDWT(NGS)=VDW                                                     WCAL3455
      CMBT(NGS)=CMB*FKCAL                                               WCAL3460
      RSV(NGS)=RTM                                                      WCAL3465
      VSV(NGS)=VTM                                                      WCAL3470
      CSV(NGS)=CTM                                                      WCAL3475
 1270 CONTINUE                                                          WCAL3480
 1275 CONTINUE                                                          WCAL3485
C     ADVANCE AND TEST LATTICE TRANSLATIONS                             WCAL3490
      GZ=GZ+1.0                                                         WCAL3495
      IF(GZ-GZMAX)1150,1150,1280                                        WCAL3500
 1280 GY=GY+1.0                                                         WCAL3505
      IF(GY-GYMAX)1145,1145,1285                                        WCAL3510
 1285 GX=GX+1.0                                                         WCAL3515
      IF(GX-GXMAX)1140,1140,1290                                        WCAL3520
C     COMPUTE AND PRINT RESULTS FOR DIRECT LATTICE SUM TO LIMIT OF SHELLWCAL3525
 1290 SGK=SG*FKCAL                                                      WCAL3530
      IF(IPRC-1)1295,1295,1300                                          WCAL3535
 1295 PRINT 40,SGK,SVDW,WR,RMAX,NG,NSRB                                 WCAL3540
   40 FORMAT(X,4F15.6,2I15)                                             WCAL3545
C     ADVANCE AND TEST LOOP THROUGH SHELLS                              WCAL3550
 1300 IR=IR+1                                                           WCAL3555
      IF(IR-NR)1120,1120,1305                                           WCAL3560
C     SORT AND PRINT RESULTS FOR A LIMITED NUMBER OF SHORTEST DISTANCES WCAL3565
 1305 IF(NGS)1355,1355,1310                                             WCAL3570
 1310 IF(IPRC-1)1315,1315,1355                                          WCAL3575
 1315 PRINT 45                                                          WCAL3580
   45 FORMAT('0 GX GY GZ  I  J       GM         R   NAMES         CMB   WCAL3585
     1 VDW        REP        SRB')                                     WCAL3590
C     INITIALIZE COUNTER AND COMPUTE MAXIMUM NUMBER TO BE PRINTED       WCAL3595
      IRP=0                                                             WCAL3600
      NRPA=IABS(NRP)*10                                                 WCAL3605
C     START OUTER LOOP TO PRINT UP TO NGS LINES                         WCAL3610
      DO 1350 I=1,NGS                                                   WCAL3615
C     LOOP TO FIND SMALLEST DISTANCE                                    WCAL3620
      SML=100.                                                          WCAL3625
      DO 1325 J=1,NGS                                                   WCAL3630
      IF(RT(J)-SML)1320,1325,1325                                       WCAL3635
 1320 SML=RT(J)                                                         WCAL3640
      JS=J                                                              WCAL3645
 1325 CONTINUE                                                          WCAL3650
C     DO NOT PRINT DISTANCES IN SAME RIGID BODY OR BONDED IF NRP IS NEG WCAL3655
      IF(SRBT(JS))1330,1335,1330                                        WCAL3660
 1330 IF(NRP)1345,1335,1335                                             WCAL3665
C     TERMINATE IF LIMIT ON NUMBER TO BE PRINTED HAS BEEN REACHED       WCAL3670
 1335 IRP=IRP+1                                                         WCAL3675
      IF(IRP-NRPA)1340,1340,1355                                        WCAL3680
C     PRINT LINE                                                        WCAL3685
 1340 IA=IAT(JS)                                                        WCAL3690
      JA=JAT(JS)                                                        WCAL3695
      IA=JAC(IA)                                                        WCAL3700
      JA=JAC(JA)                                                        WCAL3705
      IGX=GXT(JS)                                                       WCAL3710
      IGY=GYT(JS)                                                       WCAL3715
      IGZ=GZT(JS)                                                       WCAL3720
      PRINT 50,IGX,IGY,IGZ,IAT(JS),JAT(JS)                              WCAL3725
     1,GMT(JS),SML,NAME(IA),NAME(JA),CMBT(JS),VDWT(JS),REPT(JS)         WCAL3730
     2,SRBT(JS)                                                         WCAL3735
   50 FORMAT(X,5I3,2F9.5,2X,A4,X,A4,3F9.3,F8.1)                         WCAL3740
C     STORE LARGE VALUE FOR DISTANCE JUST PRINTED AND CONTINUE          WCAL3745
 1345 RT(JS)=100.                                                       WCAL3750
 1350 CONTINUE                                                          WCAL3755
C     TEST FOR OVERFLOW OF STORAGE ARRAYS AND PRINT MESSAGE             WCAL3760
 1355 IF(NG-NGS)1360,1365,1360                                          WCAL3765
 1360 PRINT 55,NG,NGS                                                   WCAL3770
   55 FORMAT('0*** NUMBER OF INTERATOMIC VECTORS GENERATED IS'          WCAL3775
     1,I6,'. THIS EXCEEDS THE PRESET LIMIT OF',I6/5X,'THE INITIAL ENERGYWCAL3780
     2 CALCULATION IS CORRECT BUT DERIVATIVES, ETC. ARE NOT. ***')      WCAL3785
C     CALCULATE TOTAL COULOMB AND VAN DER WAALS ENERGY                  WCAL3790
 1365 WC=CSF+SGK+SGK                                                    WCAL3795
      WV=VSF+SPLK+SPPK+SVDW                                             WCAL3800
C     COUNT AND TIME PASSES THROUGH SLOW DIRECT-LATTICE SUM             WCAL3805
      NT(6)=NT(6)+1                                                     WCAL3810
      LTF=ICLOCK(0)                                                     WCAL3815
      LT(6)=LT(6)+LTF-LTI                                               WCAL3820
      LTI=LTF                                                           WCAL3825
C     ENTER USER ROUTINE TO CALCULATE ENERGY OF POLARIZATION, ETC       WCAL3830
      WX=0.0                                                            WCAL3835
      CALL CWX                                                          WCAL3840
C     COMPUTE ENERGY OF DISTANCES, ANGLES, AND TORSION ANGLES           WCAL3845
      IF(NCT)1370,1375,1370                                             WCAL3850
 1370 CALL GCWX                                                         WCAL3855
C     COMPUTE AND PRINT TOTAL ENERGY AND RETURN FROM FIRST ENTRY        WCAL3860
 1375 WT=WC+WV+WR+WX                                                    WCAL3865
      IF(IPRT-4)1380,1380,1385                                          WCAL3870
 1380 PRINT 60,WC,WV,WR,WX,WT                                           WCAL3875
   60 FORMAT('0       WC         WV         WR         WX         WT'  WCAL3880
     1/X,5F9.3)                                                         WCAL3885
C     COUNT AND TIME PASSES THROUGH SLOW INTERNAL ENERGY CALCULATIONS   WCAL3890
 1385 NT(8)=NT(8)+1                                                     WCAL3895
      LTF=ICLOCK(0)                                                     WCAL3900
      LT(8)=LT(8)+LTF-LTI                                               WCAL3905
      LTI=LTF                                                           WCAL3910
      GO TO 1520                                                        WCAL3915
C     MAKE FAST DIRECT LATTICE SUMS ON ENTRIES AFTER THE FIRST          WCAL3920
 1390 SG=0.0                                                            WCAL3925
      WR=0.0                                                            WCAL3930
      SVDW=0.0                                                          WCAL3935
C     START LOOP THROUGH STORAGE ARRAYS                                 WCAL3940
      IF(NGS)1490,1490,1395                                             WCAL3945
 1395 DO 1485 IG=1,NGS                                                  WCAL3950
C     PICK UP THE ATOM NUMBERS                                          WCAL3955
      I=IAT(IG)                                                         WCAL3960
      J=JAT(IG)                                                         WCAL3965
C     TEST WHETHER PARAMETERS OR ATOM COORDINATES HAVE CHANGED          WCAL3970
      IF(ICCAX.NE.0.OR.ICC(I).NE.0.OR.ICC(J).NE.0.OR.IREP.GE.4)         WCAL3975
     1 GO TO 1415                                                       WCAL3980
C     UNCHANGED. ADD TO SUM SAME TERMS USED ON PREVIOUS ENTRY           WCAL3985
 1410 WR=WR+RSV(IG)                                                     WCAL3990
      SVDW=SVDW+VSV(IG)                                                 WCAL3995
      SG=SG+CSV(IG)                                                     WCAL4000
      GO TO 1485                                                        WCAL4005
C     TERMS MAY HAVE CHANGED. PICK UP QUANTITIES NEEDED FOR CALCULATION WCAL4010
 1415 GX=GXT(IG)                                                        WCAL4015
      GY=GYT(IG)                                                        WCAL4020
      GZ=GZT(IG)                                                        WCAL4025
      IA=JAC(I)                                                         WCAL4030
      JA=JAC(J)                                                         WCAL4035
      IK=IKA(IA)                                                        WCAL4040
      JK=IKA(JA)                                                        WCAL4045
      SRB=SRBT(IG)                                                      WCAL4050
      GM=GMT(IG)                                                        WCAL4055
      DX=GX+XC(J)-XC(I)                                                 WCAL4060
      DY=GY+YC(J)-YC(I)                                                 WCAL4065
      DZ=GZ+ZC(J)-ZC(I)                                                 WCAL4070
      RR=DX*DX*A11+DY*(DY*A22+DX*A12)+DZ*(DZ*A33+DY*A23+DX*A13)         WCAL4075
      R=DSQRT(RR)                                                       WCAL4080
C     CALCULATE REPULSION AND STORE IT IF NOT IN SAME RIGID BODY        WCAL4085
      IF(SRB)1440,1420,1440                                             WCAL4090
 1420 IF(IREP.EQ.0) GO TO 1440                                          WCAL4095
      REP=0.0                                                           WCAL4100
      GO TO (1430,1425,1425,1422,1422,1422,1422),IREP                   WCAL4105
 1422 REP=GPOT(ISB,I,J,IA,JA,IK,JK,GX,GY,GZ,DX,DY,DZ,R)                 WCAL4110
      GO TO (1430,1425,1425,1435,1430,1425,1425),IREP                   WCAL4115
 1425 REP=REP+REPL(ISB,IK,JK,R)                                         WCAL4120
      GO TO (1430,1435,1430,1435,1430,1435,1430),IREP                   WCAL4125
 1430 BRIJ=BR(IK)+BR(JK)                                                WCAL4130
      REP=REP+BRIJ*DEXP((AR(IK)+AR(JK)-R)/BRIJ)                         WCAL4135
 1435 RTM=GM*REP                                                        WCAL4140
      RSV(IG)=RTM                                                       WCAL4145
      WR=WR+RTM                                                         WCAL4150
C     IF EWALD CONSTANT IS ZERO SAVE TIME BY CALCULATING UNMODIFIED TERMWCAL4155
 1440 IF(CK)1460,1445,1460                                              WCAL4160
C     CALCULATE VAN DER WAALS TERM AND STORE IT                         WCAL4165
 1445 IF(IVDW)1450,1455,1450                                            WCAL4170
 1450 VTM=-GM*PL(IK)*PL(JK)/(RR*RR*RR)                                  WCAL4175
      VSV(IG)=VTM                                                       WCAL4180
      SVDW=SVDW+VTM                                                     WCAL4185
C     CALCULATE COULOMB TERM AND STORE IT                               WCAL4190
 1455 IF(CMB)1458,1485,1458                                             WCAL4195
 1458 CTM=GM*Q(IK)*Q(JK)/R                                              WCAL4200
      CSV(IG)=CTM                                                       WCAL4205
      SG=SG+CTM                                                         WCAL4210
      GO TO 1485                                                        WCAL4215
C     EWALD CONSTANT NOT ZERO. MODIFIED TERMS MUST BE CALCULATED        WCAL4220
 1460 IF(RR-1.0D-20)1461,1461,1465                                      WCAL4225
C     TREAT SPECIAL CASE OF ZERO R, ASSUMES PAIR IN SAME RIGID BODY     WCAL4230
C     COMPUTE LIMITING VALUE OF WILLIAMS MODIFIED VAN DER WAALS TERM    WCAL4235
 1461 IF(IVDW)1462,1463,1462                                            WCAL4240
 1462 VTM=2.0*PI*CK*GM*PL(IK)*PL(JK)                                    WCAL4245
      VSV(IG)=VTM                                                       WCAL4250
      SVDW=SVDW+VTM                                                     WCAL4255
C     COMPUTE LIMITING VALUE OF EWALD MODIFIED COULOMB TERM AND STORE ITWCAL4260
 1463 IF(ICMB)1464,1485,1464                                            WCAL4265
 1464 CTM=-2.0*CK*GM*Q(IK)*Q(JK)                                        WCAL4270
      CSV(IG)=CTM                                                       WCAL4275
      SG=SG+CTM                                                         WCAL4280
      GO TO 1485                                                        WCAL4285
C     TREAT USUAL CASE OF NON-ZERO R                                    WCAL4290
 1465 XM=SGRPIK*R                                                       WCAL4295
C     CALCULATE MODIFIED VAN DER WAALS TERM AND STORE IT                WCAL4300
      IF(IVDW)1470,1475,1470                                            WCAL4305
 1470 VDW=-PL(IK)*PL(JK)/(RR*RR*RR)                                     WCAL4310
      XXM=XM*XM                                                         WCAL4315
      VTM=GM*VDW*((0.5*XXM*XXM+XXM+1.0)*DEXP(-XXM)-SRB)                 WCAL4320
      VSV(IG)=VTM                                                       WCAL4325
      SVDW=SVDW+VTM                                                     WCAL4330
C     CALCULATE MODIFIED COULOMB TERM AND STORE IT                      WCAL4335
 1475 IF(CMB)1480,1485,1480                                             WCAL4340
 1480 CMB=Q(IK)*Q(JK)/R                                                 WCAL4345
      CTM=CMB*GM*(DERFC(XM)-SRB)                                        WCAL4350
      CSV(IG)=CTM                                                       WCAL4355
      SG=SG+CTM                                                         WCAL4360
 1485 CONTINUE                                                          WCAL4365
C     CALCULATE VARIOUS CONTRIBUTIONS TO ENERGY                         WCAL4370
 1490 SGK=SG*FKCAL                                                      WCAL4375
      WC=CSF+SGK+SGK                                                    WCAL4380
      WV=VSF+SPLK+SPPK+SVDW                                             WCAL4385
C     COUNT AND TIME PASSES THROUGH FAST DIRECT-LATTICE SUM             WCAL4390
      NT(7)=NT(7)+1                                                     WCAL4395
      LTF=ICLOCK(0)                                                     WCAL4400
      LT(7)=LT(7)+LTF-LTI                                               WCAL4405
      LTI=LTF                                                           WCAL4410
C     BYPASS INTERNAL ENERGY CALCULATIONS WHEN PREDICTED TO BE UNCHANGEDWCAL4415
 1495 GO TO (1500,1515,1500,1515,1500,1515,1500,1515),IBYP              WCAL4420
C     ENTER USER ROUTINE TO CALCULATE ENERGY OF POLARIZATION, ETC       WCAL4425
 1500 WX=0.0                                                            WCAL4430
      CALL CWX                                                          WCAL4435
      IF(NCT)1505,1510,1505                                             WCAL4440
C     COMPUTE ENERGY OF DISTANCES ANGLES AND TORSION ANGLES             WCAL4445
 1505 CALL GCWX                                                         WCAL4450
C     COUNT AND TIME PASSES THROUGH FAST INTERNAL ENERGY CALCULATIONS   WCAL4455
 1510 NT(9)=NT(9)+1                                                     WCAL4460
      LTF=ICLOCK(0)                                                     WCAL4465
      LT(9)=LT(9)+LTF-LTI                                               WCAL4470
      LTI=LTF                                                           WCAL4475
C     COMPUTE TOTAL ENERGY AND RETURN FROM FAST SUMMATIONS              WCAL4480
 1515 WT=WC+WV+WR+WX                                                    WCAL4485
 1520 WCALC=WT                                                          WCAL4490
 1525 RETURN                                                            WCAL4495
      END                                                               WCAL4500


      SUBROUTINE GCWX3 (IACT,IASV,IAZ,ICC,ICT,IDZ                       GCWX   5
     1,ISV,(IBR,JASV,JSV,KASV,LASV,PC                                   GCWX  10
     2,WSV,JAC,NAME)                                                    GCWX  15
      IMPLICIT REAL*8(A-H,O-Z)                                          GCWX  20
      DIMENSION IACT(1),IASV(1),IAZ(6,1),ICC(1),ICT(4,1),IDZ(4,1)       GCWX  25
     1,ISV(1),(IBR(4,1),JASV(1),JSV(1),KASV(1),LASV(1),PC(1)            GCWX  30
     2,WSV(1),JAC(1),NAME(1)                                            GCWX  35
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C     /DUBL/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, TIMOUT                GCWX  40
      COMMON/DUBL/A(6),AC(9),ACB(9),ASV(6),CA(9),CAB(9),CK                GCWX  45
     1,CKKCAL,CRA(9),DAA,DATE,FKCAL,WR,PI,PICK,PICKZ,PIDKSQ               GCWX  50
     2,PINHZ,QLIM(5),QMAX,RDWSS(9),RLIM(5),RM(9),RMAX,RTPIZ               GCWX  55
     3,SA(6),STGWO,SQTPDK,SQTPI,SQTPIK,TM(9),TPI,TRT(3),TV(3)             GCWX  60
     4,UT(9),UV(3),UW(3),WC,WOBS,WS(9),WV,WX,XYZA(3),XYZAS(3)             GCWX  65
     5,XYZDS(3),ZMC                                                       GCWX  70
C     /MAX/ USED BY MAIN, WMIN, WDYN, WPRE, WCALC, AND GCWX               GCWX  75
      COMMON/MAX/NPCMAX,NAMAX,NKAMAX,NSMAX,NRBMAX,NPXMAX,NCTMAX,NBCMAX    GCWX  80
     1,NMAX,NFSMAX,NGSMAX,NPSMAX,NPMAX,NOSMAX,NOMAX,NVMAX,ND,NB,NSD,NSP   GCWX  85
C     /ITGR/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, IBYPAS, TIMOUT        GCWX  90
      COMMON/ITGR/IBK,ICCAX,ICENT,ICMB,IGEM,ILSQ,INOL,INK,IPLM,IPRC       GCWX  95
     1,IPRT,IRBA,IREP,IRSC,ISB,ISW,IVDW,INGT,IZAM,JC,KPW,KPWS,LT(9)       GCWX 100
     2,MODE,NA,NAC,NAF,NBC,NCT,NKA,NOS,NP,NPC,NPR,NPS,NPX,NQ,ISETA        GCWX 105
     3,NR,NRB,NRP,NS,NT(9),NV,NVA,NVC,NVD,NVR,NVUS(9),NVX                 GCWX 110
      RETURN                                                              GCWX 115
C                                                                         GCWX 120
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS       GCWX 125
C                                                                         GCWX 130
C     GENERAL CALCULATION OF EXTRA ENERGY OF BOND DISTANCES, ANGLES,      GCWX 135
C     AND TORSION ANGLES.                                                 GCWX 140
C     THESE ARE GENERATED FROM THE CONNECTION TABLES IACT AND ICT.        GCWX 145
C     IACT(J),J=1,NCT IS THE NUMBER OF A BACKBONE ATOM, I.E. AN ATOM      GCWX 150
C     CONNECTED TO MORE THAN ONE OTHER ATOM. ICT(I,J),I=1,4 IS THE        GCWX 155
C     NUMBER OF EACH OF FOUR ATOMS BONDED TO THE BACKBONE ATOM IACT(J).   GCWX 160
C                                                                         GCWX 165
      ENTRY GCWX                                                          GCWX 170
      IF(ISW)500,725,500                                                  GCWX 175
C     ON FIRST ENTRY OF CYCLE CALCULATE ALL QUANTITIES, PRINT THEM,       GCWX 180
C        AND SET UP TABLES FOR USE ON SUBSEQUENT ENTRIES                  GCWX 185
  500 M=0                                                                 GCWX 190
C     BOND DISTANCES                                                      GCWX 195
      IF(IPRC-1)505,505,510                                               GCWX 200
  505 PRINT 5                                                             GCWX 205
    5 FORMAT('0BOND DISTANCES'/25X,'IA  JA',14X,'DIJ        WD')          GCWX 210
  510 DO 555 I=1,NCT                                                      GCWX 215
      IA=IACT(I)                                                          GCWX 220
      DO 550 J=1,4                                                        GCWX 225
      JA=ICT(J,I)                                                         GCWX 230
      IF(JA.EQ.0) GO TO 550                                               GCWX 235
      IF(JA.GT.IA) GO TO 520                                              GCWX 240
      DO 515 K=1,NCT                                                      GCWX 245
      IF(JA.EQ.IACT(K)) GO TO 550                                         GCWX 250
  515 CONTINUE                                                            GCWX 255
  520 DIJ=DST(IA,JA)                                                      GCWX 260
      IDZJI=IDZ(J,I)                                                      GCWX 265
      IF(IDZJI)530,525,530                                                GCWX 270
  525 WD=0.0                                                              GCWX 275
      GO TO 540                                                           GCWX 280
  530 WD=PC(IDZJI+1)*(DIJ-PC(IDZJI))**2*50.0                              GCWX 285
      WX=WX+WD                                                            GCWX 290
      M=M+1                                                               GCWX 295
      IF(M.GT.MMAX) GO TO 540                                             GCWX 300
      IASV(M)=IA                                                          GCWX 305
      JASV(M)=JA                                                          GCWX 310
      ISV(M)=I                                                            GCWX 315
      JSV(M)=J                                                            GCWX 320
      WSV(M)=WD                                                           GCWX 325
  540 IF(IPRC-1)545,545,550                                               GCWX 330
  545 PRINT 10,NAME(JAC(IA)),NAME(JAC(JA)),IA,JA,DIJ,WD                   GCWX 335
   10 FORMAT(2(X,A4),13X,2I4,8X,2F9.4)                                    GCWX 340
  550 CONTINUE                                                            GCWX 345
  555 CONTINUE                                                            GCWX 350
      NDST=MIN0(M,MMAX)                                                   GCWX 355
C     BOND ANGLES                                                         GCWX 360
      IF(IPRC-1)560,560,565                                               GCWX 365
  560 PRINT 15                                                            GCWX 370
   15 FORMAT('0BOND ANGLES'/25X,'IA  JA  KA',9X,'AIJK        WA')         GCWX 375
  565 DO 615 J=1,NCT                                                      GCWX 380
      JA=IACT(J)                                                          GCWX 385
      N=0                                                                 GCWX 390
      DO 610 I=1,3                                                        GCWX 395
      IA=ICT(I,J)                                                         GCWX 400
      IF(IA)570,615,570                                                   GCWX 405
  570 IP=I+1                                                              GCWX 410
      DO 605 K=IP,4                                                       GCWX 415
      N=N+1                                                               GCWX 420
      KA=ICT(K,J)                                                         GCWX 425
      IF(KA)575,610,575                                                   GCWX 430
  575 AIJK=ANG(IA,JA,KA)                                                  GCWX 435
      IAZNJ=IAZ(N,J)                                                      GCWX 440
      IF(IAZNJ)585,580,585                                                GCWX 445
  580 WA=0.0                                                              GCWX 450
      GO TO 595                                                           GCWX 455
  585 WA=PC(IAZNJ+1)*(AIJK-PC(IAZNJ))**2*0.5                              GCWX 460
      WX=WX+WA                                                            GCWX 465
      M=M+1                                                               GCWX 470
      IF(M.GT.MMAX) GO TO 595                                             GCWX 475
      IASV(M)=IA                                                          GCWX 480
      JASV(M)=JA                                                          GCWX 485
      KASV(M)=KA                                                          GCWX 490
      ISV(M)=N                                                            GCWX 495
      JSV(M)=J                                                            GCWX 500
      WSV(M)=WA                                                           GCWX 505
  595 IF(IPRC-1)600,600,605                                               GCWX 510
  600 PRINT 20,NAME(JAC(IA)),NAME(JAC(JA)),NAME(JAC(KA))                  GCWX 515
     1,IA,JA,KA,AIJK,WA                                                   GCWX 520
   20 FORMAT(3(X,A4),8X,3I4,4X,F9.2,F9.4)                                 GCWX 525
  605 CONTINUE                                                            GCWX 530
  610 CONTINUE                                                            GCWX 535
  615 CONTINUE                                                            GCWX 540
      NANG=MIN0(M,MMAX)-NDST                                              GCWX 545
C     CONFORMATION ANGLES                                                 GCWX 550
      RAD=0.017453292520                                                  GCWX 555
      IF(IPRC-1)620,620,625                                               GCWX 560
  620 PRINT 25                                                            GCWX 565
   25 FORMAT('0CONFORMATION ANGLES'                                       GCWX 570
     1/25X,'IA  JA  KA  LA        CNF        WCF')                       GCWX 575
  625 DO 715 J=1,NCT                                                      GCWX 580
      JA=IACT(J)                                                          GCWX 585
      DO 710 K=1,4                                                        GCWX 590
      KA=ICT(K,J)                                                         GCWX 595
      IF(KA-JA)710,710,630                                                GCWX 600
  630 DO 705 N=1,NCT                                                      GCWX 605
      IF(KA-IACT(N))705,635,705                                           GCWX 610
  635 DO 700 I=1,4                                                        GCWX 615
      IA=ICT(I,J)                                                         GCWX 620
      IF(IA-KA)640,700,640                                                GCWX 625
  640 IF(IA)645,700,645                                                   GCWX 630
  645 DO 695 L=1,4                                                        GCWX 635
      LA=ICT(L,N)                                                         GCWX 640
      IF(LA-JA)655,695,655                                                GCWX 645
  655 IF(LA)660,695,660                                                   GCWX 650
  660 CNF=CONF(IA,JA,KA,LA)                                               GCWX 655
      ITKJ=ITBR(K,J)                                                      GCWX 660
      IF(ITKJ)668,670,675                                                 GCWX 665
  668 CALL WCNF(IA,JA,KA,LA,CNF,ITKJ,WCF)                                 GCWX 670
      GO TO 676                                                           GCWX 675
  670 WCF=0.0                                                             GCWX 680
      GO TO 685                                                           GCWX 685
  675 WCF=PC(ITKJ)*WRAG(RAD*CNF,PC(ITKJ+1))                               GCWX 690
  676 WX=WX+WCF                                                           GCWX 695
      M=M+1                                                               GCWX 700
      IF(M.GT.MMAX) GO TO 685                                             GCWX 705
      IASV(M)=IA                                                          GCWX 710
      JASV(M)=JA                                                          GCWX 715
      KASV(M)=KA                                                          GCWX 720
      LASV(M)=LA                                                          GCWX 725
      ISV(M)=K                                                            GCWX 730
      JSV(M)=J                                                            GCWX 735
      WSV(M)=WCF                                                          GCWX 740
  685 IF(IPRC-1)690,690,695                                               GCWX 745
  690 PRINT 30,NAME(JAC(IA)),NAME(JAC(JA)),NAME(JAC(KA)),NAME(JAC(LA))    GCWX 750
     1,IA,JA,KA,LA,CNF,WCF                                                GCWX 755
   30 FORMAT(4(X,A4),3X,4I4,F9.2,F9.4)                                    GCWX 760
  695 CONTINUE                                                            GCWX 765
  700 CONTINUE                                                            GCWX 770
      GO TO 710                                                           GCWX 775
  705 CONTINUE                                                            GCWX 780
  710 CONTINUE                                                            GCWX 785
  715 CONTINUE                                                            GCWX 790
      NCNF=MIN0(M,MMAX)-NANG-NDST                                         GCWX 795
      IF(M.LE.MMAX) GO TO 845                                             GCWX 800
      PRINT 35,M,MMAX                                                     GCWX 805
   35 FORMAT('0*** NUMBER OF INTRAMOLECULAR DISTANCES, ANGLES, AND CONFOGCWX 810
     1RMATION ANGLES CONTRIBUTING TO THE ENERGY IS',I4,'.'/5X,'THIS EXCEGCWX 815
     2EDS THE PRESET LIMIT OF',I4,'. THE INITIAL ENERGY CALCULATION IS CGCWX 820
     3CORRECT BUT DERIVATIVES, ETC. ARE NOT. ***')                        GCWX 825
      GO TO 845                                                           GCWX 830
C     FAST CALCULATION USED AFTER FIRST ENTRY                             GCWX 835
  725 M=0                                                                 GCWX 840
      IF(NDST)730,760,730                                                 GCWX 845
C     BOND DISTANCES                                                      GCWX 850
  730 DO 755 L=1,NDST                                                     GCWX 855
      M=M+1                                                               GCWX 860
      IA=IASV(M)                                                          GCWX 865
      JA=JASV(M)                                                          GCWX 870
      IF(ICCAX)750,735,750                                                GCWX 875
  735 IF(ICC(IA))750,740,750                                              GCWX 880
  740 IF(ICC(JA))750,745,750                                              GCWX 885
C     ATOMS HAVE NOT MOVED SINCE LAST ENTRY. ADD TERM USED PREVIOUSLY     GCWX 890
  745 WX=WX+WSV(M)                                                        GCWX 895
      GO TO 755                                                           GCWX 900
C     ATOMS HAVE MOVED. RECALCULATE TERM AND SAVE IT                      GCWX 905
  750 I=ISV(M)                                                            GCWX 910
      J=JSV(M)                                                            GCWX 915
      DIJ=DST(IA,JA)                                                      GCWX 920
      IDZJI=IDZ(J,I)                                                      GCWX 925
      WD=PC(IDZJI+1)*(DIJ-PC(IDZJI))**2*50.0                              GCWX 930
      WSV(M)=WD                                                           GCWX 935
      WX=WX+WD                                                            GCWX 940
  755 CONTINUE                                                            GCWX 945
  760 IF(NANG)765,800,765                                                 GCWX 950
C     BOND ANGLES                                                         GCWX 955
  765 DO 795 L=1,NANG                                                     GCWX 960
      M=M+1                                                               GCWX 965
      IA=IASV(M)                                                          GCWX 970
      JA=JASV(M)                                                          GCWX 975
      KA=KASV(M)                                                          GCWX 980
      IF(ICCAX)790,770,790                                                GCWX 985
  770 IF(ICC(IA))790,775,790                                              GCWX 990
  775 IF(ICC(JA))790,780,790                                              GCWX 995
  780 IF(ICC(KA))790,785,790                                              GCWX1000
C     ATOMS HAVE NOT MOVED SINCE LAST ENTRY. ADD TERM USED PREVIOUSLY     GCWX1005
  785 WX=WX+WSV(M)                                                        GCWX1010
      GO TO 795                                                           GCWX1015
C     ATOMS HAVE MOVED. RECALCULATE TERM AND SAVE IT                      GCWX1020
  790 N=ISV(M)                                                            GCWX1025
      J=JSV(M)                                                            GCWX1030
      AIJK=ANG(IA,JA,KA)                                                  GCWX1035
      IAZNJ=IAZ(N,J)                                                      GCWX1040
      WA=PC(IAZNJ+1)*(AIJK-PC(IAZNJ))**2*0.5                              GCWX1045
      WSV(M)=WA                                                           GCWX1050
      WX=WX+WA                                                            GCWX1055
  795 CONTINUE                                                            GCWX1060
  800 IF(NCNF)805,845,805                                                 GCWX1065
C     CONFORMATION ANGLES                                                 GCWX1070
  805 DO 840 L=1,NCNF                                                     GCWX1075
      M=M+1                                                               GCWX1080
      IA=IASV(M)                                                          GCWX1085
      JA=JASV(M)                                                          GCWX1090
      KA=KASV(M)                                                          GCWX1095
      LA=LASV(M)                                                          GCWX1100
      IF(ICCAX)835,810,835                                                GCWX1105
  810 IF(ICC(IA))835,815,835                                              GCWX1110
  815 IF(ICC(JA))835,820,835                                              GCWX1115
  820 IF(ICC(KA))835,825,835                                              GCWX1120
  825 IF(ICC(LA))835,830,835                                              GCWX1125
C     ATOMS HAVE NOT MOVED SINCE LAST ENTRY. ADD TERM USED PREVIOUSLY     GCWX1130
  830 WX=WX+WSV(M)                                                        GCWX1135
      GO TO 840                                                           GCWX1140
C     ATOMS HAVE MOVED. RECALCULATE TERM AND SAVE IT                      GCWX1145
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  835 K=ISV(M)                                                          GCWX1150
      J=JSV(M)                                                          GCWX1155
      CNF=CONF(IA,JA,KA,LA)                                             GCWX1160
      ITKJ=ITBR(K,J)                                                    GCWX1165
      IF(ITKJ)836,838,838                                               GCWX1170
  836 CALL WCNF(IA,JA,KA,LA,CNF,ITKJ,WCF)                               GCWX1175
      GO TO 839                                                         GCWX1180
  838 WCF=PC(ITKJ)*WRAG(RAD*CNF,PC(ITKJ+1))                             GCWX1185
  839 WSV(M)=WCF                                                        GCWX1190
      WX=WX+WCF                                                         GCWX1195
  840 CONTINUE                                                          GCWX1200
  845 RETURN                                                            GCWX1205
      END                                                               GCWX1210


      FUNCTION ANG(I,J,K)                                               ANG    5
C     COMPUTE THE ANGLE IN DEGREES DEFINED BY ATOMS I, J, AND K.        ANG   10
C     ATOM J IS THE VERTEX.                                             ANG   15
      IMPLICIT REAL*8(A-H,O-Z)                                          ANG   20
      DIMENSION V1(3),V2(3)                                             ANG   25
      CALL VEC(J,I,V1)                                                  ANG   30
      CALL VEC(J,K,V2)                                                  ANG   35
      ANG=AVV(V1,V2)                                                    ANG   40
      RETURN                                                            ANG   45
      END                                                               ANG   50


      FUNCTION AVV(X,Y)                                                 AVV    5
C     COMPUTE THE ANGLE IN DEGREES BETWEEN VECTORS X AND Y.             AVV   10
C     VECTORS ARE REFERRED TO CRYSTAL COORDINATE SYSTEM.                AVV   15
      IMPLICIT REAL*8(A-H,O-Z)                                          AVV   20
C     /AB/ USED BY WPRE, WCALC, AVV, CONF, DST, NORM, UNIT              AVV   25
      COMMON/AB/AA(9),A11,A22,A33,A12,A13,A23,BB(9),B11,B22,B33,B12,B13 AVV   30
     1,B23,VA                                                           AVV   35
      DIMENSION X(3),Y(3),Z(3)                                          AVV   40
      CALL NORM(X,Y,Z)                                                  AVV   45
      AVV=DATAN2(VA*DSQRT(VMV(Z,AA,Z)),VMV(X,AA,Y))*57.29577951         AVV   50
      RETURN                                                            AVV   55
      END                                                               AVV   60


      SUBROUTINE AXELBX(NN,A,B,ID,DL,IFAIL)                             AXEL   5
      REAL*8 A(ID,1),B(ID,1),DL(1),X,Y                                  AXEL  10
C PROGRAM AUTHOR G. W. WESTLEY                                          AXEL  15
C  COMPUTING TECHNOLOGY CENTER, UNION CARBIDE CORP., NUCLEAR DIV.,      AXEL  20
C  OAK RIDGE, TENN.                                                     AXEL  25
C     THIS PROGRAM REDUCES THE GENERAL PROBLEM A * X  = LAMDA * B * X   AXEL  30
C     WHERE A IS SYM. AND B IS SYM. AND POS.DEF.  TO THE STANDARD FORM  AXEL  35
C     P * Z = LAMDA *Z                                                  AXEL  40
C                                                                       AXEL  45
C     THE MATRICES A AND B NEED ONLY BE DEFINED FOR THE UPPER TRIANGULAAXEL  50
C     PORTION.                                                          AXEL  55
C                                                                       AXEL  60
C     ON RETURN B WILL HOLD THE ORIGIONAL B IN THE UPPER PORTION AND    AXEL  65
C     THE OFF DIAGONAL ELEMENTS OF THE CHOLESKY DECOMPOSITION MATRIX    AXEL  70
C     L IN THE LOWER PORTION. THE SINGLY DIMENSIONED ARRAY DL WILL HOLDAXEL  75
C     DIAGONAL ELEMENTS OF L.                                           AXEL  80
C                                                                       AXEL  85
C     ON RETURN A WILL HOLD THE LOWER PORTION OF THE SYM. MATRIX P IN TAXEL  90
C     LOWER TRIANGULAR PORTION  AND THE OFF DIAGONAL ELEMENTS OF THE ORAXEL  95
C     MARTIX A IN THE UPPER PORTION  ----   THE DIAGONAL ELEMENTS OF A AXEL 100
C     LOST..                                                            AXEL 105
C                                                                       AXEL 110
C     N IS THE ORDER OF A  AND ID IS THE DIMENSION SIZE OF A IN THE CALAXEL 115
C     PROGRAM.                                                          AXEL 120
C     IF N IS NEGATIVE THEN CHOLESKY DECOMPOSITION IS ASSUMED COMPLETE AXEL 125
C     AND ONLY THE FORMATION OF P IS LEFT.                              AXEL 130
C                                                                       AXEL 135
C     IFAIL IS A FLAG WHICH INDICATES COMPLETION IF IT IS 0  AND IN-    AXEL 140
C     DICATES TERMINATION DUE TO B FAILING TO BE POS. DEF.(POSSIBLY BE- AXEL 145
C     CAUSE OF ROUND-OFF ERRORS)  IF IT IS 1.                           AXEL 150
C                                                                       AXEL 155
C                                                                       AXEL 160
C     ******************************************************************AXEL 165
      N=NN                                                              AXEL 170
      IF (N.GE.0) GO TO 500                                             AXEL 175
      N=-N                                                              AXEL 180
      GO TO 525                                                         AXEL 185
  500 DO 520 I=1,N                                                      AXEL 190
          DO 520 J=I,N                                                  AXEL 195
             X=B(I,J)                                                   AXEL 200
             K=I-1                                                      AXEL 205
  505        IF (K.LT.1) GO TO 510                                      AXEL 210
             X=X-B(I,K)*B(J,K)                                          AXEL 215
             K=K-1                                                      AXEL 220
             GO TO 505                                                  AXEL 225
  510        CONTINUE                                                   AXEL 230
             IF (I.NE.J) GO TO 515                                      AXEL 235
             IF (X.LE.0.000) GO TO 570                                  AXEL 240
             Y = DSQRT(X)                                               AXEL 245
             DL(I)=Y                                                    AXEL 250
             GO TO 520                                                  AXEL 255
  515        B(J,I)=X/Y                                                 AXEL 260
  520        CONTINUE                                                   AXEL 265
C     ******************************************************************AXEL 270
C                                                                       AXEL 275
C                                                                       AXEL 280
C     THE CHOLESKY DECOMPOSITION IS COMPLETE AND THE FORMATION OF P IS AXEL 285
C                                                                       AXEL 290
C     THE FIRST PORTION COMPLETES THE FIRST PART OF THE MATRIX P BY     AXEL 295
C     SOLVING THE SYSTEM  LX = A.                                       AXEL 300
C                                                                       AXEL 305
C                                                                       AXEL 310
C     ******************************************************************AXEL 315
  525 DO 540 I=1,N                                                      AXEL 320
          Y=DL(I)                                                       AXEL 325
          DO 540 J=I,N                                                  AXEL 330
             X=A(I,J)                                                   AXEL 335
             K=I-1                                                      AXEL 340
  530        IF (K.LT.1) GO TO 535                                      AXEL 345
             X=X-B(I,K)*A(J,K)                                          AXEL 350
             K=K-1                                                      AXEL 355
             GO TO 530                                                  AXEL 360
  535        CONTINUE                                                   AXEL 365
  540        A(J,I)=X/Y                                                 AXEL 370
C                                                                       AXEL 375
C                                                                       AXEL 380
C     THE TRANSPOSE OF THE UPPER TRIANGLE OF  L-INVERSE A HAS BEEN FORMAXEL 385
C     THE LOWER TRIANGLE OF THE MATRIX A.                               AXEL 390
C                                                                       AXEL 395
C                                                                       AXEL 400
C     ******************************************************************AXEL 405
C                                                                       AXEL 410
C                                                                       AXEL 415
C     THIS PORTION COMPLETES THE FORMATION OF P BY SOLVING THE SYSTEM   AXEL 420
C     P * (L-TRANSPOSE) = X.                                            AXEL 425
C                                                                       AXEL 430
C                                                                       AXEL 435
C     ******************************************************************AXEL 440
      DO 565 J=1,N                                                      AXEL 445
         DO 565 I=J,N                                                   AXEL 450
             X=A(I,J)                                                   AXEL 455
             K=I-1                                                      AXEL 460
  545        IF (K.LT.J) GO TO 550                                      AXEL 465
             X=X-A(K,J)*B(I,K)                                          AXEL 470
             K=K-1                                                      AXEL 475
             GO TO 545                                                  AXEL 480
  550        CONTINUE                                                   AXEL 485
             K=J-1                                                      AXEL 490
  555        IF (K.LT.1) GO TO 560                                      AXEL 495
             X=X-A(J,K)*B(I,K)                                          AXEL 500
             K=K-1                                                      AXEL 505
             GO TO 555                                                  AXEL 510
  560        CONTINUE                                                   AXEL 515
             A(I,J)=X/DL(I)                                             AXEL 520
  565        CONTINUE                                                   AXEL 525
      IFAIL = 0                                                         AXEL 530
      RETURN                                                            AXEL 535
C                                                                       AXEL 540
C                                                                       AXEL 545
C     THE SYMMETRIC MATRIX P HAS BEEN RETURNED                          AXEL 550
C                                                                       AXEL 555
C                                                                       AXEL 560
C                                                                       AXEL 565
  570 IFAIL = 1                                                         AXEL 570
C                                                                       AXEL 575
C     THE PROCEDURE FAILED BECAUSE B WAS NOT POS. DEF.                  AXEL 580
C                                                                       AXEL 585
      RETURN                                                            AXEL 590
      END


      SUBROUTINE AXES(U,V,X)                                            AXES   5
C     STORE THREE ORTHOGONAL UNIT VECTORS X(I,1),X(I,2), AND X(I,3)     AXES  10
C        GIVEN VECTORS U AND V.                                         AXES  15
C     VECTORS ARE REFERRED TO CRYSTAL AXIS SYSTEM                       AXES  20
C     X(I,1) IS PARALLEL TO U                                           AXES  25
C     X(I,2) IS IN THE PLANE OF U AND V                                 AXES  30
C     X(I,3) IS PARALLEL TO U CROSS V                                   AXES  35
      IMPLICIT REAL*8(A-H,O-Z)                                          AXES  40
      DIMENSION U(3),V(3),W(9),X(9)                                     AXES  45
      CALL UNIT(U,W(1))                                                 AXES  50
      CALL NORM(W(1),V,W(7))                                            AXES  55
      CALL NORM(W(7),W(1),W(4))                                         AXES  60
      CALL UNIT(W(4),W(4))                                              AXES  65
      CALL UNIT(W(7),W(7))                                              AXES  70
      DO 500 I=1,9                                                      AXES  75
  500 X(I)=W(I)                                                         AXES  80
      RETURN                                                            AXES  85
      END                                                               AXES  90


      SUBROUTINE CNSTRI (AR,BR,PC,PL,PX,Q                               CNST   5
     1,SXR,SYR,SZR,TR)                                                  CNST  10
      IMPLICIT REAL*8(A-H,O-Z)                                          CNST  15
      DIMENSION AR(1),BR(1),PC(1),PL(1),PX(1),Q(1)                      CNST  20
     1,SXR(1),SYR(1),SZR(1),TR(3,1)                                     CNST  25
      RETURN                                                            CNST  30
C                                                                       CNST  35
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS     CNST  40
C                                                                       CNST  45
C     SET VARIABLES IN TERMS OF COMMON PARAMETERS AND EXTRA PARAMETERS  CNST  50
C     DUMMY ROUTINE TO BE REPLACED BY USER                              CNST  55
C                                                                       CNST  60
      ENTRY CNSTRN                                                      CNST  65
      RETURN                                                            CNST  70
      END                                                               CNST  75


      FUNCTION CONF(I,J,K,L)                                            CONF   5
C     COMPUTE THE CONFORMATION ANGLE IN DEGREES FOR THE SEQUENCE OF     CONF  10
C     ATOMS NUMBERED I, J, K, AND L.                                    CONF  15
      IMPLICIT REAL*8(A-H,O-Z)                                          CONF  20
C     /AB/ USED BY WPRE, WCALC, AVV, CONF, DST, NORM, UNIT              CONF  25
      COMMON/AB/AA(9),A11,A22,A33,A12,A13,A23,BB(9),B11,B22,B33,B12,B13 CONF  30
     1,B23,VA                                                           CONF  35
      DIMENSION V1(3),V2(3),V3(3),V4(3),V5(3)                           CONF  40
      CALL VEC(I,J,V1)                                                  CONF  45
      CALL VEC(J,K,V2)                                                  CONF  50
      CALL VEC(K,L,V3)                                                  CONF  55
      CALL NORM(V1,V2,V4)                                               CONF  60
      CALL NORM(V2,V3,V5)                                               CONF  65
      CONF=DSIGN(AVV(V4,V5),VMV(V3,AA,V4))                              CONF  70
      RETURN                                                            CONF  75
      END                                                               CONF  80


      SUBROUTINE CWXI (PC,PX,Q,TR,XC                                    CWXI   5
     1,YC,ZC)                                                           CWXI  10
      IMPLICIT REAL*8(A-H,O-Z)                                          CWXI  15
      DIMENSION PC(1),PX(1),Q(1),TR(3,1),XC(1)                          CWXI  20
     1,YC(1),ZC(1)                                                      CWXI  25
      RETURN                                                            CWXI  30
C                                                                       CWXI  35
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS     CWXI  40
C                                                                       CWXI  45
C     CALCULATE EXTRA ENERGY WX, THE INTERNAL ENERGY OF POLARIZATION,ETCCWXI  50
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C     DUMMY ROUTINE TO BE REPLACED BY USER                              CWXI  55
C                                                                       CWXI  60
      ENTRY CWX                                                         CWXI  65
      RETURN                                                            CWXI  70
      END                                                               CWXI  75


      SUBROUTINE DIFV(X,Y,Z)
C     VECTOR - VECTOR                                                   DIFV   5
C     Z(3)=X(3)-Y(3)                                                    DIFV  10
      IMPLICIT REAL*8(A-H,O-Z)                                          DIFV  15
      DIMENSION X(3),Y(3),Z(3)                                          DIFV  20
      DO 500 I=1,3                                                      DIFV  25
  500 Z(I)=X(I)-Y(I)                                                    DIFV  30
      RETURN                                                            DIFV  35
      END                                                               DIFV  40
                                                                        DIFV  45


      FUNCTION DST(I,J)
C     COMPUTE THE DISTANCE IN ANGSTROMS BETWEEN ATOMS I AND J.          DST    5
      IMPLICIT REAL*8(A-H,O-Z)                                          DST   10
C     /AB/ USED BY WPRE, WCALC, AVV, CONF, DST, NORM, UNIT              DST   15
      COMMON/AB/AA(9),A11,A22,A33,A12,A13,A23,BB(9),B11,B22,B33,B12,B13 DST   20
     1,B23,VA                                                           DST   25
      DIMENSION V(3)                                                    DST   30
      CALL VECT(I,J,V)                                                  DST   35
      DST=DSQRT(V(1)**2*A11+V(2)*(V(2)*A22+V(1)*A12)                    DST   40
     1+V(3)*(V(3)*A33+V(2)*A23+V(1)*A13))                               DST   45
      RETURN                                                            DST   50
      END                                                               DST   55
                                                                        DST   60


      SUBROUTINE GMADD(A,B,R,N,M)
      IMPLICIT REAL*8(A-H,O-Z)                                          GMAD   5
C     ******************************************************************GMAD  10
C                                                                       GMAD  15
C        SUBROUTINE GMADD                                               GMAD  20
C                                                                       GMAD  25
C        PURPOSE                                                        GMAD  30
C           ADD TWO GENERAL MATRICES TO FORM RESULTANT GENERAL MATRIX   GMAD  35
C                                                                       GMAD  40
C        USAGE                                                          GMAD  45
C           CALL GMADD(A,B,R,N,M)                                       GMAD  50
C                                                                       GMAD  55
C        DESCRIPTION OF PARAMETERS                                      GMAD  60
C           A - NAME OF FIRST INPUT MATRIX                              GMAD  65
C           B - NAME OF SECONC INPUT MATRIX                             GMAD  70
C           R - NAME OF OUTPUT MATRIX                                   GMAD  75
C           N - NUMBER OF ROWS IN A,B,R                                 GMAD  80
C           M - NUMBER OF COLUMNS IN A,B,R                              GMAD  85
C                                                                       GMAD  90
C        REMARKS                                                        GMAD  95
C           ALL MATRICES MUST BE STORED AS GENERAL MATRICES             GMAD 100
C                                                                       GMAD 105
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GMAD 110
C           NONE                                                        GMAD 115
C                                                                       GMAD 120
C        METHOD                                                         GMAD 125
C           ADDITION IS PERFORMED ELEMENT BY ELEMENT                    GMAD 130
C                                                                       GMAD 135
C     ******************************************************************GMAD 140
C                                                                       GMAD 145
      DIMENSION A(1),B(1),R(1)                                          GMAD 150
C                                                                       GMAD 155
C        CALCULATE NUMBER OF ELEMENTS                                   GMAD 160
C                                                                       GMAD 165
      NM=N*M                                                            GMAD 170
C                                                                       GMAD 175
C        ADD MATRICES                                                   GMAD 180
C                                                                       GMAD 185
      DO 500 I=1,NM                                                     GMAD 190
  500 R(I)=A(I)+B(I)                                                    GMAD 195
      RETURN                                                            GMAD 200
      END                                                               GMAD 205
                                                                        GMAD 210


      SUBROUTINE GMPRD(A,B,R,N,M,L)
      IMPLICIT REAL*8(A-H,O-Z)                                          GMPR   5
C     ******************************************************************GMPR  10
C                                                                       GMPR  15
C        SUBROUTINE GMPRD                                               GMPR  20
C                                                                       GMPR  25
C        PURPOSE                                                        GMPR  30
C           MULTIPLY TWO GENERAL MATRICES TO FORM A RESULTANT GENERAL   GMPR  35
C           MATRIX                                                      GMPR  40
C                                                                       GMPR  45
C        USAGE                                                          GMPR  50
C           CALL GMPRD(A,B,R,N,M,L)                                     GMPR  55
C                                                                       GMPR  60
C        DESCRIPTION OF PARAMETERS                                      GMPR  65
C           A - NAME OF FIRST INPUT MATRIX                              GMPR  70
C           B - NAME OF SECOND INPUT MATRIX                             GMPR  75
C           R - NAME OF OUTPUT MATRIX                                   GMPR  80
C           N - NUMBER OF ROWS IN A                                     GMPR  85
C           M - NUMBER OF COLUMNS IN A AND ROWS IN B                    GMPR  90
C           L - NUMBER OF COLUMNS IN B                                  GMPR  95
C                                                                       GMPR 100
C        REMARKS                                                        GMPR 105
C           ALL MATRICES MUST BE STORED AS GENERAL MATRICES             GMPR 110
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         GMPR 115
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX B         GMPR 120
C           NUMBER OF COLUMNS OF MATRIX A MUST BE EQUAL TO NUMBER OF ROWGMPR 125
C           OF MATRIX B                                                 GMPR 130
C                                                                       GMPR 135
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GMPR 140
C           NONE                                                        GMPR 145
C                                                                       GMPR 150
C        METHOD                                                         GMPR 155
C           THE M BY L MATRIX B IS PREMULTIPLIED BY THE N BY M MATRIX A GMPR 160
C           AND THE RESULT IS STORED IN THE N BY L MATRIX R.            GMPR 165
C                                                                       GMPR 170
C                                                                       GMPR 175
C     ******************************************************************GMPR 180
C
      DIMENSION A(1),B(1),R(1)                                          GMPR 185
C                                                                       GMPR 190
      IR=0                                                              GMPR 195
      IK=-M                                                             GMPR 200
      DO 500 K=1,L                                                      GMPR 205
      IK=IK+M                                                           GMPR 210
      DO 500 J=1,N                                                      GMPR 215
      IR=IR+1                                                           GMPR 220
      JI=J-N                                                            GMPR 225
      IB=IK                                                             GMPR 230
      R(IR)=0                                                           GMPR 235
      DO 500 I=1,M                                                      GMPR 240
      JI=JI+N                                                           GMPR 245
      IB=IB+1                                                           GMPR 250
  500 R(IR)=R(IR)+A(JI)*B(IB)                                           GMPR 255
      RETURN                                                            GMPR 260
      END                                                               GMPR 265
                                                                        GMPR 270


      SUBROUTINE GMTRA(A,R,N,M)
      IMPLICIT REAL*8(A-H,O-Z)                                          GMTR   5
C     ******************************************************************GMTR  10
C                                                                       GMTR  15
C        SUBROUTINE GMTRA                                               GMTR  20
C                                                                       GMTR  25
C        PURPOSE                                                        GMTR  30
C           TRANSPOSE A GENERAL MATRIX                                  GMTR  35
C                                                                       GMTR  40
C        USAGE                                                          GMTR  45
C           CALL GMTRA(A,R,N,M)                                         GMTR  50
C                                                                       GMTR  55
C        DESCRIPTION OF PARAMETERS                                      GMTR  60
C           A - NAME OF MATRIX TO BE TRANSPOSED                         GMTR  65
C           R - NAME OF RESULTANT MATRIX                                GMTR  70
C           N - NUMBER OF ROWS OF A AND COLUMNS OF R                    GMTR  75
C           M - NUMBER OF COLUMNS OF A AND ROWS OF R                    GMTR  80
C                                                                       GMTR  85
C        REMARKS                                                        GMTR  90
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         GMTR  95
C           MATRICES A AND R MUST BE STORED AS GENERAL MATRICES         GMTR 100
C                                                                       GMTR 105
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GMTR 110
C           NONE                                                        GMTR 115
C                                                                       GMTR 120
C        METHOD                                                         GMTR 125
C           TRANSPOSE N BY M MATRIX A TO FORM M BY N MATRIX R           GMTR 130
C                                                                       GMTR 135
C                                                                       GMTR 140
C     ******************************************************************GMTR 145
      DIMENSION A(1),R(1)                                               GMTR 150
C                                                                       GMTR 155
      IR=0                                                              GMTR 160
      DO 500 I=1,N                                                      GMTR 165
      IJ=I-N                                                            GMTR 170
      DO 500 J=1,M                                                      GMTR 175
      IJ=IJ+N                                                           GMTR 180
      IR=IR+1                                                           GMTR 185
  500 R(IR)=A(IJ)                                                       GMTR 190
      RETURN                                                            GMTR 195
      END                                                               GMTR 200
                                                                        GMTR 205


      FUNCTION GPOT(AR,BR,IACT,ICT,ISC,JAC,PC,PL,PX,Q,SYM,XC,YC,ZC)     GPOT   5
      IMPLICIT REAL*8(A-H,O-Z)                                          GPOT  10
      DIMENSION AR(1),BR(1),IACT(1),ICT(4,1),ISC(1),JAC(1),PC(1),PL(1)  GPOT  15
     1,PX(1),Q(1),SYM(12,1),XC(1),YC(1),ZC(1)                           GPOT  20
      RETURN                                                            GPOT  25
C                                                                       GPOT  30
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS     GPOT  35
C                                                                       GPOT  40
C     USER ROUTINE TO CALCULATE A GENERAL NON-BONDED ENERGY TERM        GPOT  45
C     ENTERED ONLY IF IREP.GE.4                                         GPOT  50
C                                                                       GPOT  55
      ENTRY GPOT(ISB,I,J,IA,JA,IK,JK,GX,GY,GZ,DX,DY,DZ,R)               GPOT  60
      REAL*4 GX,GY,GZ                                                   GPOT  65
      GPOT=0.0D0                                                        GPOT  70
      RETURN                                                            GPOT  75
      END                                                               GPOT  80


      SUBROUTINE GTPRD(A,B,R,N,M,L)
      IMPLICIT REAL*8(A-H,O-Z)                                          GTPR   5
C     ******************************************************************GTPR  10
C                                                                       GTPR  15
C        SUBROUTINE GTPRD                                               GTPR  20
C                                                                       GTPR  25
C        PURPOSE                                                        GTPR  30
C           PREMULTIPLY A GENERAL MATRIX BY THE TRANSPOSE OF ANOTHER    GTPR  35
C           GENERAL MATRIX                                              GTPR  40
C                                                                       GTPR  45
C        USAGE                                                          GTPR  50
C           CALL GTPRD(A,B,R,N,M,L)                                     GTPR  55
C                                                                       GTPR  60
C        DESCRIPTION OF PARAMETERS                                      GTPR  65
C           A - NAME OF FIRST INPUT MATRIX                              GTPR  70
C           B - NAME OF SECOND INPUT MATRIX                             GTPR  75
C           R - NAME OF OUTPUT MATRIX                                   GTPR  80
C           N - NUMBER OF ROWS IN A AND B                               GTPR  85
C           M - NUMBER OF COLUMNS IN A AND ROWS IN R                    GTPR  90
C           L - NUMBER OF COLUMNS IN B AND R                            GTPR  95
C                                                                       GTPR 100
C        REMARKS                                                        GTPR 105
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         GTPR 110
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX B         GTPR 115
C           ALL MATRICES MUST BE STORED AS GENERAL MATRICES             GTPR 120
C                                                                       GTPR 125
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GTPR 130
C           NONE                                                        GTPR 135
C                                                                       GTPR 140
C        METHOD                                                         GTPR 145
C           MATRIX TRANSPOSE OF A IS NOT ACTUALLY CALCULATED. INSTEAD,  GTPR 150
```

```
C           ELEMENTS OF MATRIX A ARE TAKEN COLUMNWISE RATHER THAN
C           ROWWISE FOR POSTMULTIPLICATION BY MATRIX B.
C
C     ..................................................................
      DIMENSION A(1),B(1),R(1)
C
      IR=0
      IK=-N
      DO 500 K=1,L
      IJ=0
      IK=IK+N
      DO 500 J=1,M
      IB=IK
      IB=IB+1
      R(IR)=0
      DO 500 I=1,N
      IJ=IJ+1
      IB=IB+1
  500 R(IR)=R(IR)+A(IJ)*B(IB)
      RETURN
      END


      SUBROUTINE HOUSEH(A,ID,N,D,E)
C     HOUSEHOLDER REDUCTION OF MATRIX TO TRIDIAGONAL FORM BEFORE VALVEC
C PROGRAM AUTHOR G. W. WESTLEY
C  COMPUTING TECHNOLOGY CENTER, UNION CARBIDE CORP., NUCLEAR DIV.,
C  OAK RIDGE, TENN.
C
      REAL*8 A(ID,1),D(1),E(1),F,G,HH,H,TOL
      TOL = 16.D0**(-51)
      I = N
  500 L = I-2
      F = A(I,I-1)
      G = 0.D0D
      IF (L.EQ.0) GO TO 510
      DO 505 K=1,L
  505    G = G + A(I,K)*A(I,K)
  510 H = G + F*F
      IF (G.LE.TOL) GO TO 540
      L = L+1
      G = -DSQRT(H)
      IF (F.LT.0.0) G = -G
      E(I) = G
      H = H - F*G
      A(I,I-1) = F-G
      F = 0.D0D
      DO 530 J=1,L
         A(J,I) = A(I,J)/H
         G = 0.D0D
         DO 515 K=1,J
515         G = G + A(J,K)*A(I,K)
         IF (J.EQ.L) GO TO 525
         JP1 = J+1
         DO 520 K=JP1,L
520         G = G + A(K,J)*A(I,K)
525      E(J) = G/H
530      F = F + G*A(J,I)
      HH = F/(H+H)
      DO 535 J=1,L
         F = A(I,J)
         E(J) = E(J) - HH*F
         G = E(J)
         DO 535 K=1,J
535         A(J,K) = A(J,K) - F*E(K) - G*A(I,K)
      GO TO 545
540   E(I) = F
      H = 0.D0D
545   D(I) = H
      I = I-1
      IF (I.GE.2) GO TO 500
      D(1) = 0.D0D
      E(1) = 0.D0D
      DO 575 I=1,N
         L = I-1
         IF (D(I).EQ.0.D0D) GO TO 565
         DO 560 J=1,L
            G = 0.D0D
            DO 550 K=1,L
550            G = G + A(I,K)*A(K,J)
            DO 555 K=1,L
555            A(K,J) = A(K,J) - G*A(K,I)
560      CONTINUE
565      D(I) = A(I,I)
         A(I,I) =1.D0D
         IF (L.EQ.0) GO TO 575
         DO 570 J=1,L
            A(I,J) =0.D0D
570         A(J,I) =0.D0D
575   CONTINUE
      RETURN
      END


      FUNCTION IBYPAS(I,J,KPC)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION KPC(1)
C     /ITGR/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, IBYPAS, TIMOUT
      COMMON/ITGR/IBK,ICCAX,ICENT,ICMB,IGEM,ILSG,IMOL,INK,IPLM,IPRC
     1,IPRT,IRBA,IREP,IRSC,ISB,ISW,IVDW,IWGT,IZAM,JC,KPW,KPWS,LT(9)
     2,MODE,NA,NAC,NAF,NBC,NCT,NKA,NOS,NP,NPC,NPR,NPS,NPX,NS,ISETA
     3,NR,NRB,NRP,NS,NT(9),NV,NVA,NVC,NVD,NVR,NVUS(9),NVX
      DATA IP,JP/0,0/
C
C     SET INDICATOR FOR BYPASSING RECIPROCAL SUMS, DIRECT SUMS, OR GCWX
C     THIS REDUCES REPETITION OF IDENTICAL CALCULATIONS IN OBTAINING
C        SECOND DERIVATIVES WITH RESPECT TO COMMON PARAMETERS
C     IBYPAS IS SET AT INTEGER FROM 0 TO 7. A ZERO ONE-BIT FORCES ENTRY
C        TO GCWX. A ZERO TWO-BIT FORCES CALC OF DIRECT-LATTICE SUM. A
C        ZERO FOUR-BIT FORCES BOTH RECIPROCAL AND DIRECT SUMS
C     IP AND JP ARE VALUES OF I AND J ON PREVIOUS ENTRY
C
      IF(J-JP)540,500,540
C     J UNCHANGED. START LOOP TO TEST IP AND THEN I
  500 IREC=1
      IDIR=1
      IWX=1
      DO 535 L=1,2
C     NO BYPASS UNLESS BOTH IP AND I ARE COMMON PARAMETERS
      IF(IP-NPC)505,505,545
C     IF IP IS ZERO THIS IS INITIAL VALUE TO BE IGNORED
  505 IF(IP)510,530,510
C     TEST KIND OF COMMON PARAMETER. IF KPC IS ZERO DO NOT BYPASS
  510 KPCIP=KPC(IP)+1
      GO TO (545,515,520,525),KPCIP
C     COULOMB OR VAN DER WAALS. INCLUDE BOTH RECIPROCAL AND DIRECT SUMS
  515 IREC=0
C     REPULSION PARAMETER. INCLUDE DIRECT-LATTICE SUM
  520 IDIR=0
      GO TO 530
C     INTRAMOLECULAR ENERGY PARAMETER. INCLUDE INTERNAL ENERGY CALC
  525 IWX=0
C     SUBSTITUTE I FOR IP AND REPEAT
  530 IP=I
  535 CONTINUE
C     SET VALUE OF IBYPAS
      IBY=IWX+2*IDIR+4*IREC
      GO TO 550
C     J HAS CHANGED. DO NOT BYPASS ANY PART OF ENERGY CALCULATION
  540 JP=J
  545 IP=I
      IBY=0
  550 IBYPAS=IBY
      RETURN
      END


      SUBROUTINE INVRS(X,D,Z)
      IMPLICIT REAL*8(A-H,O-Z)
C     GIVEN 3 BY 3 MATRIX X, STORE DETERMINANT AT D AND INVERSE AT Z.
C     Z MAY BE THE SAME AS X.
      DIMENSION X(9),XX(9),Z(9),ZZ(9)
      DO 500 I=1,9
  500 XX(I)=X(I)
      ZZ(1)=XX(5)*XX(9)-XX(6)*XX(8)
      ZZ(2)=XX(3)*XX(8)-XX(2)*XX(9)
      ZZ(3)=XX(2)*XX(6)-XX(3)*XX(5)
      ZZ(4)=XX(6)*XX(7)-XX(4)*XX(9)
      ZZ(5)=XX(1)*XX(9)-XX(3)*XX(7)
      ZZ(6)=XX(3)*XX(4)-XX(1)*XX(6)
      ZZ(7)=XX(4)*XX(8)-XX(5)*XX(7)
      ZZ(8)=XX(2)*XX(7)-XX(1)*XX(8)
      ZZ(9)=XX(1)*XX(5)-XX(2)*XX(4)
      DD=XX(1)*ZZ(1)+XX(4)*ZZ(2)+XX(7)*ZZ(3)
      IF(DD)502,510,502
  502 DO 505 I=1,9
  505 Z(I)=ZZ(I)/DD
  510 D=DD
      RETURN
      END


      SUBROUTINE LOK(I,J,IR,N,M,MS)
      IMPLICIT REAL*8(A-H,O-Z)
C     ..................................................................
C        SUBROUTINE LOK (FORMERLY LOC)
C        PURPOSE
C           COMPUTE A VECTOR SUBSCRIPT FOR AN ELEMENT IN A MATRIX OF
C           SPECIFIED STORAGE MODE
C
C        USAGE
C           CALL LOK (I,J,IR,N,M,MS)
C
C        DESCRIPTION OF PARAMETERS
C           I   - ROW NUMBER OF ELEMENT
C           J   - COLUMN NUMBER  OF ELEMENT
C           IR  - RESULTANT VECTOR SUBSCRIPT
C           N   - NUMBER OF ROWS IN MATRIX
C           M   - NUMBER OF COLUMNS IN MATRIX
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX
C                 0 - GENERAL
C                 1 - SYMMETRIC
C                 2 - DIAGONAL
C
C        REMARKS
C           NONE
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           NONE
C
C        MEYHOD
C           MS=0     SUBSCRIPT IS COMPUTED FOR A MATRIX WITH N*M ELEMENTS
C                    IN STORAGE (GENERAL MATRIX)
C           MS=1     SUBSCRIPT IS COMPUTED FOR A MATRIX WITH N*(N+1)/2 IN
C                    STORAGE (UPPER TRIANGLE OF SYMMETRIC MATRIX). IF
C                    ELEMENT IS IN LOWER TRIANGULAR PORTION, SUBSCRIPT IS
C                    CORRESPONDING ELEMENT IN UPPER TRIANGLE.
C           MS=2     SUBSCRIPT IS COMPUTED FOR A MATRIX WITH N ELEMENTS
C                    IN STORAGE (DIAGONAL ELEMENTS OF DIAGONAL MATRIX).
C                    IF ELEMENT IS NOT ON DIAGONAL (AND THEREFORE NOT IN
C                    STORAGE), IR IS SET TO ZERO.
C     ..................................................................
C
C
      IX=I
      JX=J
      IF(MS-1) 500,505,520
```

```
  500 IRX=N*(JX-1)+IX                                                   LOK  245
      GO TO 530                                                         LOK  250
  505 IF(IX-JX) 510,515,515                                             LOK  255
  510 IRX=IX+(JX*JX-JX)/2                                               LOK  260
      GO TO 530                                                         LOK  265
  515 IRX=JX+(IX*IX-IX)/2                                               LOK  270
      GO TO 530                                                         LOK  275
  520 IRX=0                                                             LOK  280
      IF(IX-JX) 530,525,530                                             LOK  285
  525 IRX=IX                                                            LOK  290
  530 IR=IRX                                                            LOK  295
      RETURN                                                            LOK  300
      END                                                               LOK  305


      SUBROUTINE MASTER(NST)                                            MAST   5
C     USER ROUTINE TO SET THE OVERALL STORAGE AVAILABLE TO BE           MAST  10
C     ALLOCATED BY THE MAIN PROGRAM                                     MAST  15
C                                                                       MAST  20
      IMPLICIT REAL*8(A-H,O-Z)                                          MAST  25
      COMMON/S/S(12000)                                                 MAST  30
C     THE FOLLOWING CONSTANT MUST AGREE WITH THE ABOVE DIMENSION        MAST  35
      NST=12000                                                         MAST  40
      RETURN                                                            MAST  45
      END                                                               MAST  50


      SUBROUTINE MCPY(A,R,N,M,MS)                                       MCPY   5
      IMPLICIT REAL*8(A-H,O-Z)                                          MCPY  10
C     ..................................................................MCPY  15
C                                                                       MCPY  20
C        SUBROUTINE MCPY                                                MCPY  25
C                                                                       MCPY  30
C        PURPOSE                                                        MCPY  35
C           COPY ENTIRE MATRIX                                          MCPY  40
C                                                                       MCPY  45
C        USAGE                                                          MCPY  50
C           CALL MCPY (A,R,N,M,MS)                                      MCPY  55
C                                                                       MCPY  60
C        DESCRIPTION OF PARAMETERS                                      MCPY  65
C           A - NAME OF INPUT MATRIX                                    MCPY  70
C           R - NAME OF OUTPUT MATRIX                                   MCPY  75
C           N - NUMBER OF ROWS IN A OR R                                MCPY  80
C           M - NUMBER OF COLUMNS IN A OR R                             MCPY  85
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A (AND R) MCPY  90
C                 0 - GENERAL                                           MCPY  95
C                 1 - SYMMETRIC                                         MCPY 100
C                 2 - DIAGONAL                                          MCPY 105
C                                                                       MCPY 110
C        REMARKS                                                        MCPY 115
C           NONE                                                        MCPY 120
C                                                                       MCPY 125
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MCPY 130
C           LOK (FORMERLY LOC)                                          MCPY 135
C                                                                       MCPY 140
C        METHOD                                                         MCPY 145
C           EACH ELEMENT OF MATRIX A IS MOVED TO THE CORRESPONDING      MCPY 150
C           ELEMENT OF MATRIX R                                         MCPY 155
C                                                                       MCPY 160
C     ..................................................................MCPY 165
C                                                                       MCPY 170
      DIMENSION A(1),R(1)                                               MCPY 175
C                                                                       MCPY 180
C        COMPUTE VECTOR LENGTH, IT                                      MCPY 185
C                                                                       MCPY 190
      CALL LOK(N,M,IT,N,M,MS)                                           MCPY 195
C                                                                       MCPY 200
C        COPY MATRIX                                                    MCPY 205
C                                                                       MCPY 210
      DO 500 I=1,IT                                                     MCPY 215
  500 R(I)=A(I)                                                         MCPY 220
      RETURN                                                            MCPY 225
      END                                                               MCPY 230


      SUBROUTINE MINV(A,N,D,L,M)                                        MINV   5
      IMPLICIT REAL*8(A-H,O-Z)                                          MINV  10
C                                                                       MINV  15
C     ..................................................................MINV  20
C                                                                       MINV  25
C        SUBROUTINE MINV                                                MINV  30
C                                                                       MINV  35
C        PURPOSE                                                        MINV  40
C           INVERT A MATRIX                                             MINV  45
C                                                                       MINV  50
C        USAGE                                                          MINV  55
C           CALL MINV(A,N,D,L,M)                                        MINV  60
C                                                                       MINV  65
C        DESCRIPTION OF PARAMETERS                                      MINV  70
C           A - INPUT MATRIX, DESTROYED IN COMPUTATION AND REPLACED BY  MINV  75
C               RESULTANT INVERSE.                                      MINV  80
C           N - ORDER OF MATRIX A                                       MINV  85
C           D - 0.0 IF SINGULAR, 1.0 IF ALL RIGHT.                      MINV  90
C           L - WORK VECTOR OF LENGTH N                                 MINV  95
C           M - WORK VECTOR OF LENGTH N                                 MINV 100
C                                                                       MINV 105
C        REMARKS                                                        MINV 110
C           MATRIX A MUST BE A GENERAL MATRIX                           MINV 115
C                                                                       MINV 120
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MINV 125
C           NONE                                                        MINV 130
C                                                                       MINV 135
C        METHOD                                                         MINV 140
C           THE STANDARD GAUSS-JORDAN METHOD IS USED.                   MINV 145
C                                                                       MINV 150
C     ..................................................................MINV 155
C                                                                       MINV 160
      DIMENSION A(1),L(1),M(1)                                          MINV 165
C                                                                       MINV 170
C     ..................................................................MINV 175
C                                                                       MINV 180
C        SEARCH FOR LARGEST ELEMENT                                     MINV 185
C                                                                       MINV 190
      D=1.0                                                             MINV 195
      NK=-N                                                             MINV 200
      DO 590 K=1,N                                                      MINV 205
      NK=NK+N                                                           MINV 210
      L(K)=K                                                            MINV 215
      M(K)=K                                                            MINV 220
      KK=NK+K                                                           MINV 225
      BIGA=A(KK)                                                        MINV 230
      DO 510 J=K,N                                                      MINV 235
      IZ=N*(J-1)                                                        MINV 240
      DO 510 I=K,N                                                      MINV 245
      IJ=IZ+I                                                           MINV 250
  500 IF(DABS(BIGA)-DABS(A(IJ))) 505,510,510                            MINV 255
  505 BIGA=A(IJ)                                                        MINV 260
      L(K)=I                                                            MINV 265
      M(K)=J                                                            MINV 270
  510 CONTINUE                                                          MINV 275
C                                                                       MINV 280
C        INTERCHANGE ROWS                                               MINV 285
C                                                                       MINV 290
      J=L(K)                                                            MINV 295
      IF(J-K) 525,525,515                                               MINV 300
  515 KI=K-N                                                            MINV 305
      DO 520 I=1,N                                                      MINV 310
      KI=KI+N                                                           MINV 315
      HOLD=-A(KI)                                                       MINV 320
      JI=KI-K+J                                                         MINV 325
      A(KI)=A(JI)                                                       MINV 330
  520 A(JI) =HOLD                                                       MINV 335
C                                                                       MINV 340
C        INTERCHANGE COLUMNS                                            MINV 345
C                                                                       MINV 350
  525 I=M(K)                                                            MINV 355
      IF(I-K) 540,540,530                                               MINV 360
  530 JP=N*(I-1)                                                        MINV 365
      DO 535 J=1,N                                                      MINV 370
      JK=NK+J                                                           MINV 375
      JI=JP+J                                                           MINV 380
      HOLD=-A(JK)                                                       MINV 385
      A(JK)=A(JI)                                                       MINV 390
  535 A(JI) =HOLD                                                       MINV 395
C                                                                       MINV 400
C        DIVIDE COLUMN BY MINUS PIVOT (VALUE OF PIVOT ELEMENT IS        MINV 405
C        CONTAINED IN BIGA)                                             MINV 410
C                                                                       MINV 415
  540 IF(BIGA) 550,545,550                                              MINV 420
  545 D=0.0                                                             MINV 425
      RETURN                                                            MINV 430
  550 DO 560 I=1,N                                                      MINV 435
      IF(I-K) 555,560,555                                               MINV 440
  555 IK=NK+I                                                           MINV 445
      A(IK)=A(IK)/(-BIGA)                                               MINV 450
  560 CONTINUE                                                          MINV 455
C                                                                       MINV 460
C        REDUCE MATRIX                                                  MINV 465
C                                                                       MINV 470
      DO 575 I=1,N                                                      MINV 475
      IK=NK+I                                                           MINV 480
      IJ=I-N                                                            MINV 485
      DO 575 J=1,N                                                      MINV 490
      IJ=IJ+N                                                           MINV 495
      IF(I-K) 565,575,565                                               MINV 500
  565 IF(J-K) 570,575,570                                               MINV 505
  570 KJ=IJ-I+K                                                         MINV 510
      A(IJ)=A(IK)*A(KJ)+A(IJ)                                           MINV 515
  575 CONTINUE                                                          MINV 520
C                                                                       MINV 525
C        DIVIDE ROW BY PIVOT                                            MINV 530
C                                                                       MINV 535
      KJ=K-N                                                            MINV 540
      DO 585 J=1,N                                                      MINV 545
      KJ=KJ+N                                                           MINV 550
      IF(J-K) 580,585,580                                               MINV 555
  580 A(KJ)=A(KJ)/BIGA                                                  MINV 560
  585 CONTINUE                                                          MINV 565
C                                                                       MINV 570
C        REPLACE PIVOT BY RECIPROCAL                                    MINV 575
C                                                                       MINV 580
      A(KK)=1.0/BIGA                                                    MINV 585
  590 CONTINUE                                                          MINV 590
C                                                                       MINV 595
C        FINAL ROW AND COLUMN INTERCHANGE                               MINV 600
C                                                                       MINV 605
      K=N                                                               MINV 610
  595 K=(K-1)                                                           MINV 615
      IF(K) 630,630,600                                                 MINV 620
  600 I=L(K)                                                            MINV 625
      IF(I-K) 615,615,605                                               MINV 630
  605 JQ=N*(K-1)                                                        MINV 635
      JR=N*(I-1)                                                        MINV 640
      DO 610 J=1,N                                                      MINV 645
      JK=JQ+J                                                           MINV 650
      HOLD=A(JK)                                                        MINV 655
      JI=JR+J                                                           MINV 660
      A(JK)=-A(JI)                                                      MINV 665
  610 A(JI) =HOLD                                                       MINV 670
  615 J=M(K)                                                            MINV 675
      IF(J-K) 595,595,620                                               MINV 680
  620 KI=K-N                                                            MINV 685
      DO 625 I=1,N                                                      MINV 690
      KI=KI+N                                                           MINV 695
      HOLD=A(KI)                                                        MINV 700
      JI=KI-K+J                                                         MINV 705
      A(KI)=-A(JI)                                                      MINV 710
  625 A(JI) =HOLD                                                       MINV 715
      GO TO 595                                                         MINV 720
  630 RETURN                                                            MINV 725
      END                                                               MINV 730
```

```
      SUBROUTINE MM(X,Y,Z)
C     MULTIPLY TWO MATRICES
C     Z(3,3)=X(3,3)*Y(3,3). Z MAY BE THE SAME AS X OR Y
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION X(3,3),Y(3,3),Z(3,3),W(3,3)
      DO 510 I=1,3
      DO 505 K=1,3
      W(I,K)=0.0
      DO 500 J=1,3
      W(I,K)=W(I,K)+X(I,J)*Y(J,K)
  500 CONTINUE
  505 CONTINUE
  510 CONTINUE
      DO 520 J=1,3
      DO 515 I=1,3
      Z(I,J)=W(I,J)
  515 CONTINUE
  520 CONTINUE
      RETURN
      END


      SUBROUTINE MPRD(A,B,R,N,M,MSA,MSB,L)
      IMPLICIT REAL*8(A-H,O-Z)
C     ..................................................................
C
C        SUBROUTINE MPRD
C
C        PURPOSE
C           MULTIPLY TWO MATRICES TO FORM A RESULTANT MATRIX
C
C        USAGE
C           CALL MPRD(A,B,R,N,M,MSA,MSB,L)
C
C        DESCRIPTION OF PARAMETERS
C           A - NAME OF FIRST INPUT MATRIX
C           B - NAME OF SECOND INPUT MATRIX
C           R - NAME OF OUTPUT MATRIX
C           N - NUMBER OF ROWS IN A AND R
C           M - NUMBER OF COLUMNS IN A AND ROWS IN B
C           MSA - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A
C                 0 - GENERAL
C                 1 - SYMMETRIC
C                 2 - DIAGONAL
C           MSB - SAME AS MSA EXCEPT FOR MATRIX B
C           L - NUMBER OF COLUMNS IN B AND R
C
C        REMARKS
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRICES A OR B
C           NUMBER OF COLUMNS OF MATRIX A MUST BE EQUAL TO NUMBER OF ROW
C           OF MATRIX B
C
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           LOK (FORMERLY LOC)
C
C        METHOD
C           THE M BY L MATRIX B IS PREMULTIPLIED BY THE N BY M MATRIX A
C           AND THE RESULT IS STORED IN THE N BY L MATRIX R. THIS IS A
C           ROW INTO COLUMN PRODUCT.
C           THE FOLLOWING TABLE SHOWS THE STORAGE MODE OF THE OUTPUT
C           MATRIX FOR ALL COMBINATIONS OF INPUT MATRICES
C                    A                B                R
C                 GENERAL          GENERAL          GENERAL
C                 GENERAL          SYMMETRIC        GENERAL
C                 GENERAL          DIAGONAL         GENERAL
C                 SYMMETRIC        GENERAL          GENERAL
C                 SYMMETRIC        SYMMETRIC        GENERAL
C                 SYMMETRIC        DIAGONAL         GENERAL
C                 DIAGONAL         GENERAL          GENERAL
C                 DIAGONAL         SYMMETRIC        GENERAL
C                 DIAGONAL         DIAGONAL         DIAGONAL
C     ..................................................................
C
      DIMENSION A(1),B(1),R(1)
C
C        SPECIAL CASE FOR DIAGONAL BY DIAGONAL
C
      MS=MSA*10+MSB
      IF(MS-22) 510,500,510
  500 DO 505 I=1,N
  505 R(I)=A(I)*B(I)
      RETURN
C
C        ALL OTHER CASES
C
  510 IR=1
      DO 540 K=1,L
      DO 540 J=1,N
      R(IR)=0
      DO 535 I=1,M
      IF(MS) 515,525,515
  515 CALL LOK(J,I,IA,N,M,MSA)
      CALL LOK(I,K,IB,M,L,MSB)
      IF(IA) 520,535,520
  520 IF(IB) 530,535,530
  525 IA=N*(I-1)+J
      IB=M*(K-1)+I
  530 R(IR)=R(IR)+A(IA)*B(IB)
  535 CONTINUE
  540 IR=IR+1
      RETURN
      END


      SUBROUTINE MV(X,Y,Z)
C     MATRIX * VECTOR
C     Z(3)=X(3,3)*Y(3). Z MAY BE THE SAME AS Y
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION X(3,3),Y(3),Z(3),W(3)
      DO 505 I=1,3
      W(I)=0.0
      DO 500 J=1,3
      W(I)=W(I)+X(I,J)*Y(J)
  500 CONTINUE
  505 CONTINUE
      DO 510 I=1,3
      Z(I)=W(I)
  510 CONTINUE
      RETURN
      END


      SUBROUTINE NORM(X,Y,Z)
C     STORE A VECTOR Z NORMAL TO VECTORS X AND Y
C     VECTORS ARE REFERRED TO THE CRYSTAL COORDINATE SYSTEM.
C     TO OBTAIN THE CROSS PRODUCT X*Y MULTIPLY Z BY THE DIRECT CELL
C     VOLUME.
      IMPLICIT REAL*8(A-H,O-Z)
C     /AB/ USED BY MPRE, WCALC, AVY, CONF, DST, NORM, UNIT
      COMMON/AB/AA(9),A11,A22,A33,A12,A13,A23,BB(9),B11,B22,B33,B12,B13
     1,B23,VA
      DIMENSION X(3),Y(3),Z(3),XX(6),YY(6),ZZ(3)
      DO 500 I=1,3
      XX(I)=X(I)
      XX(I+3)=XX(I)
      YY(I)=Y(I)
      YY(I+3)=YY(I)
  500 CONTINUE
      DO 505 I=1,3
      ZZ(I)=XX(I+1)*YY(I+2)-XX(I+2)*YY(I+1)
  505 CONTINUE
      CALL MV(BB,ZZ,Z)
      RETURN
      END


      SUBROUTINE REJECT(ISB,HX,HY,HZ,IREJ)
C     AVOID CALCULATION OF SPACE-GROUP ABSENCES IN RECIPROCAL SUM
C     DUMMY ROUTINE TO BE REPLACED BY USER
C     IREJ=0 ON ENTRY. SET IREJ=1 TO OMIT A SPACE-GROUP ABSENCE.
      RETURN
      END


      FUNCTION REPLI(AR,BR,PC,PL,PX,Q)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION AR(1),BR(1),PC(1),PL(1),PX(1),Q(1)
      RETURN
C
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS
C
C     USER ROUTINE TO CALCULATE REPULSION ENERGY
C     ENTERED ONLY IF IREP=2
C
      ENTRY REPL(ISB,IK,JK,R)
      REPL=0.0D0
      RETURN
      END


      SUBROUTINE SETA(ISETA,A)
C     CONSTRAIN LATTICE PARAMETERS AS SPECIFIED BY ISETA
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A(6)
      ISA=ISETA+1
      GO TO (40,30,20,10),ISA
C     RHOMBOHEDRAL AXES
   10 A(5)=A(4)
      A(6)=A(4)
C     CUBIC AXES
   20 A(3)=A(1)
C     HEXAGONAL OR TETRAGONAL AXES
   30 A(2)=A(1)
C     NO CONSTRAINT FOR ORTHORHOMBIC, MONOCLINIC, OR TRICLINIC AXES
   40 RETURN
      END


      SUBROUTINE SUMV(X,Y,Z)
C     VECTOR + VECTOR
C     Z(3)=X(3)+Y(3)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION X(3),Y(3),Z(3)
      DO 500 I=1,3
  500 Z(I)=X(I)+Y(I)
      RETURN
      END


      SUBROUTINE TIMOUT
C     ANALYZE AND PRINT TIMES FOR VARIOUS PARTS OF ENERGY CALCULATION
      IMPLICIT REAL*8(A-H,O-Z)
C     /DUBL/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, TIMOUT
      COMMON/DUBL/A(6),AC(9),ACD(9),ASV(6),CA(9),CAB(9),CK
     1,CKKCAL,CRA(9),DAA,DATE,FKCAL,WR,PI,PICK,PICKZ,PIDKSQ
     2,PINHZ,QLIM(5),QMAX,RDWSS(9),RLIM(5),RM(9),RMAX,RTPIZ
     3,SA(5),SIGWD,SQTPDK,SQTPI,SQTPIK,TM(9),TPI,TRT(5),TV(3)
     4,UT(9),UV(3),UW(3),WC,WDBS,WS(9),WV,WX,XYZA(3),XYZAS(3)
     5,XYZOS(3),ZMC
C     /ITGR/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, IBYPAS, TIMOUT
      COMMON/ITGR/IBK,ICCAX,ICENT,ICMB,IGEM,ILSG,IMOL,INK,IPLN,IPRC
     1,IPRT,IRBA,IREP,IRSC,ISB,ISW,IVDW,IWGT,IZAN,JC,KPW,KPWS,LT(9)
     2,MODE,NA,NAC,NAF,NBC,NCT,NKA,NOS,NP,NPC,NPR,NPS,NPX,NQ,ISETA
     3,NR,NRB,NRP,NS,NT(9),NV,NVA,NVC,NVD,NYR,NYUS(9),NYX
      DIMENSION SEC(9),AVT(9),AL(7),BT(7)
      DATA AL/0.0D0,1.0300,1.2200,1.5600,1.7700,1.9600,2.1400/
      DATA BT/0.0D0,1.2000,1.4800,1.7100,1.5100,2.0500,2.2700/
      TOTALT=0.0
      DO 510 I=1,9
      SEC(I)=FLOAT(LT(I))/100.0
```

```
      TOTALT=TOTALT+SEC(I)                                              TIMO 110
      IF(NT(I))500,505,500                                              TIMO 115
  500 AVT(I)=SEC(I)/FLOAT(NT(I))                                        TIMO 120
      GO TO 510                                                         TIMO 125
  505 AVT(I)=0.0                                                        TIMO 130
  510 CONTINUE                                                          TIMO 135
      PRINT 5                                                           TIMO 140
    5 FORMAT('0NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGTIMO 145
     1Y CALCULATION FOR THIS CYCLE'/12X,'    NT        SEC       AVT')  TIMO 150
      PRINT 10,(NT(I),SEC(I),AVT(I),I=1,9)                              TIMO 155
   10 FORMAT(' INITIAL     ',I6,F9.2,F9.4/                              TIMO 160
     2' COORDINATES',I6,F9.2,F9.4/                                      TIMO 165
     3' SLOW RECIP ',I6,F9.2,F9.4/                                      TIMO 170
     4' FAST RECIP ',I6,F9.2,F9.4/                                      TIMO 175
     5' UNIT CELL  ',I6,F9.2,F9.4/                                      TIMO 180
     6' SLOW DIRECT',I6,F9.2,F9.4/                                      TIMO 185
     7' FAST DIRECT',I6,F9.2,F9.4/                                      TIMO 190
     8' SLOW CONFIG',I6,F9.2,F9.4/                                      TIMO 195
     9' FAST CONFIG',I6,F9.2,F9.4)                                      TIMO 200
      PRINT 15,TOTALT                                                   TIMO 205
   15 FORMAT('0TOTAL TIME (SEC) ',F9.2)                                 TIMO 210
      IF(CK)550,550,515                                                 TIMO 215
  515 IF(QMAX)550,550,520                                               TIMO 220
  520 PRINT 20                                                          TIMO 225
   20 FORMAT('0SUMMATION LIMITS FOR MINIMUM TIME'/                      TIMO 230
     1 4X,'DEL IS PROPORTIONAL TO RELATIVE ERROR OF RESULT'/            TIMO 235
     2 4X,'PRQ IS RECOMMENDED QLIM'/                                    TIMO 240
     3 4X,'PRR IS RECOMMENDED RLIM'/                                    TIMO 245
     4 4X,'PRK IS RECOMMENDED VALUE OF CK'/                             TIMO 250
     5 4X,'PRT IS PREDICTED TOTAL TIME PER CYCLE FOR RECIPROCAL AND DIRETIMO 255
     6CT SUMS'/                                                         TIMO 260
     7'0     DEL        PRQ        PRR        PRK        PRT')         TIMO 265
      FLF=SEC(4)+SEC(3)                                                 TIMO 270
      IF(FLF)525,525,530                                                TIMO 275
  525 FLF=0.005                                                         TIMO 280
  530 FLG=SEC(7)+SEC(6)                                                 TIMO 285
      IF(FLG)535,535,540                                                TIMO 290
  535 FLG=0.005                                                         TIMO 295
  540 CF=FLF/QMAX**3                                                    TIMO 300
      CG=FLG/RMAX**3                                                    TIMO 305
      CFCG=(CF/CG)**0.166667                                            TIMO 310
      SCFCG=DSQRT(CF*CG)                                                TIMO 315
      DO 545 I=2,7                                                      TIMO 320
      ALBT=AL(I)*BT(I)                                                  TIMO 325
      SQALBT=DSQRT(ALBT)                                                TIMO 330
      PRQ=SQALBT/CFCG                                                   TIMO 335
      PRR=SQALBT*CFCG                                                   TIMO 340
      PRK=DSQRT(AL(I)/BT(I))/CFCG                                       TIMO 345
      PRT=2.0*SCFCG*ALBT*SQALBT                                         TIMO 350
      PRINT 25,I,PRQ,PRR,PRK,PRT                                        TIMO 355
   25 FORMAT(' 1.0E-',I1,3F9.5,F9.2)                                    TIMO 360
  545 CONTINUE                                                          TIMO 365
  550 RETURN                                                            TIMO 370
      END                                                               TIMO 375


      SUBROUTINE TRANS(X,Z)                                             TRAN   5
C     STORE AT Z(3,3) THE TRANSPOSE OF X(3,3). X AND Z MAY BE THE SAME. TRAN  10
      IMPLICIT REAL*8(A-H,O-Z)                                          TRAN  15
      DIMENSION X(9),Y(9),Z(9)                                          TRAN  20
      DO 500 I=1,9                                                      TRAN  25
  500 Y(I)=X(I)                                                         TRAN  30
      HOLD=Y(2)                                                         TRAN  35
      Y(2)=Y(4)                                                         TRAN  40
      Y(4)=HOLD                                                         TRAN  45
      HOLD=Y(3)                                                         TRAN  50
      Y(3)=Y(7)                                                         TRAN  55
      Y(7)=HOLD                                                         TRAN  60
      HOLD=Y(6)                                                         TRAN  65
      Y(6)=Y(8)                                                         TRAN  70
      Y(8)=HOLD                                                         TRAN  75
      DO 505 I=1,9                                                      TRAN  80
  505 Z(I)=Y(I)                                                         TRAN  85
      RETURN                                                            TRAN  90
      END                                                               TRAN  95


      SUBROUTINE TRANSF(A,B,D,ID,N,NORM)                                TRAN   5
C     TRANSFORM EIGENVECTORS AFTER AXELBX, HOUSEH, AND VALVEC           TRAN  10
      REAL*8 A(ID,1),B(ID,1),D(1),X,C                                   TRAN  15
C     ******************************************************************TRAN  20
C                                                                       TRAN  25
C                                                                       TRAN  30
C     THE COLUMNS OF A ARE THE EIGENVECTORS OF P.                       TRAN  35
C                                                                       TRAN  40
C     THE DIAGONAL ELEMENTS OF L ARE IN THE ARRAY D.                    TRAN  45
C     THE OFF-DIAGONAL ELEMENTS OF L ARE IN THE LOWER PORTION OF B.     TRAN  50
C                                                                       TRAN  55
C     ******************************************************************TRAN  60
C                                                                       TRAN  65
      DO 510 J=1,NORM                                                   TRAN  70
         C = 0.0D0                                                      TRAN  75
         DO 500 I=1,N                                                   TRAN  80
  500       C = C + A(I,J)**2                                           TRAN  85
         C = DSQRT(C)                                                   TRAN  90
         DO 505 I=1,N                                                   TRAN  95
  505       A(I,J) = A(I,J)/C                                           TRAN 100
  510    CONTINUE                                                       TRAN 105
  515 DO 530 J=1,NORM                                                   TRAN 110
         A(N,J)= A(N,J)/D(N)                                            TRAN 115
         I = N-1                                                        TRAN 120
  520    IF (I.LT.1) GO TO 530                                          TRAN 125
         X = A(I,J)                                                     TRAN 130
         KK = I+1                                                       TRAN 135
         DO 525 K = KK,N                                                TRAN 140
  525       X = X - B(K,I)*A(K,J)                                       TRAN 145
         A(I,J) = X/D(I)                                                TRAN 150
         I = I-1                                                        TRAN 155
         GO TO 520                                                      TRAN 160
  530    CONTINUE                                                       TRAN 165
      RETURN                                                            TRAN 170
      END
```

```
      SUBROUTINE UNIT(X,Z)                                              UNIT   5
C     STORE AT Z A UNIT VECTOR IN THE DIRECTION OF X. Z MAY BE SAME AS XUNIT  10
C     VECTORS ARE REFERRED TO CRYSTAL AXIS SYSTEM                       UNIT  15
      IMPLICIT REAL*8(A-H,O-Z)                                          UNIT  20
C     /AB/ USED BY WPRE, WCALC, AVV, CONF, DST, NORM, UNIT              UNIT  25
      COMMON/AB/AA(9),A11,A22,A33,A12,A13,A23,BB(9),B11,B22,B33,B12,B13 UNIT  30
     1,B23,VA                                                           UNIT  35
      DIMENSION X(3),Y(3),Z(3)                                          UNIT  40
      DO 500 I=1,3                                                      UNIT  45
  500 Y(I)=X(I)                                                         UNIT  50
      D=DSQRT(Y(1)**2*A11+Y(2)*(Y(2)*A22+Y(1)*A12)+Y(3)*(Y(3)*A33       UNIT  55
     1+Y(2)*A23+Y(1)*A13))                                              UNIT  60
      DO 505 I=1,3                                                      UNIT  65
  505 Z(I)=Y(I)/D                                                       UNIT  70
      RETURN                                                            UNIT  75
      END                                                               UNIT  80


      SUBROUTINE VALVEC(D,E,A,IC,N,ID)                                  VALV   5
C     GET EIGENVALUES AND EIGENVECTORS OF TRIDIAGONAL MATRIX FROM HOUSEHVALV  10
C PROGRAM AUTHOR G. W. WESTLEY                                          VALV  15
C  COMPUTING TECHNOLOGY CENTER, UNION CARBIDE CORP.. NUCLEAR DIV..      VALV  20
C  OAK RIDGE, TENN.                                                     VALV  25
C                                                                       VALV  30
      REAL*8 A(ID,1),D(1),E(1),B,C,F,G,H,R,S,P,Q,TOL                    VALV  35
      IC = 0                                                            VALV  40
      TOL = 16.D0**(-14)                                                VALV  45
      DO 500 I=2,N                                                      VALV  50
  500    E(I-1) = E(I)                                                  VALV  55
      E(N) =0.0D0                                                       VALV  60
      F = 0.0D0                                                         VALV  65
      B = 0.0D0                                                         VALV  70
      DO 550 L=1,N                                                      VALV  75
         J = 0                                                          VALV  80
         H = TOL*(DABS(D(L)) + DABS(E(L)))                              VALV  85
         IF (B.LT.H) B = H                                              VALV  90
         DO 505 M = L,N                                                 VALV  95
            IF (DABS(E(M)).LE.B) GO TO 510                              VALV 100
  505       CONTINUE                                                    VALV 105
  510    IF (M.EQ.L) GO TO 550                                          VALV 110
  515    IF (J.GE.30) GO TO 575                                         VALV 115
         J = J+1                                                        VALV 120
         P = (D(L+1) - D(L))/(2.0D0*E(L))                               VALV 125
         R = DSQRT(P*P + 1.0D0)                                         VALV 130
         Q = P+R                                                        VALV 135
         IF (P.LT.0.0D0) Q = Q - 2.0D0*R                                VALV 140
         H = D(L) - E(L) / Q                                            VALV 145
         DO 520 I=L,N                                                   VALV 150
  520       D(I) = D(I)-H                                               VALV 155
         F = F+H                                                        VALV 160
         P = D(M)                                                       VALV 165
         C = 1.0D0                                                      VALV 170
         S = 0.0D0                                                      VALV 175
         I = M                                                          VALV 180
  525    I = I-1                                                        VALV 185
         IF (I.LT.L) GO TO 545                                          VALV 190
         G = C*E(I)                                                     VALV 195
         H = C*P                                                        VALV 200
         IF (DABS(P).GE.DABS(E(I))) GO TO 530                           VALV 205
         C = P/E(I)                                                     VALV 210
         R = DSQRT(C*C + 1.0D0)                                         VALV 215
         E(I+1) = S*E(I)*R                                              VALV 220
         S = 1.0D0/R                                                    VALV 225
         C = C/R                                                        VALV 230
         GO TO 535                                                      VALV 235
  530    C = E(I)/P                                                     VALV 240
         R = DSQRT(C*C + 1.0D0)                                         VALV 245
         E(I+1) = S*R*P                                                 VALV 250
         S = C/R                                                        VALV 255
         C = 1.0D0/R                                                    VALV 260
  535    P = C*D(I) - S*G                                               VALV 265
         D(I+1) = H + S*(C*G + S*D(I))                                  VALV 270
         DO 540 K=1,N                                                   VALV 275
            H = A(K,I+1)                                                VALV 280
            A(K,I+1) = S*A(K,I) + C*H                                   VALV 285
  540       A(K,I) = C*A(K,I) - S*H                                     VALV 290
         GO TO 525                                                      VALV 295
  545    CONTINUE                                                       VALV 300
         E(L) = S*P                                                     VALV 305
         D(L) = C*P                                                     VALV 310
         IF (DABS(E(L)).GT.B) GO TO 515                                 VALV 315
  550    D(L) = D(L)+ F                                                 VALV 320
      DO 570 I=1,N                                                      VALV 325
         K = I                                                          VALV 330
         P = D(I)                                                       VALV 335
         IF (I.EQ.N) GO TO 560                                          VALV 340
         II=I+1                                                         VALV 345
         DO 555 J=II,N                                                  VALV 350
            IF (D(J).LE.P) GO TO 555                                    VALV 355
            K = J                                                       VALV 360
            P = D(J)                                                    VALV 365
  555       CONTINUE                                                    VALV 370
  560    IF (K.EQ.I) GO TO 570                                          VALV 375
         D(K) = D(I)                                                    VALV 380
         D(I) = P                                                       VALV 385
         DO 565 J=1,N                                                   VALV 390
            P = A(J,I)                                                  VALV 395
            A(J,I) = A(J,K)                                             VALV 400
  565       A(J,K) = P                                                  VALV 405
  570    CONTINUE                                                       VALV 410
      RETURN                                                            VALV 415
  575 IC = 1                                                            VALV 420
      RETURN                                                            VALV 425
      END                                                               VALV 430


      SUBROUTINE VECI (XC,YC,ZC)                                        VECI   5
      IMPLICIT REAL*8(A-H,O-Z)                                          VECI  10
      DIMENSION XC(1),YC(1),ZC(1)                                       VECI  15
      DIMENSION V(3)                                                    VECI  20
      RETURN                                                            VECI  25
```

```
C
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS
C
C     OBTAIN VECTOR V FROM ATOM I TO ATOM J.
C     COMPONENTS OF V ARE REFERRED TO CRYSTAL COORDINATE SYSTEM.
C
      ENTRY VEC(I,J,V)
      V(1)=XC(J)-XC(I)
      V(2)=YC(J)-YC(I)
      V(3)=ZC(J)-ZC(I)
      RETURN
      END

      FUNCTION VMV(X1,Q,X2)
C     TRANSPOSED VECTOR * MATRIX * VECTOR
C     VMV=X1(3)*Q(3,3)*X2(3)     TO  EVALUATE QUADRATIC OR BILINEAR FORM
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION X1(3),Q(3,3),X2(3)
      T1=0.D0
      DO 500 J=1,3
  500 T1=T1+X1(J)*(X2(1)*Q(J,1)+X2(2)*Q(J,2)+X2(3)*Q(J,3))
      VMV=T1
      RETURN
      END

      SUBROUTINE WCNF( IKA,JAC,PC)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION IKA(1),JAC(1),PC(1)
      RETURN
C
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS
C
C     USER ROUTINE TO CALCULATE ENERGY, WCF, OF TORSION ANGLE IN
C     DEGREES, CNF, DEFINED BY ATOMS IA, JA, KA, AND LA, CALLED ONCE
C     FOR EACH CONFORMATION ANGLE ABOUT BOND JA-KA IF THE CORRESPONDING
C     ITBR.LT.0
C
      ENTRY WCNF(IA,JA,KA,LA,CNF,ITKJ,WCF)
      RETURN
      END

      FUNCTION WRAG(X,B)
C     EVALUATE WRAP-AROUND GAUSSIAN
      IMPLICIT REAL*8(A-H,O-Z)
      DATA TPI/6.2831853071795860D/
      F=DEXP(-0.5*(X/B)**2)
      TPN=0.0
  500 TPN=TPN+TPI
      G=F+DEXP(-0.5*((X+TPN)/B)**2)+DEXP(-0.5*((X-TPN)/B)**2)
      IF(G-F)505,510,505
  505 F=G
      GO TO 500
  510 WRAG=G
      RETURN
      END
```

9.2 Glossary of Symbols

```
      SUBROUTINE GLOSS
C     A(6)          LATTICE PARAMEYERS, ANGSTROMS AND COSINES
C     A11           AA(1)=A(1)**2
C     A12           2*AA(2)=2*A(1)*A(2)*A(6)
C     A13           2*AA(3)=2*A(1)*A(3)*A(5)
C     A22           AA(2)=A(2)**2
C     A23           2*AA(6)=2*A(2)*A(3)*A(4)
C     A33           AA(3)=A(3)**2
C     AA(9)         METRIC FOR DIRECT LATTICE
C     AC(9)         AA*UT, TRANSPOSE MATRIX FOR CARTESIAN TRANSFORMATION
C     ACB(9)        CARTESIAN TRANSFORMATION MATRIX FROM FIRST RIGID BODY
C     ACZ(9,NRB)    MATRICES FOR CARTESIAN TRANS BASED ON INPUT LATTICE
C     AF            TERM A OF STRUCTURE FACTOR FOR COULOMB ENERGY
C     AFV           TERM A OF STRUCTURE FACTOR FOR VAN DER WAALS ENERGY
C     AIJK          BOND ANGLE, DEGREES
C     AKE(NV*NV)    KINETIC ENERGY MATRIX, INVERSE OF USUAL G MATRIX
C     AKEIJ         AKE(I,J)
C     AL(7)         TABULATED VALUES OF XM FOR VARIOUS RELATIVE ERRORS
C     ALBT          AL(I)*BT(I)
C     AM(NV*NV)     MATRIX OF LEAST-SQUARES NORMAL EQUATIONS FOR ONE SUBS
C     AMASS(NKA)    ATOMIC MASS IN PHYSICAL ATOMIC WEIGHT UNITS
C     AN(NV*NV)     MATRIX OF LEAST-SQUARES NORMAL EQUATIONS
C     ANG           SUBROUTINE TO CALCULATE BOND ANGLE
C     ANIJ          AN(IJ)
C     AR(NKA)       ATOMIC RADIUS FOR REPULSION, ANGSTROM UNITS
C     ARE           ACCEPTABLE RATIO OF EIGENVALUES FOR PRINC COMP ANAL
C     ARG           ARGUMENT FOR SIN OR COS IN STRUCTURE FACTOR CALC
C     ASV(6)        LATTICE PARAMETERS SAVED FROM PREVIOUS ENTRY TO WCALC
C     AVT(9)        AVERAGE TIME IN EACH BRANCH OF WCALC, SECONDS
C     AXEL.BX       SUBROUTINE TO PREPARE FOR SOLVING GENERAL EIG PROBLEM
C     AXES          SUBROUTINE TO GENERATE ORTHOGONAL UNIT VECTOR TRIPLE
C     B1            RECIPROCAL LATTICE CONSTANT
C     B11           BB(1)
C     B12           2*BB(2)
C     B13           2*BB(3)
C     B2            RECIPROCAL LATTICE CONSTANT
C     B22           BB(2)
C     B23           2*BB(6)
C     B3            RECIPROCAL LATTICE CONSTANT
C     B33           BB(3)
C     BB(9)         METRIC FOR RECIPROCAL LATTICE
C     BF            TERM B OF STRUCTURE FACTOR FOR COULOMB ENERGY
C     BFV           TERM B OF STRUCTURE FACTOR FOR VAN DER WAALS ENERGY
C     BR(NKA)       ATOMIC SOFTNESS COEFFICIENT FOR REPULSION, ANGSTROMS
C     BRIJ          BR(IA)+BR(JA)
C     BT(7)         TABULATED VALUES OF YM FOR VARIOUS RELATIVE ERRORS
C     BTR(NV*NOS)   TRANSPOSED MATRIX OF SECOND DERIVATIVES
C     BXMAX         MAXIMUM VALUE OF ATOM COORD IN BASIC ASYMMETRIC UNIT
C     BXMIN         MINIMUM VALUE OF ATOM COORD IN BASIC ASYMMETRIC UNIT
C     BYMAX         MAXIMUM VALUE OF ATOM COORD IN BASIC ASYMMETRIC UNIT
C     BYMIN         MINIMUM VALUE OF ATOM COORD IN BASIC ASYMMETRIC UNIT
C     BZMAX         MAXIMUM VALUE OF ATOM COORD IN BASIC ASYMMETRIC UNIT
C     BZMIN         MINIMUM VALUE OF ATOM COORD IN BASIC ASYMMETRIC UNIT
C     CA(9)         INVERSE OF CARTESIAN TRANSFORMATION MATRIX
C     CAB(9)        TRANSFORM BASIC CARTESIAN TO CRYSTAL, INVERSE OF ACB
C     CF            TOTAL TIME PER UNIT VOLUME OF RECIPROCAL SPACE
C     CFCG          SIXTH ROOT OF (CF/CG)
C     CG            TOTAL TIME PER UNIT VOLUME OF DIRECT SPACE
C     CHAR(NS)      CHARACTER OF NORMAL MODE WITH RESPECT TO EACH SYM OP
C     CK            CONSTANT K IN EWALD SUMMATION METHOD
C     CKKCAL        -FKCAL*CK
C     CMB           COULOMB TERM
C     CMBI(NGS)     COULOMB TERM SAVED FOR OUTPUT, KCAL/MOLE
C     CMPR          CONSTANT ADDED TO DIAG EL OF AN FOR MARQUARDTS COMP.
C     CNF           CONFORMATION ANGLE, DEGREES
C     CNSTRN        USER SUBROUTINE TO CONSTRAIN PARAMETERS
C     CONF          SUBROUTINE TO CALCULATE CONFORMATION ANGLE
C     COSARG        COS(ARG)
C     CRA(9)        MATRIX CAWRM*ACZ
C     CSF           RTPIZV*SF, SCALED RECIPROCAL COULOMB SUM
C     CSV(NGS)      MODIFIED COULOMB TERM SAVED FOR NEXT ENTRY
C     CTM           MODIFIED COULOMB TERM INCLUDING MULTIPLICITY
C     CWX           USER SUBROUTINE TO CALCULATE EXTRA ENERGY
C     CX            COS(SXR(J))
C     CXMAX         MAXIMUM VALUE OF ATOM COORD IN UNIT CELL
C     CXMIN         MINIMUM VALUE OF ATOM COORD IN UNIT CELL
C     CY            COS(SYR(J))
C     CYMAX         MAXIMUM VALUE OF ATOM COORD IN UNIT CELL
C     CYMIN         MINIMUM VALUE OF ATOM COORD IN UNIT CELL
C     CZ            COS(SZR(J))
C     CZMAX         MAXIMUM VALUE OF ATOM COORD IN UNIT CELL
C     CZMIN         MINIMUM VALUE OF ATOM COORD IN UNIT CELL
C     D             DETERMINANT OF MATRIX AC
C     DAA           DETERMINANT OF DIRECT LATTICE METRIC
C     DATE          ALPHANUMERIC CALENDAR DATE
C     DDWIJ         D**2 W / D P(I) D P(J)
C     DET           DETERMINANT OF INVERSE OF WMAT
C     DCAN          DIAGONAL ELEMENT OF AN
C     DGF           NUMBER OF DEGREES OF FREEDOM NO-NV (OR 1 IF NO=NV)
C     DIAG          DIAGONAL ELEMENT OF INVERSE AN
C     DIFV          SUBROUTINE TO SUBTRACT TWO 3*1 VECTORS
C     DIJ           BOND DISTANCE
C     DKT(9)        TABLE OF DAMPING FACTORS SET BY DATA STATEMENT
C     DKTKQI        DKT(KQI)
C     DP(NP)        INCREMENTS FOR NUMERICAL DERIVS WITH RESPECT TO P
C     DPC(NPC)      INCREMENTS FOR NUMERICAL DERIVS WITH RESPECT TO PC
C     DPX(NPX)      INCREMENTS FOR NUMERICAL DERIVS WITH RESPECT TO PX
C     DST           SUBROUTINE TO CALCULATE INTERATOMIC DISTANCE
C     DW(NP)        D/DP, FIRST DERIVATIVES OF ENERGY
C     DWDQ(NV)      DERIVATIVES OF ENERGY WITH RESPECT TO VARIABLE
C     DWMI          -DW(I)
C     DX            COMPONENT OF INTERATOMIC DISTANCE IN CRYSTAL COORDS
C     DXI           TERM IN DX
C     DXQ(NV,NA)    DERIVS OF ATOM CART COORDS WITH RESPECT TO VARIABLES
C     DY            COMPONENT OF INTERATOMIC DISTANCE IN CRYSTAL COORDS
C     DYC(NO)       -DW(J) FOR THOSE P(J)'S USED AS OBSERVATIONS
C     DYI           TERM IN DY
C     DYQ(NV,NA)    DERIVS OF ATOM CART COORDS WITH RESPECT TO VARIABLES
C     DZ            COMPONENT OF INTERATOMIC DISTANCE IN CRYSTAL COORDS
C     DZI           TERM IN DZ
C     DZQ(NV,NA)    DERIVS OF ATOM CART COORDS WITH RESPECT TO VARIABLES
C     EL1M          LOWER LIMIT FOR ACCEPTABLE EIGENVALUES
C     EPS(NP)       CURRENT PARAMETER INCREMENTS FOR MODE 3
C     EPSC          FACTOR USED TO SET INITIAL VALUES OF EPS IN MODE 3
C     EPSL          FACTOR APPLIED TO VBEST FOR VECTOR SEARCH IN MODE 3
C     ERR(NV)       CALCULATED PARAMETER ERRORS
C     EVAL(NV)      EIGENVALUES OF NORMAL EQUATION MATRIX
C     EVEC(NV*NV)   EIGENVECTORS OF NORMAL EQUATION MATRIX
C     EXIT          LIBRARY SUBROUTINE YO TERMINATE JOB
C     EXPYYM        EXP(-YYM)
C     FKCAL         332.17, FACTOR TO CONVERT ENERGY TO KCAL/MOLE
C     FLF           TOTAL TIME FOR FAST RECIPROCAL LATTICE SUMS
C     FLG           TOTAL TIME FOR FAST DIRECT LATTICE SUMS
C     FM            1.0 FOR NON-CENTROSYMMETRIC, 2.0 FOR CENTRO STRUCTURE
C     FMC(NA*NS)    MULTIPLICITY OF ATOM IN STRUCTURE FACTOR CALCULATION
C     FNS           FLOATING NS, THE NUMBER OF EQUIVALENT POSITIONS
C     FREQ(NV)      VIBRATIONAL FREQUENCIES, WAVE NUMBERS
C     FSQ           COULOMB STRUCTURE FACTOR SQUARED
C     FSQV          VAN DER WAALS STRUCTURE FACTOR SQUARED
C     GCMX          SUBROUTINE FOR GENERAL CALC OF CONFORMATION ENERGY
C     GM            MULTIPLICITY OF DIRECT LATTICE TERM
C     GMADD         SUBROUTINE FOR GENERAL MATRIX ADDITION
C     GMI           FACTOR IN MULTIPLICITY OF DIRECT LATTICE TERM
C     GMPRD         SUBROUTINE FOR GENERAL MATRIX PRODUCT
C     GMT(NGS)      MULTIPLICITY SAVED FOR NEXT ENTRY
C     GMTRA         SUBROUTINE FOR GENERAL MATRIX TRANSPOSE
C     GPOT          USER SUBROUTINE FOR GENERAL NONBONDED POTENTIAL
C     GTPRD         SUBROUTINE FOR GENERAL MATRIX TRANSPOSE PRODUCT
C     GX            LATTICE TRANSLATION FOR DIRECT LATTICE SUM
C     GXMAX         MAXIMUM POSSIBLE LATTICE TRANSLATION
C     GXMIN         MINIMUM POSSIBLE LATTICE TRANSLATION
C     GXT(NGS)      LATTICE TRANSLATION SAVED FOR NEXT ENTRY
C     GY            LATTICE TRANSLATION FOR DIRECT LATTICE SUM
C     GYMAX         MAXIMUM POSSIBLE LATTICE TRANSLATION
C     GYMIN         MINIMUM POSSIBLE LATTICE TRANSLATION
C     GYT(NGS)      LATTICE TRANSLATION SAVED FOR NEXT ENTRY
C     GZ            LATTICE TRANSLATION FOR DIRECT LATTICE SUM
C     GZMAX         MAXIMUM POSSIBLE LATTICE TRANSLATION
C     GZMIN         MINIMUM POSSIBLE LATTICE TRANSLATION
C     GZT(NGS)      LATTICE TRANSLATION SAVED FOR NEXT ENTRY
C     HBXY          TERM USED TO CALCULATE QQ
C     HBX2          TERM USED YO CALCULATE QQ
C     HBYZ          TERM USED TO CALCULATE QQ
C     HM            1, 2, 4, OR 6, MULTIPLICITY FOR RECIP LATTICE TERM
C     HMI(NFS)      SAVED MULTIPLICITY OF RECIPROCAL LATTICE TERM
C     HOUSEH        SUBROUTINE TO CONVERT MATRIX TO TRIDIAGONAL FORM
C     HX            INDEX FOR RECIPROCAL LATTICE SUM
C     HXM           1 OR 2, MULTIPLICITY ASSOCIATED WITH HX
C     HXMAX         UPPER LIMIT ON INDEX FOR SHELL IN RECIPROCAL SPACE
C     HXMIN         LOWER LIMIT ON INDEX FOR SHELL IN RECIPROCAL SPACE
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C     HXNEG          1 IF SYMMETRY REQUIRES NEGATIVE INDEX, OTHERWISE 0      GLOS 805
C     HXT(NFS)       SAVED INDEX OF RECIPROCAL LATTICE TERM                  GLOS 810
C     HY             INDEX FOR RECIPROCAL LATTICE SUM                        GLOS 815
C     HYM            1, 2, OR 4. MULTIPLICITY ASSOCIATED WITH HX AND HY      GLOS 820
C     HYMAX          UPPER LIMIT ON INDEX FOR SHELL IN RECIPROCAL SPACE      GLOS 825
C     HYMIN          LOWER LIMIT ON INDEX FOR SHELL IN RECIPROCAL SPACE      GLOS 830
C     HYNEG          1 IF SYMMETRY REQUIRES NEGATIVE INDEX, OTHERWISE 0      GLOS 835
C     HYT(NFS)       SAVED INDEX OF RECIPROCAL LATTICE TERM                  GLOS 840
C     HZ             INDEX FOR RECIPROCAL LATTICE SUM                        GLOS 845
C     HZMAX          UPPER LIMIT ON INDEX FOR SHELL IN RECIPROCAL SPACE      GLOS 850
C     HZMIN          LOWER LIMIT ON INDEX FOR SHELL IN RECIPROCAL SPACE      GLOS 855
C     HZNEG          1 IF SYMMETRY REQUIRES NEGATIVE INDEX, OTHERWISE 0      GLOS 860
C     HZT(NFS)       SAVED INDEX OF RECIPROCAL LATTICE TERM                  GLOS 865
C     IACT(NCT)      IDENTIFYING NUMBER OF BACKBONE ATOM IN CONNECTION TABGLOS 870
C     IASV(MMAX)     INDEX SAVED FOR LATER CALC OF CONFORMATION ENERGY       GLOS 875
C     IAT(NGS)       INDEX OF ATOM IN UNIT CELL SAVED FOR NEXT ENTRY         GLOS 880
C     IAZ(6,NCT)     IDENT NUMBERS OF COMMON PARAM USED TO CALCULATE WA      GLOS 885
C     IAZNJ          IAZ(N,J)                                                GLOS 890
C     IB             INDICATOR SET TO 1 IF ANY P IS OUTSIDE LIMITS           GLOS 895
C     IBK            BREAK INDICATOR. 1 TERMINATES WCALC AFTER XYZR IS SETGLOS 900
C     IBPC           INDICATOR TO BYPASS READING COMMON PARAMETERS           GLOS 905
C     IBY            INDICATOR FOR BYPASSING RECIP SUMS, DIRECT SUMS, GCWXGLOS 910
C     IBYP           IBY+1                                                   GLOS 915
C     IBYPAS         SUBROUTINE TO GENERATE IBY, THE BYPASS INDICATOR        GLOS 920
C     IC             NUMBER OF CURRENT CYCLE                                 GLOS 925
C     ICA            INDICATOR OF CHANGE IN LATTICE PARAM SINCE LAST ENTRYGLOS 930
C     ICC(NA*NS)     INDICATOR OF CHANGE IN ATOM COORDS                      GLOS 935
C     ICCAX          OVERALL INDICATOR OF CHANGE IN COMMON, LATTICE, EXTRAGLOS 940
C     ICENT          1 FOR NONCENTRO, 2 FOR CENTROSYMMETRIC STR FAC CALC     GLOS 945
C     ICLOCK         LIBRARY ROUTINE TO READ CENTRAL PROCESSOR TIME          GLOS 950
C     ICMB           COULOMB ENERGY INDICATOR. 0 OMIT, 1 INCLUDE             GLOS 955
C     ICPC           INDICATOR OF CHANGE IN COMMON PARAM SINCE LAST ENTRY GLOS 960
C     ICPX           INDICATOR OF CHANGE IN EXTRA PARAM SINCE LAST ENTRY     GLOS 965
C     ICT(4,NCT)     IDENT NUMBERS OF ATOMS CONNECTED TO ATOM IACT           GLOS 970
C     IDAY           LIBRARY SUBROUTINE TO OBTAIN CALENDAR DATE              GLOS 975
C     IDD            INDICATOR. 0 IF DDWIJ HAS NOT BEEN SET, 1 IF IT HAS     GLOS 980
C     IDIR           INDICATOR FOR DIRECT SUM. 0 INCLUDE, 1 BYPASS           GLOS 985
C     IDZ(4,NCT)     IDENT NUMBERS OF COMMON PARAM USED TO CALCULATE WD      GLOS 990
C     IDZJI          IDZ(J,I)                                                GLOS 995
C     IFL            INDICATOR FOR AT LEAST ONE FAILURE IN MODE 3            GLOS1000
C     IFST           FIRST STEP INDICATOR FOR STEEPEST DESCENTS              GLOS1005
C     IG             INDEX FOR FAST DIRECT LATTICE SUMS                      GLOS1010
C     IGEM           INDICATOR FOR GEMINAL ATOM TERMS. 0 INCLUDE, 1 OMIT     GLOS1015
C     IGX            CELL TRANSLATION IN INTEGER FORM FOR PRINTING           GLOS1020
C     IGY            CELL TRANSLATION IN INTEGER FORM FOR PRINTING           GLOS1025
C     IGZ            CELL TRANSLATION IN INTEGER FORM FOR PRINTING           GLOS1030
C     IH             INDEX OVER TERMS IN FAST RECIPROCAL LATTICE SUM         GLOS1035
C     IKA(NA)        INDICATES KIND OF EACH ATOM IN LIST. 0 FOR EXTRA ATOMGLOS1040
C     ILSQ           LEAST-SQUARES INDICATOR. 1 TO REQUIRE LEAST SQUARES     GLOS1045
C     IMOL           ISOLATED MOLECULE INDICATOR. 1 FOR MOL, 0 FOR CRYSTALGLOS1050
C     INK            PL(INK+1) IS FIRST PARAMETER OF CURRENT SUBSTANCE       GLOS1055
C     INVRS          SUBROUTINE TO INVERT 3*3 MATRIX                         GLOS1060
C     IOUT(NV)       PARAMETER NUMBER OF VARIABLES SAVED FOR OUTPUT          GLOS1065
C     IPLM           PARAMETER LIMIT INDICATOR. 1 USE LIMITS, 0 DO NOT       GLOS1070
C     IPRC           OUTPUT PRINT IND MODIFIED FOR FIRST OR LAST CYCLE       GLOS1075
C     IPRT           OUTPUT PRINT INDICATOR                                  GLOS1080
C     IQ             INDEX WHICH COUNTS SHELLS IN RECIPROCAL SPACE           GLOS1085
C     IR             INDEX OVER SHELLS IN DIRECT SPACE                       GLOS1090
C     IRB(NA)        NUMBER OF RIGID BODY TO WHICH ATOM BELONGS              GLOS1095
C     IRBA           INDICATOR FOR RIGID BODIES. 0 GENERAL; 1 MONATOMIC      GLOS1100
C     IRBC(NA*NS)    NUMBER OF RIGID BODY TO WHICH ATOM IN CELL BELONGS      GLOS1105
C     IREC           INDICATOR FOR RECIPROCAL SUM. 0 INCLUDE, 1 BYPASS       GLOS1110
C     IREJ           REJECTION INDICATOR FOR RECIP SUM. 0 ACCEPT, 1 REJECTGLOS1115
C     IREP           REPULSION INDICATOR FOR STANDARD, REPL, AND/OR GPOT     GLOS1120
C     IRGT           DIRECTION INDICATOR FOR STEEPEST DESCENTS               GLOS1125
C     IRP            COUNTER FOR PRINTING INTERATOMIC DISTANCES              GLOS1130
C     IRSC           INDICATOR FOR RELAXING SYMMETRY CONSTRAINTS             GLOS1135
C     IS             SWITCH. 0 FOR SETTING BTR(IM), 1 FOR SETTING UMAT(IN)GLOS1140
C     ISB            INTEGER WHICH IDENTIFIES EACH SUBSTANCE                 GLOS1145
C     ISBP(NP)       SUBSTANCE IDENT FOR EACH PARAM. ZERO FOR COMMON PAR     GLOS1150
C     ISC(NA*NS)     NUMBER OF SYMMETRY POSIT FOR ATOM IN UNIT CELL          GLOS1155
C     ISETA          LATTICE PARAMETER CONSTRAINT INDICATOR                  GLOS1160
C     ISTG           STAGE COUNTER FOR MODE 3                                GLOS1165
C     ISTP           STEPPING INDICATOR FOR STEEPEST DESCENTS                GLOS1170
C     ISU            INDICATOR FOR AT LEAST ONE SUCCESS IN MODE 3            GLOS1175
C     ISV(MMAX)      INDEX SAVED FOR LATER CALC OF CONFORMATION ENERGY       GLOS1180
C     ISW            SWITCH. 1 FOR FIRST ENTRY TO WCALC ON CYCLE, 0 LATER GLOS1185
C     ITBR(4,NCT)    IDENT NUMBERS OF COMMON PARAM USED TO CALCULATE WCF     GLOS1190
C     ITKJ           ITBR(K,J)                                               GLOS1195
C     ITYPE(133)     TABLE SPECIFYING WORD SIZE FOR ARRAYS                   GLOS1200
C     IU(NRB)        NUMBER OF ATOM USED TO DEFINE AXES OF COORD SYSTEM      GLOS1205
C     IUJ            IU(J)                                                   GLOS1210
C     IV(NRB)        NUMBER OF ATOM USED TO DEFINE AXES OF COORD SYSTEM      GLOS1215
C     IVDW           VAN DER WAALS INDICATOR. 0 OMIT, 1 INCLUDE              GLOS1220
C     IVJ            IV(J)                                                   GLOS1225
C     IW(NRB)        NUMBER OF ATOM USED TO DEFINE AXES OF COORD SYSTEM      GLOS1230
C     IWGT           WEIGHT INDICATOR. 1 USE WEIGHT IN MODE 0, 0 DO NOT      GLOS1235
C     IWJ            IW(J)                                                   GLOS1240
C     IWT            WEIGHT INDICATOR. 1 IF WGT MATRIX IS USED, 0 IF NOT     GLOS1245
C     IWX            INDICATOR FOR CONFORMATION ENERGY. 0 INCLUDE, 1 OMIT    GLOS1250
C     IZ(NRB)        NUMBER OF ATOM WHICH DEFINES ORIGIN OF COORD SYSTEM     GLOS1255
C     IZAM           ALLOWS USER TO SET ZAM(I). IGNORED IF ZERO.             GLOS1260
C     IZJ            IZ(J)                                                   GLOS1265
C     JAC(NA*NS)     NUMBER OF INPUT ATOM FOR ATOM IN UNIT CELL              GLOS1270
C     JASV(MMAX)     INDEX SAVED FOR LATER CALC OF CONFORMATION ENERGY       GLOS1275
C     JAT(NGS)       INDEX OF ATOM IN UNIT CELL SAVED FOR NEXT ENTRY         GLOS1280
C     JC             SAME AS IC BUT IN COMMON                                GLOS1285
C     JOTS(NOS)      JOTS(I) IS OVERALL PARAM NUMBER OF OBS I                GLOS1290
C     JOUT(NO)       PARAMETER NUMBERS OF OBSERVATIONS SAVED FOR OUTPUT      GLOS1295
C     JS             INDEX OF SMALLEST INTERATOMIC DISTANCE FOUND            GLOS1300
C     JSV(MMAX)      INDEX SAVED FOR LATER CALC OF CONFORMATION ENERGY       GLOS1305
C     KADR(133)      HEXADECIMAL ADDRESS OF EACH ARRAY IN S                  GLOS1310
C     KASV(MMAX)     INDEX SAVED FOR LATER CALC OF CONFORMATION ENERGY       GLOS1315
C     KP(NP)         OBSERVATION SELECTION INTEGERS. 1 IF USED, 0 IF NOT     GLOS1320
C     KPC(NPC)       KIND OF PC. 1 Q OR PL, 2 AR OR BR, 3 FOR GCWX, 0        GLOS1325
C     KPCIP          KPC(IP)                                                 GLOS1330
C     KPI            KIND OF PARAM IN MAP MODE. -1 NONE, 0 COMMON, 1 REG     GLOS1335
C     KPJ            KIND OF PARAM IN MAP MODE. -1 NONE, 0 COMMON, 1 REG     GLOS1340
C     KPK            KIND OF PARAM IN MAP MODE. -1 NONE, 0 COMMON, 1 REG     GLOS1345
C     KPS(NPS)       OBSERVATION SELECTION INTEGERS FOR ONE SUBSTANCE        GLOS1350
C     KPW            INDICATOR FOR WOBS. 0 NOT USED, 1 USED, -1 SOMETIMES GLOS1355
C     KPWS           INDICATOR FOR WOBS. USED TO SET KPW                     GLOS1360
C     KQ(NP)         VARIABLE SELECTION INTEGERS. 1 TO 9 IF VARIED, ELSE 0GLOS1365
C     KQC(NPC)       VARIABLE SELECTION INTEGERS FOR COMMON PARAMETERS       GLOS1370
C     KQI            KQ(I)                                                   GLOS1375
C     KQS(NPS)       VARIABLE SELECTION INTEGERS FOR ONE SUBSTANCE           GLOS1380
C     KRSC           SWITCH. ALLOWS RELAXATION OF SYM CONSTRNTS ONCE ONLY GLOS1385
C     L1(133)        TABLE SELECTING LIMIT USED TO SET DIMENSIONS            GLOS1390
C     L2(133)        TABLE SELECTING LIMIT USED TO SET DIMENSIONS            GLOS1395
C     LASV(MMAX)     INDEX SAVED FOR LATER CALC OF CONFORMATION ENERGY       GLOS1400
C     LBCI(NBC)      LBCI(K) AND LBCJ(K) DEFINE A BONDED PAIR OF ATOMS       GLOS1405
C     LBCJ(NBC)      LBCI(K) AND LBCJ(K) DEFINE A BONDED PAIR OF ATOMS       GLOS1410
C     LI(NP)         LI(I) IS INDEX OF P(I) IN LIST OF THOSE VARIED          GLOS1415
C     LIM(32)        DYNAMIC DIMENSIONS USED TO SET UP ARRAY STORAGE         GLOS1420
C     LPI            PARAMETER INDEX IN MAPPING MODE                         GLOS1425
C     LPJ            PARAMETER INDEX IN MAPPING MODE                         GLOS1430
C     LPK            PARAMETER INDEX IN MAPPING MODE                         GLOS1435
C     LS             1 FOR LEAST-SQUARES, 0 FOR DIRECT SOLUTION OF EQUATNSGLOS1440
C     LT(9)          ACCUMULATED TIMES IN VARIOUS BRANCHES OF WCALC          GLOS1445
C     LTF            CURRENT CLOCK TIME, HUNDREDTHS OF SECONDS               GLOS1450
C     LTI            CLOCK TIME SAVED FROM PREVIOUS READING                  GLOS1455
C     M              COUNTER FOR DISTANCES, ANGLES, AND CONFORMATION ANGS GLOS1460
C     MCPY           SUBROUTINE TO COPY MATRIX                               GLOS1465
C     MINV           SUBROUTINE TO INVERT MATRIX                             GLOS1470
C     MJ(NP)         IF P(J) IS OBSERVATION I THEN MJ(J)=I                   GLOS1475
C     MM             SUBROUTINE TO MULTIPLY 3*3 MATRICES                     GLOS1480
C     MMAX           DIMENSION WHICH PLACES UPPER LIMIT ON M                 GLOS1485
C     MODE           OVERALL CONTROL INTEGER. -1, 0, 1, 2, 3, OR 4           GLOS1490
C     MPI            NUMBER OF PARAMETER IN MAPPING MODE                     GLOS1495
C     MPJ            NUMBER OF PARAMETER IN MAPPING MODE                     GLOS1500
C     MPK            NUMBER OF PARAMETER IN MAPPING MODE                     GLOS1505
C     MPRD           SUBROUTINE FOR MATRIX PRODUCT                           GLOS1510
C     MV             SUBROUTINE TO MULTIPLY 3*3 MATRIX TIMES 3*1 VECTOR      GLOS1515
C     NA             NUMBER OF ATOMS IN ASYMMETRIC UNIT. INCLUDES EXTRAS     GLOS1520
C     NAC            NUMBER OF ATOMS IN UNIT CELL                            GLOS1525
C     NAF            NUMBER OF ATOMS INCLUDED IN STRUCTURE FACTOR CALC       GLOS1530
C     NAMA(6)        ALPHANUMERIC CONSTANTS 'A, B, C, COSA, COSB, COSG'      GLOS1535
C     NAMARY(133)    ALPHANUMERIC NAMES OF ARRAYS WITH DYNAMIC DIMENSIONS GLOS1540
C     NAMAX          DIMENSION WHICH PLACES UPPER LIMIT ON NA                GLOS1545
C     NAME(NA)       ALPHANUMERIC ATOM NAME                                  GLOS1550
C     NAMK(NKA)      ALPHANUMERIC NAME OF EACH (CHEMICAL) KIND OF ATOM       GLOS1555
C     NAMLIM(32)     NAMES OF LIMITS USED TO SET DIMENSIONS                  GLOS1560
C     NAMP(NP)       ALPHANUMERIC NAME OF PARAMETERS IN OVERALL LIST         GLOS1565
C     NAMPC(NPC)     ALPHANUMERIC NAMES OF COMMON PARAMETERS                 GLOS1570
C     NAMPX(NPX)     ALPHANUMERIC NAMES OF EXTRA PARAMETERS                  GLOS1575
C     NAMR(3)        ALPHANUMERIC CONSTANTS 'RX, RY, RZ'                     GLOS1580
C     NAMS(NS)       ALPHANUMERIC NAME OF SYMMETRY OPERATION                 GLOS1585
C     NAMT(3)        ALPHANUMERIC CONSTANTS 'TX, TY, TZ'                     GLOS1590
C     NANG           NUMBER OF BOND ANGLES                                   GLOS1595
C     NB             DATA SET REFERENCE NUMBER FOR AUXILIARY STORAGE         GLOS1600
C     NBC            NUMBER OF BONDED CONTACTS IN LIST TO BE EXCLUDED        GLOS1605
C     NBCMAX         DIMENSION WHICH PLACES UPPER LIMIT ON NBC               GLOS1610
C     NC             NUMBER OF CYCLES OF ADJUSTMENT TO BE MADE               GLOS1615
C     NCNF           NUMBER OF CONFORMATION ANGLES                           GLOS1620
C     NCS            NUMBER OF CYCLES IN SUMMARY. NCS=MIN0(NC,8)             GLOS1625
C     NCT            NUMBER OF ENTRIES IN CONNECTION TABLE                   GLOS1630
C     NCTMAX         DIMENSION WHICH PLACES UPPER LIMIT ON NCT               GLOS1635
C     NCY            NC+1                                                    GLOS1640
C     NCYS           NCS+1, NUMBER OF COLUMNS IN SUMMARY OUTPUT              GLOS1645
C     ND             DATA SET REFERENCE NUMBER FOR AUXILIARY STORAGE         GLOS1650
C     NDST           NUMBER OF BOND DISTANCES                                GLOS1655
C     NE             ERROR INDICATOR SET BY VALVEC                           GLOS1660
C     NF             TOTAL NUMBER OF TERMS IN RECIPROCAL LATTICE SUMS        GLOS1665
C     NFS            NUMBER OF RECIP LAT TERMS STORED. LIMITED TO NFSMAX     GLOS1670
C     NFSMAX         DIMENSION WHICH PLACES UPPER LIMIT ON NFS               GLOS1675
C     NG             TOTAL NUMBER OF TERMS IN DIRECT LATTICE SUMS            GLOS1680
C     NGS            NUMBER OF DIR LAT TERMS STORED. LIMITED TO NGSMAX       GLOS1685
C     NGSMAX         DIMENSION WHICH PLACES UPPER LIMIT ON NGS               GLOS1690
C     NKA            NUMBER OF (CHEMICAL) KINDS OF ATOMS                     GLOS1695
C     NKAMAX         DIMENSION WHICH PLACES UPPER LIMIT ON NKA               GLOS1700
C     NO             NUMBER OF PARAMETERS USED AS OBSERVATIONS               GLOS1705
C     NOBS(NO)       ALPHANUMERIC NAMES OF OBSERVATIONS SAVED FOR OUTPUT GLOS1710
C     NOMAX          DIMENSION WHICH PLACES UPPER LIMIT ON NO                GLOS1715
C     NONE           ALPHANUMERIC CONSTANT 'NONE'                            GLOS1720
C     NOS            NUMBER OF OBSERVATIONS FOR CURRENT SUBSTANCE            GLOS1725
C     NOSMAX         DIMENSION WHICH PLACES UPPER LIMIT ON NOS               GLOS1730
C     NOSS(NOS)      ALPHANUMERIC NAMES OF OBSERVATIONS FOR ONE SUBSTANCE GLOS1735
C     NOUT(NV)       ALPHANUMERIC NAMES OF VARIABLES FOR OUTPUT              GLOS1740
C     NOV            NUMBER OF OBSERVATIONS WHICH ARE ALSO VARIABLES         GLOS1745
C     NP             OVERALL NUMBER OF PARAMETERS                            GLOS1750
C     NPC            NUMBER OF PARAMETERS COMMON TO SEVERAL SUBSTANCES       GLOS1755
C     NPCA           NPC+7                                                   GLOS1760
C     NPCMAX         DIMENSION WHICH PLACES UPPER LIMIT ON NPC               GLOS1765
C     NPMAX          DIMENSION WHICH PLACES UPPER LIMIT ON NP                GLOS1770
C     NPR            6*NRB                                                   GLOS1775
C     NPS            NUMBER OF PARAMETERS FOR CURRENT SUBSTANCE              GLOS1780
C     NPSMAX         DIMENSION WHICH PLACES UPPER LIMIT ON NPS               GLOS1785
C     NPX            NUMBER OF EXTRA PARAMETERS FOR ONE SUBSTANCE            GLOS1790
C     NPXMAX         DIMENSION WHICH PLACES UPPER LIMIT ON NPX               GLOS1795
C     NQ             NUMBER OF LIMITS FOR RECIPROCAL LATTICE SUMS            GLOS1800
C     NR             NUMBER OF LIMITS FOR DIRECT LATTICE SUMS                GLOS1805
C     NRB            NUMBER OF RIGID BODIES FOR ONE SUBSTANCE                GLOS1810
C     NRBMAX         DIMENSION WHICH PLACES UPPER LIMIT ON NRB               GLOS1815
C     NRP            MAXIMUM NUMBER OF CONTACTS TO BE PRINTED IS NRP/10      GLOS1820
C     NRPA           MAXIMUM NUMBER OF DISTANCES TO BE PRINTED               GLOS1825
C     NS             NUMBER OF SYMMETRY POSITIONS IN CELL                    GLOS1830
C     NSD            DATA SET REFERENCE NUMBER FOR FINAL SUMMARY OUTPUT      GLOS1835
C     NSF            NS/2 FOR CENTROSYMMETRY, NS FOR NON-CENTRO              GLOS1840
C     NSMAX          DIMENSION WHICH PLACES UPPER LIMIT ON NS                GLOS1845
C     NSO            DATA SET REFERENCE NUMBER FOR SUMMARY OUTPUT            GLOS1850
C     NSP            DATA SET REFERENCE NUMBER FOR STANDARD PRINTER OUTPUTGLOS1855
C     NSRB           NUMBER OF TERMS IN SAME RIGID BODY OR BONDED CONTACTSGLOS1860
C     NST            NUMBER OF 8-BYTE WORDS AVAILABLE FOR ARRAYS             GLOS1865
C     NSTG           NUMBER OF STAGES PER CYCLE IN MODE 3                    GLOS1870
C     NSU            NUMBER OF TIMES EACH SUMMARY IS TO BE PUT OUT           GLOS1875
C     NT(9)          COUNTERS FOR ENTRIES TO VARIOUS BRANCHES OF WCALC       GLOS1880
C     NV             NUMBER OF PARAMETERS TO BE VARIED                       GLOS1885
C     NVA            NUMBER OF VARIABLE LATTICE PARAMETERS                   GLOS1890
C     NVAP           NVA+1                                                   GLOS1895
C     NVC            NUMBER OF VARIABLE COMMON PARAMETERS                    GLOS1900
C     NVD            NUMBER OF DYNAMIC VARIABLES. NVD=NV-NVA                 GLOS1905
C     NVMAX          DIMENSION WHICH PLACES UPPER LIMIT ON NV                GLOS1910
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C     NVOS        NV*NOS                                                    GLOS1915
C     NVR         NUMBER OF VARIABLE RIGID BODY ROTATIONS, TRANSLATIONSGLOS1920
C     NVU         NUMBER OF EIGENVECTORS USED IN ADJUSTMENT                 GLOS1925
C     NVUS(9)     NVU SAVED FOR SUMMARY OUTPUT                              GLOS1930
C     NVV         NV*NV                                                     GLOS1935
C     NVX         NUMBER OF VARIABLE EXTRA PARAMETERS                       GLOS1940
C     NWORD(133)  NUMBER OF 8-BYTE WORDS ASSIGNED TO EACH ARRAY             GLOS1945
C     NXA         NUMBER OF EXTRA ATOMS                                     GLOS1950
C     P(NP)       OVERALL PARAMETER LIST                                    GLOS1955
C     PBASE(NP)   PARAMETERS AT START OF CYCLE OF MODE 3 SEARCH             GLOS1960
C     PC(NPC)     PARAMS COMMON TO SEVERAL SUBSTANCES. DEFINE BY CNSTRNGLOS1965
C     PCMN(NPC)   MINIMUM VALUES ALLOWED FOR COMMON PARAMETERS              GLOS1970
C     PCMX(NPC)   MAXIMUM VALUES ALLOWED FOR COMMON PARAMETERS              GLOS1975
C     PCSV(NPC)   COMMON PARAMETERS SAVED FROM PREVIOUS ENTRY TO WCALC      GLOS1980
C     PD(NV)      VECTOR OF PARAMETER CHANGES                               GLOS1985
C     PDJ         CALCULATED PARAMETER CHANGE BEFORE SCALING                GLOS1990
C     PDK         PARAMETER CHANGE SCALED AND CAMPED                        GLOS1995
C     PDLI        PARAMETER INCREMENT IN MAPPING MODE                       GLOS2000
C     PDLJ        PARAMETER INCREMENT IN MAPPING MODE                       GLOS2005
C     PDLK        PARAMETER INCREMENT IN MAPPING MODE                       GLOS2010
C     PI          3.14---                                                   GLOS2015
C     PICK        ((PI*CK*CK)**3)/12.0                                      GLOS2020
C     PICKZ       -((PI*CK)**3)*ZMC/6.0                                     GLOS2025
C     PICKZV      -(PI*CK)**3*ZMC/(6.0*VA)                                  GLOS2030
C     PIDKSQ      PI/CK**2                                                  GLOS2035
C     PINHZ       -PI**(9/2)/(3.0*ZMC)                                      GLOS2040
C     PINHZV      -PI**(9/2)/(3.0*VA*ZMC)                                   GLOS2045
C     PINI        INITIAL VALUE OF PARAMETER IN MAPPING MODE                GLOS2050
C     PINJ        INITIAL VALUE OF PARAMETER IN MAPPING MODE                GLOS2055
C     PINK        INITIAL VALUE OF PARAMETER IN MAPPING MODE                GLOS2060
C     PISAVE      PARAMETER  SAVED WHEN P(I) IS INCREMENTED                 GLOS2065
C     PJSAVE      PARAMETER SAVED WHEN P(J) IS INCREMENTED                  GLOS2070
C     PL(NKA)     VAN DER WAALS COEFFICIENT. KILOCAL AND ANGSTROM UNITSGLOS2075
C     PLJA        PL(JA)                                                    GLOS2080
C     PLMI        FINAL VALUE OF PARAMETER IN MAPPING MODE                  GLOS2085
C     PLMJ        FINAL VALUE OF PARAMETER IN MAPPING MODE                  GLOS2090
C     PLMK        FINAL VALUE OF PARAMETER IN MAPPING MODE                  GLOS2095
C     PMN(NP)     MINIMUM VALUES ALLOWED FOR PARAMETERS                     GLOS2100
C     PMX(NP)     MAXIMUM VALUES ALLOWED FOR PARAMETERS                     GLOS2105
C     PRK         OPTIMUM VALUE OF EWALD CONSTANT CK. FOR OUTPUT ONLY       GLOS2110
C     PRQ         OPTIMUM VALUE OF QLIM. FOR OUTPUT ONLY                    GLOS2115
C     PRR         OPTIMUM VALUE OF RLIM. FOR OUTPUT ONLY                    GLOS2120
C     PRT         PREDICTED TIME PER CYCLE FOR OPTIMUM SUMMATION            GLOS2125
C     PS(9,NV)    PARAMETERS SAVED FOR OUTPUT IN FINAL SUMMARY              GLOS2130
C     PSAVE       PARAMETER  SAVED WHEN P(I) IS INCREMENTED                 GLOS2135
C     PSV(NP)     PREVIOUS VALUES OF PARAMETERS SAVED                       GLOS2140
C     PSVI        ORIGINAL PARAMETER SAVED IN MAPPING MODE                  GLOS2145
C     PSVJ        ORIGINAL PARAMETER SAVED IN MAPPING MODE                  GLOS2150
C     PSVK        ORIGINAL PARAMETER SAVED IN MAPPING MODE                  GLOS2155
C     PX(NPX)     EXTRA PARAMETERS, ONE SUBSTANCE, DEFINED BY CNSTRN        GLOS2160
C     PXMN(NPX)   MINIMUM VALUES ALLOWED FOR EXTRA PARAMETERS               GLOS2165
C     PXMX(NPX)   MAXIMUM VALUES ALLOWED FOR EXTRA PARAMETERS               GLOS2170
C     PXSV(NPX)   EXTRA PARAMETERS SAVED FROM PREVIOUS ENTRY TO WCALC       GLOS2175
C     Q(NKA)      IONIC CHARGE IN PROTON UNITS                              GLOS2180
C     QH          LENGTH OF RECIPROCAL LATTICE VECTOR                       GLOS2185
C     QJA         Q(JA)                                                     GLOS2190
C     QLIM(NQ)    LIMITS OF SUCCESSIVE SHELLS IN RECIPROCAL SPACE           GLOS2195
C     QMAX        UPPER LIMIT ON SHELL IN RECIPROCAL SPACE                  GLOS2200
C     QQ          LENGTH SQUARED OF RECIPROCAL LATTICE VECTOR               GLOS2205
C     QQMAX       UPPER LIMIT ON SHELL IN RECIPROCAL SPACE, QMAX**2         GLOS2210
C     QQMIN       LOWER LIMIT ON SHELL IN RECIPROCAL SPACE                  GLOS2215
C     QQX         X TERM IN QQ                                              GLOS2220
C     QQY         X AND Y TERMS IN QQ                                       GLOS2225
C     R           INTERATOMIC DISTANCE                                      GLOS2230
C     RAD         PI/180                                                    GLOS2235
C     ROWS        SQRT(SDWS)                                                GLOS2240
C     ROWSS(9)    ROWS SAVED FOR SUMMARY OUTPUT                             GLOS2245
C     ROWST       SQRT(SDWST)                                               GLOS2250
C     REJECT      USER SUBROUTINE TO AVOID SPACE GROUP ABSENCES             GLOS2255
C     REP         REPULSION ENERGY TERM                                     GLOS2260
C     REPL        USER SUBROUTINE TO COMPUTE NONBONDED REPULSION TERM       GLOS2265
C     REPT(NGS)   REPULSION ENERGY TERM SAVED FOR OUTPUT                    GLOS2270
C     RLIM(NR)    LIMITS OF SUCCESSIVE SHELLS IN DIRECT SPACE               GLOS2275
C     RM(9)       MATRIX WHICH ROTATES RIGID BODY                           GLOS2280
C     RMAX        UPPER LIMIT ON SHELL IN DIRECT SPACE                      GLOS2285
C     RR          INTERATOMIC DISTANCE SQUARED                              GLOS2290
C     RRMAX       UPPER LIMIT ON SHELL IN DIRECT SPACE. RMAX**2             GLOS2295
C     RRMIN       LOWER LIMIT ON SHELL IN DIRECT SPACE                      GLOS2300
C     RSV(NGS)    REPULSION ENERGY TERM SAVED FOR NEXT ENTRY                GLOS2305
C     RT(NGS)     INTERATOMIC DISTANCE SAVED FOR OUTPUT                     GLOS2310
C     RYM         REPULSION ENERGY TERM INCLUDING MULTIPLICITY              GLOS2315
C     RTPIZ       FKCAL/(2.0*PI*ZMC)                                        GLOS2320
C     RTPIZV      332.17/(2.0*PI*VA*ZMC)                                    GLOS2325
C     S(NST)      OVERALL STORAGE TO BE APPORTIONED AMONG ARRAYS            GLOS2330
C     SA(6)       STANDARD ERRORS OF LATTICE PARAMETERS A                   GLOS2335
C     SAN(NV)     SCALE FACTORS WHICH MULTIPLY ROWS AND COLS OF AN          GLOS2340
C     SCFCG       SQRT(CF*CG)                                               GLOS2345
C     SDWS        DISCREPANCY FACTOR FOR ONE SUBSTANCE                      GLOS2350
C     SDWST       DISCREPANCY FACTOR SUMMED OVER ALL SUBSTANCES             GLOS2355
C     SEC(9)      TIME PER CYCLE SPENT IN EACH BRANCH OF WCALC, SECONDSGLOS2360
C     SETA        SUBROUTINE TO CONSTRAIN LATTICE SYMMETRY                  GLOS2365
C     SF          RECIPROCAL LATTICE SUM FOR COULOMB ENERGY                 GLOS2370
C     SFV         RECIPROCAL LATTICE SUM FOR VAN DER WAALS ENERGY           GLOS2375
C     SG          SUM OF MODIFIED COULOMB DIRECT LATTICE TERMS              GLOS2380
C     SGX         SUM OF MODIFIED COULOMB TERMS, KCAL/MOLE                  GLOS2385
C     SIGMA       SQRT(SDWSY/DGF)                                           GLOS2390
C     SIGWO       STANDARD ERROR OF OBSERVED ENERGY FOR ONE SUBSTANCE       GLOS2395
C     SINARG      SIN(ARG)                                                  GLOS2400
C     SLIM        LOWER LIMIT BELOW WHICH DGAN IS NOT SCALED TO UNITY       GLOS2405
C     SMC(NA*NS)  TOTAL NUMBER OF TIMES SYMMETRY PUTS ATOM IN THIS POS.GLOS2410
C     SMCMX       MAXIMUM VALUE OF SMC. USED TO DETERMINE ZMC               GLOS2415
C     SNL         VALUE OF SMALLEST INTERATOMIC DISTANCE FOUND              GLOS2420
C     SP(NP)      OVERALL LIST OF PARAMETER ERRORS USED FOR WEIGHTING       GLOS2425
C     SPL         SUM OVER UNIT CELL FOR VAN DER WAALS ENERGY               GLOS2430
C     SPLK        NEGATIVE SCALED UNIT CELL SUM FOR VAN DER WAALS           GLOS2435
C     SPP         SUM OVER UNIT CELL FOR VAN DER WAALS ENERGY               GLOS2440
C     SPPK        SUM OVER UNIT CELL FOR VAN DER WAALS ENERGY. SCALED       GLOS2445
C     SP0(NOS)    STANDARD ERRORS OF PARAMETERS USED AS OBSERVATIONS        GLOS2450
C     SQ          SUM OVER UNIT CELL FOR COULOMB ENERGY                     GLOS2455
C     SQALBT      SQRT(ALBT)                                                GLOS2460
C     SQK         NEGATIVE SCALED UNIT CELL SUM FOR COULOMB ENERGY          GLOS2465
C     SQTPOK      SQRT(PI)/CK                                               GLOS2470
C     SQTPI       SQRT(PI)                                                  GLOS2475
C     SQTPIK      SQRT(PI)*CK                                               GLOS2480
C     SRB         1 FOR CONTACT IN SAME RIGID BODY OR BONDED                GLOS2485
C     SRBT(NGS)   SRB SAVED FOR NEXT ENTRY                                  GLOS2490
C     SRR(NRB)    ERROR ASSIGNED TO OBSERVED RIGID BODY ORIENTATION         GLOS2495
C     STITLE(18)  ALPHANUMERIC TITLE FOR ONE SUBSTANCE                      GLOS2500
C     STR(NRB)    ERROR ASSIGNED TO OBSERVED RIGID BODY TRANSLATION         GLOS2505
C     SUMV        SUBROUTINE TO ADD TWO 3*1 VECTORS                         GLOS2510
C     SVDW        SUM OF MODIFIED VAN DER WAALS DIRECT LATTICE TERMS        GLOS2515
C     SX          SIN(SXR(J))                                               GLOS2520
C     SXR(NRB)    ROTATION OF EACH RIGID GROUP ABOUT X, RADIANS             GLOS2525
C     SY          SIN(SYR(J))                                               GLOS2530
C     SYM(12,NS)  COEFFICIENTS FROM EACH SYMMETRY CARD                      GLOS2535
C     SYR(NRB)    ROTATION OF EACH RIGID GROUP ABOUT Y, RADIANS             GLOS2540
C     SZ          SIN(SZR(J))                                               GLOS2545
C     SZR(NRB)    ROTATION OF EACH RIGID GROUP ABOUT Z, RADIANS             GLOS2550
C     TIMOUT      SUBROUTINE TO TO ANALYZE TIME IN BRANCHES OF WCALC        GLOS2555
C     TITLE(18)   OVERALL ALPHANUMERIC TITLE                                GLOS2560
C     TMI(9)      TEMPORARY STORAGE FOR 3*3 MATRIX                          GLOS2565
C     TMAT(NOS*NOS) OF (NV*NV), WHICHEVER IS LARGER. TEMPORARY MATRIX       GLOS2570
C     TOTALT      TOTAL TIME PER CYCLE IN WCALC, SECONDS                    GLOS2575
C     TPI         2.0*PI                                                    GLOS2580
C     TQ(NV)      AUXILIARY VECTOR USED BY EIGENVALUE ROUTINES              GLOS2585
C     TR(3,NRB)   TRANSLATIONS OF EACH RIGID BODY IN X,Y,Z. ANGSTROMS       GLOS2590
C     TRANS       SUBROUTINE TO TRANSPOSE 3*3 MATRIX                        GLOS2595
C     TRANSF      SUBROUTINE TO COMPLETE SOLUTION OF GEN EIGVAL PROBLEMGLOS2600
C     TRT(3)      VECTOR XYZR(IZJ)+CA*TR-CA*RM*ACZ*XYZ(IZJ)                 GLOS2605
C     TVT(3)      TEMPORARY STORAGE FOR VECTOR                              GLOS2610
C     UEXP        EXPONENTIAL FUNCTION WITH TEST TO AVOID UNDERFLOW         GLOS2615
C     UMAT(NOS*NOS) OR (NV*NV), WHICHEVER IS LARGER. TEMPORARY MATRIX       GLOS2620
C     US          INNER PRODUCT OF NORM VIB WITH SYM TRANSFORMED VIB        GLOS2625
C     UT(9)       ORTHOGONAL UNIT VECTOR TRIPLE                             GLOS2630
C     UU          SUM OF SQUARES OF COMPONENTS OF NORMAL VIBRATION          GLOS2635
C     UV(3)       VECTOR FROM ATOM IU TO ATOM IV                            GLOS2640
C     UW(3)       VECTOR FROM ATOM IU TO ATOM IW                            GLOS2645
C     UX(3)       UNIT VECTOR IN X DIRECTION                                GLOS2650
C     UY(3)       UNIT VECTOR IN Y DIRECTION                                GLOS2655
C     VA          DIRECT CELL VOLUME                                        GLOS2660
C     VALVEC      SUBROUTINE TO OBTAIN EIGVAL AND EIGVEC OF TRIDIAG MATGLOS2665
C     VBEST(NP)   PARAMETER CHANGES IN CYCLE OF MODE 3 SEARCH               GLOS2670
C     VBSQ        MAGNITUDE SQUARED OF VBEST IN MODE 3                      GLOS2675
C     VDW         VAN DER WAALS TERM                                        GLOS2680
C     VDWT(NGS)   VAN DER WAALS TERM SAVED FOR OUTPUT                       GLOS2685
C     VM(NV)      VECTOR OF LEAST-SQUARES NORMAL EQUATIONS FOR ONE SUBSGLOS2690
C     VN(NV)      VECTOR OF LEAST-SQUARES NORMAL EQUATIONS                  GLOS2695
C     VSF         PINHZV*SFV, SCALED RECIPROCAL VAN DER WAALS SUM           GLOS2700
C     VSV(NGS)    MODIFIED VAN DER WAALS TERM SAVED FOR NEXT ENTRY          GLOS2705
C     VTM         MODIFIED VAN DER WAALS TERM INCLUDING MULTIPLICITY        GLOS2710
C     W           CALCULATED ENERGY. KCAL/FORMULA WGT. ZAM OF EACH ATOMGLOS2715
C     WA          ENERGY CALCULATED FROM BOND ANGLE                         GLOS2720
C     WC          COULOMB ENERGY                                            GLOS2725
C     WCALC       SUBROUTINE TO MAKE ONE ENERGY CALCULATION                 GLOS2730
C     WCF         ENERGY CALCULATED FROM CONFORMATION ANGLE                 GLOS2735
C     WCNF        USER SUBROUTINE TO COMPUTE TORSION ANGLE ENERGY           GLOS2740
C     WCUR        CURRENT  VALUE OF  ENERGY DURING SEARCH FOR MINIMUM       GLOS2745
C     WD          ENERGY CALCULATED FROM BOND DISTANCE                      GLOS2750
C     WDYN        SUBROUTINE TO FREQUENCIES AND NORMAL MODES                GLOS2755
C     WGT         WEIGHT OF OBSERVED ENERGY                                 GLOS2760
C     WMAT(NOS*NOS)WEIGHT MATRIX FOR LEAST SQUARES                          GLOS2765
C     WN(NP)      ENERGY CALCULATED WITH P DECREMENTED BY DP                GLOS2770
C     WOBS        OBSERVED ENERGY. KCAL/FORMULA WGT                         GLOS2775
C     WOWC        OBSERVED ENERGY MINUS CALCULATED                          GLOS2780
C     WP(NP)      ENERGY CALCULATED WITH P INCREMENTED BY DP                GLOS2785
C     WPIJ        ENERGY CALCULATED WITH BOTH P(I) AND P(J) INCREMENTEDGLOS2790
C     WPRE        SUBROUTINE TO PREPARE FOR ENERGY CALCULATION              GLOS2795
C     WR          SUM OF REPULSION ENERGY TERMS                             GLOS2800
C     WRAG        SUBROUTINE TO CALCULATE WRAP-AROUND GAUSSIAN FUNCTIONGLOS2805
C     WS(9)       ENERGY SAVED FOR OUTPUT IN FINAL SUMMARY                  GLOS2810
C     WSV(NMAX)   WD, WA, OR WCF SAVED FOR LATER USE                        GLOS2815
C     WT          TOTAL ENERGY. KCAL/FORMULA WEIGHT                         GLOS2820
C     WTR         TRIAL VALUE OF ENERGY DURING SEARCH FOR MINIMUM           GLOS2825
C     WV          VAN DER WAALS ENERGY                                      GLOS2830
C     WX          CONFORMATION ENERGY COMPUTED BY GCWX OR CWX               GLOS2835
C     WXL         ENERGY CORRESPONDING TO XL IN STEEPEST DESCENTS           GLOS2840
C     WXN         ENERGY CORRESPONDING TO XN IN STEEPEST DESCENTS           GLOS2845
C     XC(NA*NS)   COORD OF ATOM IN UNIT CELL AFTER ROT AND TRANS            GLOS2850
C     XCSV        TRANSFORMED ATOM COORDS SAVED FROM PREVIOUS ENTRY         GLOS2855
C     XG          CURRENT STEP SIZE ALONG STEEPEST DESCENT VECTOR           GLOS2860
C     XGM         MINIMUM STEP SIZE ALONG STEEPEST DESCENT VECTOR           GLOS2865
C     XGRO        INITIAL VALUE OF STEP ALONG STEEPEST DESCENT VECTOR       GLOS2870
C     XL          PREVIOUS DISTANCE ALONG STEEPEST DESCENT VECTOR           GLOS2875
C     XM          SQRT(PI)*CK*R  -USED TO MODIFY TERMS IN EWALD SUM         GLOS2880
C     XN          NEW DISTANCE ALONG STEEPEST DESCENT VECTOR                GLOS2885
C     XXC         ATOM COORDINATE AFTER SYMMETRY TRANSFORMATION             GLOS2890
C     XXD         COORDINATE DIFFERENCE USED TO TEST FOR DUPLICATION        GLOS2895
C     XXM         PI*CK**2*R**2  -USED TO MODIFY TERMS IN EWALD SUM         GLOS2900
C     XYZ(3,NA)   FRACTIONAL COORDINATES OF ATOMS IN BASIC ASYM UNIT        GLOS2905
C     XYZA(3)     VIBRATIONAL DISPLACEMENT IN CRYSTAL COORD SYSTEM          GLOS2910
C     XYZAS(3)    XYZA AFTER SYMMETRY TRANSFORMATION                        GLOS2915
C     XYZC(3,NA)  ATOM COORDS IN BASIC CARTESIAN SYSTEM                     GLOS2920
C     XYZD(3,NA)  VECTOR DISPLACEMENT OF ATOM IN NORMAL COORDINATE          GLOS2925
C     XYZDS(3)    XYZD AFTER SYMMETRY TRANSFORMATION                        GLOS2930
C     XYZN(3,NA)  CART COORDS OF ATOMS AFTER A PARAM IS DECREMENTED         GLOS2935
C     XYZR(3,NA)  ATOM COORDS AFTER RIGID BODY TRANSLATION AND ROTATIONSGLOS2940
C     YC(NA*NS)   COORD OF ATOM IN UNIT CELL AFTER ROT AND TRANS            GLOS2945
C     YCSV        TRANSFORMED ATOM COORDS SAVED FROM PREVIOUS ENTRY         GLOS2950
C     YM          SQRT(PI)*DH/CK -USED TO MODIFY TERMS IN EWALD SUM         GLOS2955
C     YYC         ATOM COORDINATE AFTER SYMMETRY TRANSFORMATION             GLOS2960
C     YYD         COORDINATE DIFFERENCE USED TO TEST FOR DUPLICATION        GLOS2965
C     YYM         PI*DG/CK**2    -USED TO MODIFY TERMS IN EWALD SUM         GLOS2970
C     ZAM(NA)     NUMBER OF ATOMS OF EACH KIND IN FORMULA UNIT              GLOS2975
C     ZC(NA*NS)   COORD OF ATOM IN UNIT CELL AFTER ROT AND TRANS            GLOS2980
C     ZCSV        TRANSFORMED ATOM COORDS SAVED FROM PREVIOUS ENTRY         GLOS2985
C     ZMC         NUMBER OF FORMULA UNITS PER CELL                          GLOS2990
C     ZZC         ATOM COORDINATE AFTER SYMMETRY TRANSFORMATION             GLOS2995
C     ZZD         COORDINATE DIFFERENCE USED TO TEST FOR DUPLICATION        GLOS3000
      RETURN                                                                GLOS3005
      END                                                                   GLOS3010
```

9.3 Dummy System Subroutines

```
      FUNCTION ICLOCK(DUMMY)                                            ICLO   5
C     SUBSTITUTE ROUTINE. REMOVE IF LIBRARY ROUTINE IS AVAILABLE.       ICLO  10
C     OTHERWISE PROVIDE A ROUTINE TO SET ICLOCK IN UNITS OF 0.01 SEC    ICLO  15
C     OF CENTRAL PROCESSOR TIME.                                        ICLO  20
      ICLOCK=0                                                          ICLO  25
      RETURN                                                            ICLO  30
      END                                                               ICLO  35


      SUBROUTINE IDAY(NDATE)                                            IDAY   5
C     SUBSTITUTE ROUTINE. REMOVE IF LIBRARY ROUTINE IS AVAILABLE.       IDAY  10
C     OTHERWISE PROVIDE A ROUTINE TO SET NDATE AS THE ALPHANUMERIC DATE.IDAY  15
      REAL*8 NDATE,MDATE                                                IDAY  20
      DATA MDATE/'SEE IDAY'/                                            IDAY  25
      NDATE=MDATE                                                       IDAY  30
      RETURN                                                            IDAY  35
      END                                                               IDAY  40
```

9.4 User Routines for Test Problems

```
      SUBROUTINE CNSTRI (AR,BR,PC,PL,PX,Q                               CNST   5
     1,SXR,SYR,SZR,TR)                                                  CNST  10
      IMPLICIT REAL*8(A-H,O-Z)                                          CNST  15
      DIMENSION AR(1),BR(1),PC(1),PL(1),PX(1),Q(1)                      CNST  20
     1,SXR(1),SYR(1),SZR(1),TR(3,1)                                     CNST  25
C     /ITGR/ USED BY WMIN, WDYN, WPRE, WCALC, GCWX, IBYPAS, TIMOUT      CNST  30
      COMMON/ITGR/IBK,ICCAX,ICENT,ICMB,IGEM,ILSQ,IMOL,INK,IPLM,IPRC     CNST  35
     1,IPRT,IRBA,IREP,IRSC,ISB,ISW,IVDW,IWGT,IZAM,JC,KPW,KPWS,LT(9)     CNST  40
     2,MODE,NA,NAC,NAF,NBC,NCT,NKA,NOS,NP,NPC,NPR,NPS,NPX,NQ,ISETA      CNST  45
     3,NR,NRB,NRP,NS,NT(9),NV,NVA,NVC,NVD,NVR,NVUS(9),NVX               CNST  50
      RETURN                                                            CNST  55
C                                                                       CNST  60
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS     CNST  65
C                                                                       CNST  70
C     SET VARIABLES IN TERMS OF COMMON PARAMETERS AND EXTRA PARAMETERS  CNST  75
C     CNSTRN FOR TEST PROBLEMS                                          CNST  80
C                                                                       CNST  85
      ENTRY CNSTRN                                                      CNST  90
      GO TO(500,500,560,565),ISB                                        CNST  95
C     CNSTRN FOR ETHANE AND PROPANE                                     CNST 100
  500 AR(1)=PC(1)                                                       CNST 105
      AR(2)=PC(2)                                                       CNST 110
      BR(1)=PC(3)                                                       CNST 115
      BR(2)=PC(4)                                                       CNST 120
      PL(1)=PC(5)                                                       CNST 125
      PL(2)=PC(6)                                                       CNST 130
      GO TO 580                                                         CNST 135
C     CNSTRN FOR NACL                                                   CNST 140
  560 AR(1)=PC(1)                                                       CNST 145
      AR(2)=PC(2)                                                       CNST 150
      BR(1)=PC(3)                                                       CNST 155
      BR(2)=PC(4)                                                       CNST 160
      GO TO 580                                                         CNST 165
C     CNSTRN FOR BENZENE                                                CNST 170
  565 PL(1)=PC(1)                                                       CNST 175
      PL(2)=PC(2)                                                       CNST 180
      Q(1)=-PC(9)                                                       CNST 185
      Q(2)= PC(9)                                                       CNST 190
  580 CONTINUE                                                          CNST 195
      RETURN                                                            CNST 200
      END                                                               CNST 205


      SUBROUTINE REJECT(ISB,HX,HY,HZ,IREJ)                              REJE   5
C     AVOID CALCULATION OF SPACE-GROUP ABSENCES IN RECIPROCAL SUM       REJE  10
C     IREJ=0 ON ENTRY. SET IREJ=1 TO OMIT A SPACE-GROUP ABSENCE.        REJE  15
C     REJECT FOR TESY PROBLEMS                                          REJE  20
      GO TO(545,545,500,510),ISB                                        REJE  25
C     REJECT FOR NACL                                                   REJE  30
  500 IF(AMOD(HX+HY,2.0))540,505,540                                    REJE  35
  505 IF(AMOD(HY+HZ,2.0))540,545,540                                    REJE  40
C     REJECT FOR BENZENE. PBCA                                          REJE  45
  510 IF(HX)520,515,520                                                 REJE  50
  515 IF(AMOD(HY,2.0))540,520,540                                       REJE  55
  520 IF(HY)530,525,530                                                 REJE  60
  525 IF(AMOD(HZ,2.0))540,530,540                                       REJE  65
  530 IF(HZ)545,535,545                                                 REJE  70
  535 IF(AMOD(HX,2.0))540,545,540                                       REJE  75
  540 IREJ=1                                                            REJE  80
  545 CONTINUE                                                          REJE  85
      RETURN                                                            REJE  90
      END                                                               REJE  95


      FUNCTION REPLI(AR,BR,PC,PL,PX,Q)                                  REPL   5
      IMPLICIT REAL*8(A-H,O-Z)                                          REPL  10
      DIMENSION AR(1),BR(1),PC(1),PL(1),PX(1),Q(1)                      REPL  15
      RETURN                                                            REPL  20
C                                                                       REPL  25
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS     REPL  30
C                                                                       REPL  35
C     USER ROUTINE TO CALCULATE REPULSION ENERGY                        REPL  40
C     ENTERED ONLY IF IREP=2                                            REPL  45
C                                                                       REPL  50
      ENTRY REPL(ISB,IK,JK,R)                                           REPL  55
C     REPL FOR BENZENE. POTENTIAL OF WILLIAMS & STARR (1977)            REPL  60
      B=PC(IK+JK+1)                                                     REPL  65
      C=PC(IK+JK+4)                                                     REPL  70
      REPL=1000.0*B*DEXP(-C*R)                                          REPL  75
      RETURN                                                            REPL  80
      END                                                               REPL  85


      SUBROUTINE WCNFI (IKA,JAC,PC)                                     WCNF   5
      IMPLICIT REAL*8(A-H,O-Z)                                          WCNF  10
      DIMENSION IKA(1),JAC(1),PC(1)                                     WCNF  15
      RETURN                                                            WCNF  20
C                                                                       WCNF  25
C     THE ABOVE IS CALLED ONCE FROM MAIN TO SET LOCATIONS OF ARRAYS     WCNF  30
C                                                                       WCNF  35
C     USER ROUTINE TO CALCULATE ENERGY, WCF, OF TORSION ANGLE IN        WCNF  40
C     DEGREES, CNF, DEFINED BY ATOMS IA, JA, KA, AND LA. CALLED ONCE    WCNF  45
C     FOR EACH CONFORMATION ANGLE ABOUT BOND JA-KA IF THE CORRESPONDING WCNF  50
C     ITBRSLT.0                                                         WCNF  55
C                                                                       WCNF  60
      ENTRY WCNF(IA,JA,KA,LA,CNF,ITKJ,WCF)                              WCNF  65
C     WCNF FOR ETHANE AND PROPANE                                       WCNF  70
      WCF=0.5*PC(7)*(1.0+DCOS(3.0*0.0174532925*CNF))                    WCNF  75
      RETURN                                                            WCNF  80
      END                                                               WCNF  85
```

9.5 Input Data for Test Problems

```
         4         2         2         4         2         0         1         1DATA   5
         0        50       700        12        16         1         1         1DATA  10
TEST PROBLEM 1A. ADJUST REPULSION PARAMETERS FOR NACL                     DATA  15
   0  1  4  0  0  0  0  4  0   0.0001 0.000001         0     0.002        10DATA  20
      ARNA      ARCL      BRNA      BRCL                                   DATA  25
      1.18      2.43     0.079     0.238                                   DATA  30
     0.001     0.001    0.0001    0.0001                                   DATA  35
2222                                                                      DATA  40
1000                                                                      DATA  45
  3NACL                                                                   DATA  50
  2  2  4  2  0  0  0  2  0 10  1  0  1  0  0  0  0  0  1  2               DATA  55
     0.31  2  2                                                           DATA  60
     0.64      0.72                                                       DATA  65
      6.4       7.0                                                       DATA  70
    5.628     5.628     5.628         0         0         0               DATA  75
              0  1  0  0            0  0  1  0            0  0  0 1DATA  80
              0  1  0  0          0.5  0  1  0          0.5  0  0 1DATA  85
            0.5  1  0  0            0  0  1  0          0.5  0  0 1DATA  90
            0.5  1  0  0          0.5  0  1  0            0  0  0 1DATA  95
NA                1                                                       DATA 100
CL               -1                                                       DATA 105
NA        1                         0         0         0                 DATA 110
CL        2                       0.5       0.5       0.5                 DATA 115
  1  2                                                                    DATA 120
  1  0                                                                    DATA 125
  2  0                                                                    DATA 130
  0                0         0                                            DATA 135
100000000000                                                              DATA 140
000000000000                                                              DATA 145
                                                                          DATA 150
         4         2         2         4         2         0         1DATA 155
         0        50       700        12        16         1         1DATA 160
TEST PROBLEM 1B. MAP ENERGY OF NACL                                       DATA 165
 -1  0  4  0  0  0  0  4  1   0.0001 0.000001         0     0.002        10DATA 170
1000                                                                      DATA 175
  3NACL                                                                   DATA 180
  2  2  4  2  0  0  0  2  0 10  1  0  1  0  0  0  0  0  1  2               DATA 185
     0.31  2  2                                                           DATA 190
     0.64      0.72                                                       DATA 195
      6.4       7.0                                                       DATA 200
    5.628     5.628     5.628         0         0         0               DATA 205
              0  1  0  0            0  0  1  0            0  0  0 1DATA 210
              0  1  0  0          0.5  0  1  0          0.5  0  0 1DATA 215
            0.5  1  0  0            0  0  1  0          0.5  0  0 1DATA 220
            0.5  1  0  0          0.5  0  1  0            0  0  0 1DATA 225
NA                1                                                       DATA 230
CL               -1                                                       DATA 235
NA        1                         0         0         0                 DATA 240
CL        2                       0.5       0.5       0.5                 DATA 245
  1  2                                                                    DATA 250
  1  0                                                                    DATA 255
  2  0                                                                    DATA 260
  0                0         0                                            DATA 265
100000000000                                                              DATA 270
000000000000                                                              DATA 275
 -1                                                                       DATA 280
  0  1         0.80      0.05      1.20                                   DATA 285
  1  1          5.5       0.1       6.0                                   DATA 290
                                                                          DATA 295
                                                                          DATA 300
         9        13         2         8         1         0         6 80DATA 305
         0        50       700        12        21         6         6  6DATA 310
TEST PROBLEM 2A. MINIMIZE ENERGY BY NEWTON'S METHOD                       DATA 315
   1  2  9  0  0  0  0  4  0   0.0001 0.000001         0     0.002        10DATA 320
      PLC       PLH       BCC       BCH       BHH       CCC       CCH   CHH DATA 325
      QH                                                                  DATA 330
 24.02372  5.70218 87.80210 15.65620  2.79170  3.60000  3.67000  3.74000DATA 335
    0.153                                                                 DATA 340
     0.01      0.01      0.01      0.01      0.01      0.01      0.01  0.01DATA 345
    0.001                                                                 DATA 350
112222221                                                                 DATA 355
000000000                                                                 DATA 360
  4BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.   DATA 365
   7  2  8  2  0  0  0  1  0  8  1  1  2  0  6  2  0  0  0  0              DATA 370
     0.30  2  2                                                           DATA 375
     0.44      0.51                                                       DATA 380
     4.45      5.20                                                       DATA 385
     7.44      9.55     6.92         0         0         0               DATA 390
              .0  1  0  0          .0  0  1  0          .0  0  0 1DATA 395
              .0 -1  0  0          .0  0 -1  0          .0  0  0-1DATA 400
              .5  1  0  0          .5  0 -1  0          .0  0  0-1DATA 405
              .5 -1  0  0          .5  0  1  0          .0  0  0 1DATA 410
              .0 -1  0  0          .5  0  1  0          .5  0  0-1DATA 415
              .0  1  0  0          .5  0 -1  0          .5  0  0 1DATA 420
              .5 -1  0  0          .0  0 -1  0          .5  0  0 1DATA 425
              .5  1  0  0          .0  0  1  0          .5  0  0-1DATA 430
C                                                                         DATA 435
H                                                                         DATA 440
C1        1                   -0.0569    0.1387   -0.0054                DATA 445
C2        1                   -0.1335    0.0460    0.1264                DATA 450
C3        1                   -0.0774   -0.0925    0.1295                DATA 455
H1        2                   -0.09862   0.24040  -0.00936               DATA 460
H2        2                   -0.23115   0.07965   0.21886               DATA 465
H3        2                   -0.13445  -0.16068   0.22495               DATA 470
```

```
XTRA    0                       0         0         0                                    DATA 475
  1  1  1  1  1  1  1  1  1  1  1  1  1  1                                                 DATA 480
  7  0                                                                                   DATA 485
  1     2  4 10                                                                          DATA 490
  2     1  3  5                                                                          DATA 495
  3     2  5  8                                                                          DATA 500
  8     3  9 11                                                                          DATA 505
  9     8 10 12                                                                          DATA 510
 10     1  9 13                                                                          DATA 515
  0                 0         0                                                           DATA 520
111000111000                                                                             DATA 525
000000000000                                                                             DATA 530
                                                                                         DATA 535
        9        13         2         8         1         0         1                  1DATA 540
        0        50       700        12        21         6         6                  6DATA 545
TEST PROBLEM 2B. MINIMIZE ENERGY BY MODIFIED ROSENBROCK SEARCH                           DATA 550
  3  2  9  0  0  0  0  4  0    0.0001 0.000001         0     0.002                    10DATA 555
    PLC       PLH       BCC       BCH       BHH       CCC       CCH                   CHHDATA 560
    QH                                                                                   DATA 565
 24.02372  5.70218 87.80210 15.65620  2.79170  3.60000  3.67000  3.74000DATA 570
    0.153                                                                                DATA 575
    0.01      0.01      0.01      0.01      0.01      0.01      0.01                  0.01DATA 580
    0.001                                                                                DATA 585
112222221                                                                                DATA 590
000000000                                                                                DATA 595
  4BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.                  DATA 600
  7  2  8  2  0  0  0  1  0  8  1  1  2  0  0  2  0  0  0  0                              DATA 605
    0.29  2  2                                                                           DATA 610
    0.42      0.49                                                                       DATA 615
    4.55      5.43                                                                       DATA 620
    7.44      9.55      6.92         0         0         0                              DATA 625
              .0  1  0  0              .0  0  1  0              .0  0  0  1DATA 630
              .0 -1  0  0              .0  0 -1  0              .0  0  0 -1DATA 635
              .5  1  0  0              .5  0 -1  0              .0  0  0 -1DATA 640
              .5 -1  0  0              .5  0  1  0              .0  0  0  1DATA 645
              .0 -1  0  0              .5  0  1  0              .5  0  0 -1DATA 650
              .0  1  0  0              .5  0 -1  0              .5  0  0  1DATA 655
              .5 -1  0  0              .0  0 -1  0              .5  0  0  1DATA 660
              .5  1  0  0              .0  0  1  0              .5  0  0 -1DATA 665
C                                                                                        DATA 670
H                                                                                        DATA 675
C1        1                       -0.0569    0.1387   -0.0054                            DATA 680
C2        1                       -0.1335    0.0460    0.1264                            DATA 685
C3        1                       -0.0774   -0.0925    0.1295                            DATA 690
H1        2                       -0.09862   0.24049  -0.00936                           DATA 695
H2        2                       -0.23115   0.07965   0.21886                           DATA 700
H3        2                       -0.13445  -0.16068   0.22495                           DATA 705
XTRA    0                       0         0         0                                    DATA 710
  1  1  1  1  1  1  1  1  1  1  1  1  1  1                                                 DATA 715
  7  0                                                                                   DATA 720
  0                 0         0                                                           DATA 725
111000111000                                                                             DATA 730
000000000000                                                                             DATA 735
                                                                                         DATA 740
       17         8         2        12         8         0         3                 10DATA 745
       46         0        30        30        50        24        24                 24DATA 750
TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES DATA 755
  0  1 17  0  0  0  4  0      0.01 0.000001         0     0.002                    10DATA 760
    ARC       ARH       BRC       BRH       PLC       PLH       TBR                   DCC DATA 765
    KCC       DCH       KCH      ACCC      KCCC      ACCH      KCCH                  AHCHDATA 770
    KHCH                                                                                 DATA 775
    1.711     1.234     0.1407    0.1459    22.64     4.94  0.281667               1.400DATA 780
    4.268     1.000     6.351   102.00   0.01169   109.50   0.01673               110.00DATA 785
  0.01795                                                                                DATA 790
    0.001     0.001     0.0001    0.0001    0.01      0.01      0.001                 0.001DATA 795
    0.001     0.001     0.001     0.1     0.0001      0.1     0.0001                  0.1DATA 800
    0.0001                                                                               DATA 805
22221133333333333                                                                        DATA 810
000000101010001C                                                                         DATA 815
  1ETHANE. TOTALLY SYMMETRIC                                                             DATA 820
  2  2  6  2  1  1  0  2  0 10  0  1  1  1  2  0  2  0  1  0                              DATA 825
        0  1  1                                                                          DATA 830
        0                                                                                DATA 835
       10                                                                                DATA 840
        1         1         1         0         0        -0.5                            DATA 845
              0  1  0  0              0  0  0  0              0  0  0  1DATA 850
              0  0  0  0              0  1  0  0              0  0  0 1DATA 855
              0 -1  0  0              0 -1  0  0              0  0  0 -1DATA 860
              0 -1  0  0              0  0  0  0              0  0  0 -1DATA 865
              0  0  0  0              0 -1  0  0              0  0  0 -1DATA 870
              0  1  0  0              0  1  0  0              0  0  0 -1DATA 875
C                                                            12.0039                     DATA 880
H                                                             1.0081                     DATA 885
C         1                       0         0   0.76700                                 DATA 890
H         2                 1.02162         0   1.16110                                 DATA 895
  1  2                                                                                   DATA 900
  1  0                                                                                   DATA 905
  2  0                                                                                   DATA 910
  1     5  2  3  4     8 10 10 10    14 14 14 16 16 16    -1  0  0  0                   DATA 915
  5     1  6  7  8     8 10 10 10    14 14 14 16 16 16    -1  0  0  0                   DATA 920
                                                                                         DATA 925
000000001101                                                                             DATA 930
000000000000                                                                             DATA 935
  2PROPANE. TOTALLY SYMMETRIC                                                            DATA 940
  5  2  8  2  1  1  0  5  0 10  0  1  1  1  3  0  0  0  1  0                              DATA 945
        0  1  1                                                                          DATA 950
        0                                                                                DATA 955
       10                                                                                DATA 960
        1         1         1         0         0         0                              DATA 965
              0  1  0  0              0  0  1  0              0  0  0 1DATA 970
              0  1  0  0              0  0 -1  0              0  0  0 1DATA 975
              0 -1  0  0              0  0  1  0              0  0  0 1DATA 980
              0 -1  0  0              0  0 -1  0              0  0  0 1DATA 985
C                                                            12.0039                     DATA 990
H                                                             1.0081                     DATA 995
C1        1                       0         0         0                                 DATA1000
C2        1                 1.26808         0  -0.34891                                 DATA1005
H1        2                       0   0.87588   0.65883                                 DATA1010
H21       2                 2.16177         0  -0.22315                                 DATA1015
H22       2                 1.31300   0.88090  -1.69101                                 DATA1020
  1  2  3  4  5                                                                          DATA1025
  1  0                                                                                   DATA1030
  2  0                                                                                   DATA1035
  3  0                                                                                   DATA1040
  4  0                                                                                   DATA1045
  5  0                                                                                   DATA1050
  1     2  3  3  5     8  8 10 10    12 14 14 14 14 16    -1 -1  0  0                   DATA1055
  2     1  4  5  7     8 10 10 10    14 14 14 16 16 16    -1  0  0  0                   DATA1060
  8     1  9 10 11     8 10 10 10    14 14 14 16 16 16    -1  0  0  0                   DATA1065
                                                                                         DATA1070
000000001101011101111                                                                    DATA1075
000000000000000000000                                                                    DATA1080
                                                                                         DATA1085
       17         8         2        12         6         0         3                 10DATA1090
       46         0        30        30        50        24        24                 24DATA1095
TEST PROBLEM 3B. MINIMIZE ENERGY AND CALCULATE FREQUENCIES OF MOLECULES DATA1100
  4  1 17  0  0  0  0  4  1      0.01 0.000001         0     0.002                    10DATA1105
000000101010010                                                                          DATA1110
  1ETHANE. NO SYMMETRY RESTRICTIONS. PARALLEL CARTESIAN SYSTEMS.                         DATA1115
  2  2 12  1  1  1  0  8  0 10  0  1  1  1  2  6  0  0  1  0                              DATA1120
        0  1  1                                                                          DATA1125
        0                                                                                DATA1130
       10                                                                                DATA1135
        1         1         1         0         0        -0.5                            DATA1140
E             0  1  0  0              0  0  1  0              0  0  0 1DATA1145
C3            0  0 -1  0              0  1 -1  0              0  0  0 1DATA1150
C3            0 -1  1  0              0 -1  0  0              0  0  0 1DATA1155
C2            0 -1  1  0              0  0  1  0              0  0  0 -1DATA1160
C2            0  0 -1  0              0 -1  0  0              0  0  0 -1DATA1165
C2            0  1  0  0              0  1 -1  0              0  0  0 -1DATA1170
I             0 -1  0  0              0  0 -1  0              0  0  0 -1DATA1175
S6            0  0  1  0              0 -1  1  0              0  0  0 -1DATA1180
S6            0  1 -1  0              0  1  0  0              0  0  0 -1DATA1185
M             0  1 -1  0              0  0 -1  0              0  0  0 1DATA1190
M             0  0  1  0              0  1  0  0              0  0  0 1DATA1195
M             0 -1  0  0              0 -1  1  0              0  0  0 1DATA1200
C                                                            12.0039                     DATA1205
H                                                             1.0081                     DATA1210
C         1                       0         0   0.76700                                 DATA1215
H         2                 1.02162         0   1.16110                                 DATA1220
  1  2  3  4  5  6  7  8                                                                  DATA1225
  1  0                                                                                   DATA1230
  2  0                                                                                   DATA1235
  3  0                                                                                   DATA1240
  4  0                                                                                   DATA1245
  5  0                                                                                   DATA1250
  6  0                                                                                   DATA1255
  7  0                                                                                   DATA1260
  8  0                                                                                   DATA1265
  1     5  2  3  4     8 10 10 10    14 14 14 16 16 16    -1  0  0  0                   DATA1270
  5     1  6  7  8     8 10 10 10    14 14 14 16 16 16    -1  0  0  0                   DATA1275
                                                                                         DATA1280
000000111111111111111111111111                                                           DATA1285
000000000000000000000000000000                                                           DATA1290
                                                                                         DATA1295
```

10. TEST PROBLEM OUTPUT

The following output is provided so that it can be verified that the program works properly with the test data of Section 9.5 and the user routines of Section 9.4. In order to save space here we have set the print indicator IPRT (see Section 7.3) at values which cause some of the output to be omitted, and we have further truncated parts of the printout. In running the test problems, however, the user will probably wish to leave IPRT as zero to obtain the complete output.

10.1 Sodium Chloride, Mode 0 and Mode -1

```
DYNAMIC DIMENSIONS FOR WMIN

  NPCMAX   NAMAX   NKAMAX    NSMAX  NRBMAX  NPXMAX  NCTMAX  NBCMAX
       4       2       2        4       2       0       1       1

    MMAX  NFSMAX  NGSMAX   NPSMAX   NPMAX  NOSMAX   NOMAX   NVMAX
       0      50     700       12      16       1       1       1

                    1          2          3          4          5          6          7          8          9         10
ARRAY             ACZ        AKE         AM       AMASS         AN         AR         BR        BTR       CHAR       CMBT
DIMEN-          (   9      (   0      ( NVMAX    (   1      ( NVMAX    (   1      (   1      ( NVMAX    (   1      (   1
 SIONS          *NRBMAX)   *   0  )   * NVMAX)   *NKAMAX)   * NVMAX)   *NKAMAX)   *NKAMAX)   *NOSMAX)   * NSMAX)   *NGSMAX)
WORDS              18          0          1          2          1          2          2          1          4        700
BYTES/WORD          8          8          8          8          8          8          8          8          8          4
HEX ADDRESS    00000090   00000090   00000090   00000098   000000A8   000000B0   000000C0   00000000   00000008   000000F8

                   11         12         13         14         15         16         17         18         19         20
ARRAY             CSV         DP        DPC       DPX         DW       DWDQ        DXQ        DYC        DYQ        DZQ
DIMEN-          (   1      (   1      (   1      (   1      (   1      (   1      ( NVMAX    (   1      ( NVMAX    ( NVMAX
 SIONS          *NGSMAX)   * NPMAX)   *NPCMAX)   *NPXMAX)   * NPMAX)   * NVMAX)   * NAMAX)   * NOMAX)   * NAMAX)   * NAMAX)
WORDS             700         16          4          0         16          1          2          1          2          2
BYTES/WORD          8          8          8          8          8          8          8          8          8          8
HEX ADDRESS    000008E8   000021C8   00002248   00002268   00002268   000022E8   000022F0   00002300   00002308   00002318

                   21         22         23         24         25         26         27         28         29         30
ARRAY            EPS        ERR       EVAL       EVEC        FMC       FREQ        GMT        GXT        GYT        GZT
DIMEN-          (   1      (   1      (   1      ( NVMAX    ( NAMAX    (   1      (   1      (   1      (   1      (   1
 SIONS          * NPMAX)   * NVMAX)   * NVMAX)   * NVMAX)   * NSMAX)   * NVMAX)   *NGSMAX)   *NGSMAX)   *NGSMAX)   *NGSMAX)
WORDS              16          1          1          1          8          1        700        700        700        700
BYTES/WORD          8          8          8          8          4          8          8          4          4          4
HEX ADDRESS    00002328   000023A8   00002380   00002338   000023C0   000023E0   000023E8   000039C8   000044B8   00004FA8

                   31         32         33         34         35         36         37         38         39         40
ARRAY            HMT        HXT        HTY        HZT       IACT       IASV        IAT        IAZ        ICC        ICT
DIMEN-          (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   6      ( NAMAX    (   4
 SIONS          *NFSMAX)   *NFSMAX)   *NFSMAX)   *NFSMAX)   *NCTMAX)   *  MMAX)   *NGSMAX)   *NCTMAX)   * NSMAX)   *NCTMAX)
WORDS              50         50         50         50          2          0        700          6          8          4
BYTES/WORD          4          4          4          4          4          4          4          4          4          4
HEX ADDRESS    00005A98   00005B60   00005C28   00005CF0   00005DB8   00005DC0   00005DC0   00006BB0   000068C8   000068E8

                   41         42         43         44         45         46         47         48         49         50
ARRAY            IDZ        IKA       IOUT        IRB       IRBC       ISBP        ISC        ISV       ITBR         IU
DIMEN-          (   4      (   1      (   1      (   1      ( NAMAX    (   1      ( NAMAX    (   1      (   4      (   1
 SIONS          *NCTMAX)   * NAMAX)   * NVMAX)   * NAMAX)   * NSMAX)   * NPMAX)   * NSMAX)   *  MMAX)   *NCTMAX)   *NRBMAX)
WORDS               4          2          2          2          8         16          8          0          4          2
BYTES/WORD          4          4          4          4          4          4          4          4          4          4
HEX ADDRESS    000068F8   00006908   00006918   00006920   00006940   00006980   00006980   000069A0   000069A0   000069B0

                   51         52         53         54         55         56         57         58         59         60
ARRAY             IV         IW         IZ        JAC       JASV        JAT       JDTS       JOUT        JSV       KASV
DIMEN-          (   1      (   1      (   1      ( NAMAX    (   1      (   1      (   1      (   1      (   1      (   1
 SIONS          *NRBMAX)   *NRBMAX)   *NRBMAX)   * NSMAX)   *  MMAX)   *NGSMAX)   *NOSMAX)   * NOMAX)   *  MMAX)   *  MMAX)
WORDS               2          2          2          8          0        700          2          2          0          0
BYTES/WORD          4          4          4          4          4          4          4          4          4          4
HEX ADDRESS    00006988   000069C0   000069C8   00006900   000069F0   000069F0   000074E0   000074E8   000074F0   000074F0

                   61         62         63         64         65         66         67         68         69         70
ARRAY             KP        KPC        KPS         KQ        KQC        KQS       LASV       LBCI       LBCJ         LI
DIMEN-          (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   1
 SIONS          * NPMAX)   *NPCMAX)   *NPSMAX)   * NPMAX)   *NPCMAX)   *NPSMAX)   *  MMAX)   *NBCMAX)   *NBCMAX)   * NPMAX)
WORDS              16          4         12         16          4         12          0          2          2         16
BYTES/WORD          4          4          4          4          4          4          4          4          4          4
HEX ADDRESS    000074F0   00007530   00007540   00007570   000075B0   000075C0   000075F0   000075F0   000075F8   00007600

                   71         72         73         74         75         76         77         78         79         80
ARRAY             MJ       NAME       NAMK       NAMP      NAMPC      NAMPX       NAMS       NOBS       NOSS       NOUT
DIMEN-          (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   1
 SIONS          * NPMAX)   * NAMAX)   *NKAMAX)   * NPMAX)   *NPCMAX)   *NPXMAX)   * NSMAX)   * NOMAX)   *NOSMAX)   * NVMAX)
WORDS              16          2          2         16          4          0          4          2          2          2
BYTES/WORD          4          4          4          4          4          4          4          4          4          4
HEX ADDRESS    00007640   00007680   00007688   00007690   000076D0   000076E0   000076E0   000076F0   000076F8   00007700

                   81         82         83         84         85         86         87         88         89         90
ARRAY              P      PBASE         PC       PCMN       PCMX       PCSV         PD         PL        PMN        PMX
DIMEN-          (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   1
 SIONS          * NPMAX)   * NPMAX)   *NPCMAX)   *NPCMAX)   *NPCMAX)   *NPCMAX)   * NVMAX)   *NKAMAX)   * NPMAX)   * NPMAX)
WORDS              16         16          4          4          4          4          1          2         16         16
BYTES/WORD          8          8          8          8          8          8          8          8          8          8
HEX ADDRESS    00007708   00007788   00007808   00007828   00007848   00007868   00007888   00007890   000078A0   00007920

                   91         92         93         94         95         96         97         98         99        100
ARRAY             PS        PSV         PX       PXMN       PXMX       PXSV          Q       REPT        RSV         RT
DIMEN-          (   9      (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   1      (   1
 SIONS          * NVMAX)   * NPMAX)   *NPXMAX)   *NPXMAX)   *NPXMAX)   *NPXMAX)   *NKAMAX)   *NGSMAX)   *NGSMAX)   *NGSMAX)
WORDS               9         16          0          0          0          0          2        700        700        700
BYTES/WORD          8          8          8          8          8          8          8          4          8          4
HEX ADDRESS    000079A0   000079E8   00007A68   00007A68   00007A68   00007A68   00007A68   00007A78   00008568   00009548

                  101        102        103        104        105        106        107        108        109        110
ARRAY            SAN        SMC         SP        SPW       SRBT        SSR        STR        SXR        SYM        SYR
DIMEN-          (   1      ( NAMAX    (   1      (   1      (   1      (   1      (   1      (   1      (  12      (   1
 SIONS          * NVMAX)   * NSMAX)   * NPMAX)   *NOSMAX)   *NGSMAX)   *NRBMAX)   *NRBMAX)   *NRBMAX)   * NSMAX)   *NRBMAX)
WORDS               1          8         16          1        700          2          2          2         48          2
BYTES/WORD          8          4          8          8          4          8          8          8          8          8
HEX ADDRESS    0000A638   0000A640   0000A660   0000A6E0   0000A6E8   0000B1D8   0000B1E8   0000B1F8   0000B208   00009388
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                    111        112        113        114        115        116        117        118        119        120
ARRAY               SZR       TMAT         TQ         YR       UMAT       VBEST       VDWT         VM         VN        VSV
DIMEN-            (   1    (NOSMAX    (   1    (   3    (NOSMAX    (   1    (   1    (   1    (   1    (   1
 SIONS            *NRBMAX)  *NOSMAX)  * NVMAX)  *NRBMAX)  *NOSMAX)  * NPMAX)  *NGSMAX)  * NVMAX)  * NVMAX)  *NGSMAX)
WORDS                   2          1          1          6          1         16        700          1          1        700
BYTES/WORD              8          8          8          8          8          8          4          8          8          8
HEX ADDRESS      0000B398   0000B3A8   0000B3B0   0000B3B8   0000B3E8   0000B3F0   00008470   0000BF60   0000BF68   0000BF70

                    121        122        123        124        125        126        127        128        129        130
ARRAY              WMAT         WN         WP        WSV         XC        XYZ       XYZC       XYZD       XYZN       XYZR
DIMEN-            (NOSMAX    (   1    (   1    (   1    (NAMAX    (   3    (   3    (   3    (   3    (   3
 SIONS            *NOSMAX)  * NPMAX)  * NPMAX)  *  MMAX)  * NSMAX)  * NAMAX)  * NAMAX)  * NAMAX)  * NAMAX)  * NAMAX)
WORDS                   1         16         16          0          8          6          6          6          6          6
BYTES/WORD              8          8          8          8          8          8          8          8          8          8
HEX ADDRESS      0000D550   0000D558   0000D5D8   0000D658   0000D658   0000D698   0000D6C8   0000D6F8   0000D728   0000D758

                    131        132        133
ARRAY                YC        ZAM         ZC
DIMEN-            ( NAMAX    (   1    ( NAMAX    (
 SIONS            * NSMAX)  * NAMAX)  * NSMAX)  *
WORDS                   8          2          8
BYTES/WORD              8          8          8
HEX ADDRESS      0000D788   0000D7C8   0000D7D8
```

6915 8-BYTE STORAGE LOCATIONS HAVE BEEN REQUESTED. THE PROGRAM IS DIMENSIONED FOR 12000 COMMON/S/ AND NST MAY BE DECREASED BY 5085 WORDS. THIS WILL REDUCE THE REGION USED BY 39K BYTES.

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TEST PROBLEM 1A. ADJUST REPULSION PARAMETERS FOR NACL                                   01-06-81
  MODE    NC   NPC  ILSQ  IWGT  IPLM  IPRT  NSTG  IBPC        ARE       SLIM       CMPR       XDRO       EPSC
    0     1     4     0     0     0     2     4     0   0.100D-03  0.100D-05   0.0       0.200D-02  0.100D 02
 NAMPC(I)
    ARNA      ARCL      BRNA      BRCL

   PC(I)
 1.18000   2.43000   0.07900   0.23800

  DPC(I)
 0.00100   0.00100   0.00010   0.00010

  KPC(I)
     2         2         2         2
```

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TEST PROBLEM 1A. ADJUST REPULSION PARAMETERS FOR NACL                                   01-06-81
NACL

  ISB
   3

   NA   NKA    NS ICENT HXNEG HYNEG HZNEG   NRB   NPX   NRP  ICMB  IVDW  IREP  IMOL   NCT  IRSC  IZAM  IGEM  IRBA ISETA
    2    2     4     2   0.0   0.0   0.0     2     0    10     1     0     1     0     0     0     0     0     1     2

     CK    NQ    NR
 0.31000    2     2

 QLIM(I)
 0.64000  0.72000

 RLIM(I)
 6.40000  7.00000

    A(I)
 5.62800  5.62800  5.62800  0.0       0.0       0.0

NAMS          TRANSFORMED X                          TRANSFORMED Y                          TRANSFORMED Z

          0.0      1.0*X  0.0*Y  0.0*Z       0.0      0.0*X  1.0*Y  0.0*Z       0.0      0.0*X  0.0*Y  1.0*Z
          0.0      1.0*X  0.0*Y  0.0*Z       0.5000   0.0*X  1.0*Y  0.0*Z       0.5000   0.0*X  0.0*Y  1.0*Z
          0.5000   1.0*X  0.0*Y  0.0*Z       0.0      0.0*X  1.0*Y  0.0*Z       0.5000   0.0*X  0.0*Y  1.0*Z
          0.5000   1.0*X  0.0*Y  0.0*Z       0.5000   0.0*X  1.0*Y  0.0*Z       0.0      0.0*X  0.0*Y  1.0*Z

 K  NAMK          Q        PL        AR        BR     AMASS
 1  NA       1.00000  0.0       0.0       0.0       0.0
 2  CL      -1.00000  0.0       0.0       0.0       0.0

 J  NAME    IKA    IRB          X         Y         Z
 1  NA       1      1       0.0       0.0       0.0
 2  CL       2      2       0.50000   0.50000   0.50000

 I  NAME    ISC    JAC    SMC    FMC   IRBC       XC        YC        ZC
 1  NA       1      1     1.     1.0      1   0.0       0.0       0.0
 2  CL       1      2     1.     1.0      2   0.50000   0.50000   0.50000
 3  NA       2      1     1.     1.0      3   0.0       0.50000   0.50000
 4  CL       2      2     1.     1.0      4   0.50000   1.00000   1.00000
 5  NA       3      1     1.     1.0      5   0.50000   0.0       0.50000
 6  CL       3      2     1.     1.0      6   1.00000   0.50000   1.00000
 7  NA       4      1     1.     1.0      7   0.50000   0.50000   0.0
 8  CL       4      2     1.     1.0      8   1.00000   1.00000   0.50000
ABOVE ATOMS USED TO COMPUTE STRUCTURE FACTORS

  ZMC
  4.0

 I  NAME(I)   ZAM(I)
 1    NA        1.0
 2    CL        1.0

 J  IZ(J)  IU(J)  IV(J)  IW(J)   SSR(J)   STR(J)   SXR(J)   SYR(J)   SZR(J)   TR(1,J)  TR(2,J)  TR(3,J)
 1     1      0      0      0    0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 2     2      0      0      0    0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0

 KPWS   KPW     WOBS     SIGWO
    0     0     0.0      0.0
```

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TEST PROBLEM 1A. ADJUST REPULSION PARAMETERS FOR NACL                                   01-06-81
 I  NAMP(I)       P(I)       DP(I)      PMN(I)     PMX(I)   KP(I)   KQ(I)   DKT(KQ)    SP(I)   ISBP(I)
 1     ARNA    1.180000   0.001000   0.0        0.0        0       1     1.000     0.0        0
 2     ARCL    2.430000   0.001000   0.0        0.0        0       0     0.0       0.0        0
 3     BRNA    0.079000   0.000100   0.0        0.0        0       0     0.0       0.0        0
 4     BRCL    0.238000   0.000100   0.0        0.0        0       0     0.0       0.0        0
 5     A       5.628000   0.000010   4.628000   6.628000   1       0     0.0       0.0        3
 6     B       5.628000   0.000010   4.628000   6.628000   0       0     0.0       0.0        3
 7     C       5.628000   0.000010   4.628000   6.628000   0       0     0.0       0.0        3
```

8	COSA	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	3
9	COSB	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	3
10	COSG	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	3
11	TX	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	3
12	TY	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	3
13	TZ	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	3
14	TX	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	3
15	TY	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	3
16	TZ	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	3

ND	NV	NOV	LS	IWT
1	1	0	1	0

TEST PROBLEM 1A. ADJUST REPULSION PARAMETERS FOR NACL 01-06-81
NACL

CYCLE 1

CSF	VSF	QMAX	NF
18.126419	0.0	0.640000	11
18.126419	0.0	0.720000	14

SQK	SPLK	SPPK
-205.945352	0.0	0.0

SCK	SVDW	WR	RMAX	NG	NSRB
-18.467021	0.0	41.917623	6.400000	74	0
-18.466922	0.0	41.997429	7.000000	122	0

GX	GY	GZ	I	J	GM	R	NAMES		CMB	VDW	REP	SRB
-1	-1	-1	1	4	1.00000	2.81400	NA	CL	-118.042	0.0	3.905	0.0
-1	-1	-1	1	6	1.00000	2.81400	NA	CL	-118.042	0.0	3.905	0.0
-1	-1	-1	1	8	1.00000	2.81400	NA	CL	-118.042	0.0	3.905	0.0
-1	-1	0	1	8	1.00000	2.81400	NA	CL	-118.042	0.0	3.905	0.0
-1	0	-1	1	6	1.00000	2.81400	NA	CL	-118.042	0.0	3.905	0.0
0	-1	-1	1	4	1.00000	2.81400	NA	CL	-118.042	0.0	3.905	0.0
-1	-1	0	1	7	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
-1	-1	0	2	8	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
-1	0	-1	1	5	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
-1	0	-1	2	6	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
-1	0	0	1	5	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
-1	0	0	1	7	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
-1	0	0	2	6	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
-1	0	0	2	8	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	-1	-1	1	3	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	-1	-1	2	4	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	-1	0	1	3	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	-1	0	1	7	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	-1	0	2	4	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	-1	0	2	8	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	0	-1	1	3	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	0	-1	1	5	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	0	-1	2	4	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	0	-1	2	6	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	0	0	1	3	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	0	0	1	5	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	0	0	1	7	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	0	0	2	4	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	0	0	2	6	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	0	0	2	8	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
-1	-1	-1	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.006	0.0
-1	-1	0	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.006	0.0
-1	0	-1	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.006	0.0
-1	0	0	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.006	0.0
0	-1	-1	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.006	0.0
0	-1	0	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.006	0.0
0	0	-1	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.006	0.0
0	0	0	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.006	0.0
-1	0	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
-1	0	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	-1	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	-1	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	0	-1	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	0	-1	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	0	1	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	0	1	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	1	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	1	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
1	0	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
1	0	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
-2	-1	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-2	-1	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-2	-1	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-2	0	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-2	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-2	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-2	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	-2	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	-2	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	0	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	0	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	-2	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	0	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-2	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	-2	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	0	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	0	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	0	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	-1	1	3	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	-1	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	-1	1	7	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	-1	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	-1	2	6	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	-1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	0	1	3	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	0	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	0	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	0	2	6	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	1	1	7	0.50000	6.89285	NA	NA	48.190	0.0	0.000	0.0
-1	-1	1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	-1	1	3	0.50000	6.89285	NA	NA	48.190	0.0	0.000	0.0
-1	0	-1	1	7	0.50000	6.89285	NA	NA	48.190	0.0	0.000	0.0
-1	0	-1	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	-1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	0	1	3	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	0	0	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	1	1	7	0.50000	6.89285	NA	NA	48.190	0.0	0.000	0.0
-1	0	1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	1	-1	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	1	-1	2	6	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	1	0	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	1	0	2	6	0.50000	6.89285	CL	CL	48.190	0.0	0.007	0.0
0	-1	-1	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
0	-1	-1	1	7	0.50000	6.89285	NA	NA	48.190	0.0	0.000	0.0

```
        WC          WV          WR          WX          WT
  -206.286       0.0       41.997       0.0     -164.288

TEST PROBLEM 1A. ADJUST REPULSION PARAMETERS FOR NACL                                  01-06-81
NACL

        WOBS        WCALC BEFORE CYCLE  1
       0.0       -164.2884

DERIVATIVES BEFORE CYCLE  1
                                DDW/DP(I)DP(J) FOR I=
  J  NAMP(J)  DYC(J)        1   ARNA
  5  A        28.2083   -117.1807

            RDWS                SDWS
   0.2820830 02    0.7957060 03

NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGY CALCULATION FOR THIS CYCLE
                      NT        SEC       AVT
INITIAL                5       0.01     0.0020
COORDINATES            4       0.0      0.0
SLOW RECIP             1       0.0      0.0
FAST RECIP             3       0.01     0.0033
UNIT CELL              4       0.0      0.0
SLOW DIRECT            1       0.10     0.1000
FAST DIRECT            4       0.05     0.0125
SLOW CONFIG            1       0.0      0.0
FAST CONFIG            3       0.0      0.0

TOTAL TIME (SEC)               0.17

SUMMATION LIMITS FOR MINIMUM TIME
   DEL IS PROPORTIONAL TO RELATIVE ERROR OF RESULT
   PRQ IS RECOMMENDED QLIM
   PRR IS RECOMMENDED RLIM
   PRK IS RECOMMENDED VALUE OF CK
   PRT IS PREDICTED TOTAL TIME PER CYCLE FOR RECIPROCAL AND DIRECT SUMS

   DEL        PRQ        PRR        PRK        PRT
1.0E-2    0.55994    2.20738    0.46662       0.01
1.0E-3    0.70396    2.77515    0.47565       0.02
1.0E-4    0.82261    3.24286    0.48106       0.03
1.0E-5    0.92605    3.65066    0.48484       0.04
1.0E-6    1.01937    4.01855    0.48774       0.06
1.0E-7    1.11007    4.37611    0.48902       0.07


TEST PROBLEM 1A. ADJUST REPULSION PARAMETERS FOR NACL                                  01-06-81
CYCLE  1

            RDWST               SDWST               SIGMA
   0.2820830 02    0.7957080 03    0.2820830 02

                   SAN(I)
                    1   ARNA
                   0.008534

                  EVEC(I,J)
  J     EVAL(J)     1   ARNA
  1   0.1000 01    1.000000

                  SAN(I)*EVEC(I,J)
  J     EVAL(J)     1   ARNA
  1   0.1000 01    0.008534

                          WMAT*BMAT*SAN*EVEC
  J  NAMP(J)  DYC(J)          1
  5  A        28.2083     -1.0000

PARAMETERS AFTER CYCLE  1
  I      NAMP       OLD P      CHANGE       NEW P        ERR
  1      ARNA    1.180000   -0.240725    0.939275    0.240725


TEST PROBLEM 1A. ADJUST REPULSION PARAMETERS FOR NACL                                  01-06-81
NACL

CYCLE  2

            CSF                 VSF                 QMAX                NF
        18.126419           0.0                 0.640000            11
        18.126419           0.0                 0.720000            14

            SQK                 SPLK                SPPK
     -205.945352            0.0                 0.0

            SGK                 SVDW                WR                  RMAX                NG                NSRB
      -18.467021            0.0                 29.426764           6.400000            74                0
      -18.466922            0.0                 29.506570           7.000000            122               0

GX GY GZ  I  J        GM          R    NAMES        CMB        VDW        REP        SRB
-1 -1 -1  1  4   1.00000    2.81400   NA   CL   -118.042        0.0      1.827        0.0
-1 -1 -1  1  6   1.00000    2.81400   NA   CL   -118.042        0.0      1.827        0.0
-1 -1 -1  1  8   1.00000    2.81400   NA   CL   -118.042        0.0      1.827        0.0
-1 -1  0  1  8   1.00000    2.81400   NA   CL   -118.042        0.0      1.827        0.0
-1  0 -1  1  6   1.00000    2.81400   NA   CL   -118.042        0.0      1.827        0.0
 0 -1 -1  1  4   1.00000    2.81400   NA   CL   -118.042        0.0      1.827        0.0
-1 -1  0  1  7   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
-1 -1  0  2  8   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
-1  0 -1  1  5   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
-1  0 -1  2  6   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
-1  0  0  1  5   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
-1  0  0  1  7   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
-1  0  0  2  6   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
-1  0  0  2  8   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
 0 -1 -1  1  3   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
 0 -1 -1  2  4   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
 0 -1  0  1  3   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
 0 -1  0  1  7   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
 0 -1  0  2  4   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
 0 -1  0  2  8   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
 0  0 -1  1  3   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
 0  0 -1  1  5   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
 0  0 -1  2  4   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
 0  0 -1  2  6   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
 0  0  0  1  3   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
 0  0  0  1  5   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
 0  0  0  1  7   0.50000    3.97960   NA   NA     83.468        0.0      0.000        0.0
 0  0  0  2  4   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
 0  0  0  2  6   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
 0  0  0  2  8   0.50000    3.97960   CL   CL     83.468        0.0      3.026        0.0
-1 -1 -1  1  2   1.00000    4.87399   NA   CL    -68.152        0.0      0.003        0.0
-1 -1  0  1  2   1.00000    4.87399   NA   CL    -68.152        0.0      0.003        0.0
-1  0 -1  1  2   1.00000    4.87399   NA   CL    -68.152        0.0      0.003        0.0
```

-1	0	0	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
0	-1	-1	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
0	-1	0	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
0	0	-1	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
0	0	0	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
-1	0	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
-1	0	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	-1	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	-1	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	0	-1	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	0	-1	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	0	1	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	0	1	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	1	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	1	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
1	0	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
1	0	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
-2	-1	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-2	-1	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-2	-1	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-2	0	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-2	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-2	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-2	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	-2	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	-2	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	0	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	0	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	-2	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	0	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-2	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	-2	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	0	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	0	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	0	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	-1	1	3	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	-1	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	-1	1	7	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	-1	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	-1	2	6	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	-1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	0	1	3	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	0	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	0	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	0	2	6	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	1	1	7	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	-1	1	3	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	0	-1	1	7	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	0	-1	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	-1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	0	1	3	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	0	0	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	1	1	7	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	0	1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	1	-1	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	1	-1	2	6	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	1	0	1	5	0.50000	6.89285	NA	NA	48.190	0.0	0.000	0.0
-1	1	0	2	6	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
0	-1	-1	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
0	-1	-1	1	7	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0

WC	WV	WR	WX	WT
-206.286	0.0	29.507	0.0	-176.779

TEST PROBLEM 1A. ADJUST REPULSION PARAMETERS FOR NACL 01-06-81
NACL

```
      WDBS        WCMLC BEFORE CYCLE  2
    0.0       -176.7793

DERIVATIVES BEFORE CYCLE  2
  J  NAMP(J)   DYC(J)
  5  A         8.4760

NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGY CALCULATION FOR THIS CYCLE
                    NT       SEC       AVT
INITIAL              3       0.0       0.0
COORDINATES          3       0.0       0.0
SLOW RECIP           1       0.01      0.0100
FAST RECIP           2       0.01      0.0050
UNIT CELL            3       0.0       0.0
SLOW DIRECT          1       0.10      0.1000
FAST DIRECT          2       0.03      0.0150
SLOW CONFIG          1       0.0       0.0
FAST CONFIG          2       0.0       0.0

TOTAL TIME (SEC)        0.15

SUMMATION LIMITS FOR MINIMUM TIME
   DEL  IS PROPORTIONAL TO RELATIVE ERROR OF RESULT
   PRQ  IS RECOMMENDED QLIM
   PRR  IS RECOMMENDED RLIM
   PRK  IS RECOMMENDED VALUE OF CK
   PRT  IS PREDICTED TOTAL TIME PER CYCLE FOR RECIPROCAL AND DIRECT SUMS

   DEL        PRQ        PRR        PRK        PRT
1.0E-2   0.48709    2.53751    0.40531    0.01
1.0E-3   0.61238    3.19018    0.41377    0.02
1.0E-4   0.71559    3.72785    0.41847    0.04
1.0E-5   0.80557    4.19664    0.42177    0.06
1.0E-6   0.88675    4.61954    0.42428    0.07
1.0E-7   0.96565    5.03058    0.42540    0.10

  J  NAME    IKA    IRB          X          Y          Z
  1  NA       1      1       0.0        0.0        0.0
  2  CL       2      2       0.50000    0.50000    0.50000


*****************************************************************

TEST PROBLEM 1A. ADJUST REPULSION PARAMETERS FOR NACL                    01-06-81

  MODE     NC    NPC   ILSQ   IWGT   IPLM   IPRT   NSTG   IBPC          ARE          SLIM         CMPR         XORD         EPSC
    0       1      4      0      0      0      2      4      0    0.100D-03    0.100D-05    0.0          0.200D-02    0.100D 02

     ARNA       ARCL       BRNA       BRCL
  0.93928    2.43000    0.07900    0.23800

    NO     NV    NOV     LS    IWT
     1      1      0      1      0

                    PARAMETERS AFTER EACH CYCLE
  J  NAMP    DKT      INITIAL        1
  1  ARNA   1.000    1.180000    0.939275

             NVU                        1

             RDWS 0.2821D 02

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DYNAMIC DIMENSIONS FOR WMIN

  NPCMAX    NAMAX  NKAMAX    NSMAX  NRBMAX  NPKMAX  NCTMAX  NBCMAX
       4        2       2        4       2       0       1       1

    MMAX  NFSMAX  NGSMAX  NPSMAX   NPMAX  NOSMAX   NDMAX   NVMAX
       0     30     700     12      16       1       1       1

                     1       2       3       4       5       6       7       8       9      10
ARRAY              ACZ     AKE      AM    AMASS      AN      AR      BR     BTR    CHAR     CMBT
DIMEN-           (  9    (  0    ( NVMAX  (  1    ( NVMAX  (  1    (  1    ( NVMAX  (  1    (  1
 SIONS           *NRBMAX)  *  0  )  * NVMAX)  *NKAMAX)  * NVMAX)  *NKAMAX)  *NKAMAX)  *NDSMAX)  * NSMAX)  *NGSMAX)
WORDS                18       0       1       2       1       2       2       1       4     700
BYTES/WORD            8       8       8       8       8       8       8       8       8       4
HEX ADDRESS    00000000  00000090  00000090  00000098  000000A8  00000B30  000000C0  00000030  000000D8  000000F8

                    11      12      13      14      15      16      17      18      19
ARRAY              CSV      DP     DPC     DPX      DW    DWDQ     DXQ     DYC
DIMEN-           (  1    (  1    (  1    (  1    (  1    (  1    ( NVMAX  (  1
 SIONS           *NGSMAX)  * NPMAX)  *NPCMAX)  *NPXMAX)  * NPMAX)  * NVMAX)  * NAMAX)  * NDMA
WORDS               700      16       4       0      16       1       2
BYTES/WORD            8       8       8       8       8       8       8
HEX ADDRESS    00000B68  000021C8  00002248  00002268  00002268  000022E8  0000

                    21      22      23      24      25                                      8
ARRAY              EPS     ERR    EVAL    EVEC     FMC                                  00008388
DIMEN-           (  1    (  1    (  1    ( NVMAX  ( NAMA                                 119     120
 SIONS           * NPMAX)  * NVMAX)  * NVMAX)  * NVMAX)  *                                 VN      VSV
WORDS                16       1       1       1                                        (  1    (  1
BYTES/WORD            8       8       8                                                * NVMAX)  *NGSMAX)
HEX ADDRESS    00002328  000023A8  00002380                                      700       1     700
                                                                                    4       8       8
                    31      32                                                  0000  00008470  00008F60  00008F68  00008F70
ARRAY              HMT     HXT
DIMEN-           (  1
 SIONS           *NFSMAX
WORDS                                                                     XC      126     127     128     129     130
BYTES/WORD                                                          ( NAMAX   (  3    (  3    (  3    (  3    (  3
HEX ADDRESS                                                   NMAX)  * NSMAX)  * NAMAX)  * NAMAX)  * NAMAX)  * NAMAX)  * NAMAX)
                                                                 0       8       6       6       6       6       6
                                                                 8       8       8       8       8       8       8
                                                          00000D08  0000D658  0000D658  00000698  0000D6C8  0000D6F8  0000D728  0000D758

                                          132     133
                                          ZAM      ZC
                                       NMAX   (  1    ( NAMAX   (
                                    * NSMAX)  * NAMAX)  * NSMAX)  *
                                          8       2       8
                                          8       8       8
                                 ...S/WORD
                                 HEX ADDRESS  0000D788  0000D7C8  0000D708

    6915 8-BYTE STORAGE LOCATIONS HAVE BEEN REQUESTED. THE PROGRAM IS DIMENSIONED FOR   12000
 COMMON/S/ AND NST MAY BE DECREASED BY  5095 WORDS. THIS WILL REDUCE THE REGION USED BY  39K BYTES.
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TEST PROBLEM 1B. MAP ENERGY OF NACL                                                    01-06-81

  MODE     NC    NPC   ILSQ   IWGT   IPLM   IPRT   NSTG   IBPC        ARE        SLIM        CMPR        XDRD        EPSC
    -1      0      4      0      0      0      2      4      1   0.100D-03   0.100D-05   0.0         0.200D-02   0.100D 02

 NAMPC(I)
    ARNA      ARCL      BRNA      BRCL

   PC(I)
 0.93928   2.43000   0.07900   0.23800

   DPC(I)
 0.00100   0.00100   0.00010   0.00010

   KPC(I)
      2         2         2         2
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TEST PROBLEM 1B. MAP ENERGY OF NACL                                                    01-06-81
NACL

   ISB
     3

    NA    NKA     NS  ICENT  HXNEG  HYNEG  HZNEG    NRB    NPK    NRP   ICMB   IVDW   IREP   INUL    NCT   IRSC   IZAM   IGEM   IRBA  ISETA
     2      2      4      2    0.0    0.0    0.0      2      0     10      1      0      1      0      0      0      0      0      1      2

       CK     NQ     NR
 0.31000      2      2

  QLIM(I)
 0.64000   0.72000

  RLIM(I)
 6.40000   7.00000

    A(I)
 5.62800   5.62800   5.62800   0.0       0.0       0.0
NAMS          TRANSFORMED X                    TRANSFORMED Y                    TRANSFORMED Z

          0.0      1.0*X   0.0*Y   0.0*Z      0.0      0.0*X   1.0*Y   0.0*Z      0.0      0.0*X   0.0*Y   1.0*Z
          0.0      1.0*X   0.0*Y   0.0*Z      0.5000   0.0*X   1.0*Y   0.0*Z      0.5000   0.0*X   0.0*Y   1.0*Z
          0.5000   1.0*X   0.0*Y   0.0*Z      0.0      0.0*X   1.0*Y   0.0*Z      0.5000   0.0*X   0.0*Y   1.0*Z
          0.5000   1.0*X   0.0*Y   0.0*Z      0.5000   0.0*X   1.0*Y   0.0*Z      0.0      0.0*X   0.0*Y   1.0*Z

 K  NAMK          Q        PL        AR        BR      AMASS
 1  NA        1.00000   0.0       0.0       0.0       0.0
 2  CL       -1.00000   0.0       0.0       0.0       0.0

 J  NAME    IKA    IRB          X         Y         Z
 1  NA       1      1       0.0       0.0       0.0
 2  CL       2      2       0.50000   0.50000   0.50000

 I  NAME    ISC    JAC    SMC    FMC   IRBC        XC        YC        ZC
 1  NA       1      1     1.     1.0      1   0.0       0.0       0.0
 2  CL       1      2     1.     1.0      2   0.50000   0.50000   0.50000
 3  NA       2      1     1.     1.0      3   0.0       0.50000   0.50000
 4  CL       2      2     1.     1.0      4   0.50000   1.00000   1.00000
 5  NA       3      1     1.     1.0      5   0.50000   0.0       0.50000
 6  CL       3      2     1.     1.0      6   1.00000   0.50000   1.00000
 7  NA       4      1     1.     1.0      7   0.50000   0.50000   0.0
 8  CL       4      2     1.     1.0      8   1.00000   1.00000   0.50000
ABOVE ATOMS USED TO COMPUTE STRUCTURE FACTORS

   ZMC
   4.0
```

I	NAME(I)	ZAM(I)
1	NA	1.0
2	CL	1.0

J	IZ(J)	IU(J)	IV(J)	IW(J)	SSR(J)	STR(J)	SXR(J)	SYR(J)	SZR(J)	TR(1,J)	TR(2,J)	TR(3,J)
1	1	0	0	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	2	0	0	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

KPWS	KPW	WOBS	SIGWD
0	0	0.0	0.0

TEST PROBLEM 18. MAP ENERGY OF NACL 01-06-81
NACL

KPI	MPI	LPI	PINI	PDLI	PLMI
-1	0	16	0.0	0.0	0.0

KPJ	MPJ	LPJ	PINJ	PDLJ	PLMJ
0	1	1	0.80000	0.05000	1.20000

KPK	MPK	LPK	PINK	PDLK	PLMK
1	1	5	5.50000	0.10000	6.00000

TEST PROBLEM 18. MAP ENERGY OF NACL 01-06-81
NACL

CYCLE 0

CSF	VSF	QMAX	NF
18.126419	0.0	0.640000	11
18.126419	0.0	0.720000	14

SQK	SPLK	SPPK
-235.945352	0.0	0.0

SGK	SVDW	WR	RMAX	NG	NSRB
-18.467021	0.0	29.426764	6.400000	74	0
-18.466922	0.0	29.506570	7.000000	122	0

GX	GY	GZ	I	J	GM	R	NAMES		CMB	VDW	REP	SRB
-1	-1	-1	1	4	1.00000	2.81400	NA	CL	-118.042	0.0	1.827	0.0
-1	-1	-1	1	6	1.00000	2.81400	NA	CL	-118.042	0.0	1.827	0.0
-1	-1	-1	1	8	1.00000	2.81400	NA	CL	-118.042	0.0	1.827	0.0
-1	-1	0	1	8	1.00000	2.81400	NA	CL	-118.042	0.0	1.827	0.0
-1	0	-1	1	6	1.00000	2.81400	NA	CL	-118.042	0.0	1.827	0.0
0	-1	-1	1	4	1.00000	2.81400	NA	CL	-118.042	0.0	1.827	0.0
-1	-1	0	1	7	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
-1	-1	0	2	8	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
-1	0	-1	1	5	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
-1	0	-1	2	6	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
-1	0	0	1	5	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
-1	0	0	1	7	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
-1	0	0	2	6	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
-1	0	0	2	8	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	-1	-1	1	3	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	-1	-1	2	4	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	-1	0	1	3	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	-1	0	1	7	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	-1	0	2	4	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	-1	0	2	8	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	0	-1	1	3	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	0	-1	1	5	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	0	-1	2	4	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	0	-1	2	6	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	0	0	1	3	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	0	0	1	5	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	0	0	1	7	0.50000	3.97960	NA	NA	83.468	0.0	0.000	0.0
0	0	0	2	4	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	0	0	2	6	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
0	0	0	2	8	0.50000	3.97960	CL	CL	83.468	0.0	3.026	0.0
-1	-1	-1	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
-1	-1	0	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
-1	0	-1	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
-1	0	0	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
0	-1	-1	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
0	-1	0	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
0	0	-1	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
0	0	0	1	2	1.00000	4.87399	NA	CL	-68.152	0.0	0.003	0.0
-1	0	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
-1	0	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	-1	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	-1	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	0	-1	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	0	-1	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	0	1	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	0	1	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
0	1	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
0	1	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
1	0	0	1	1	0.50000	5.62800	NA	NA	59.021	0.0	0.000	0.0
1	0	0	2	2	0.50000	5.62800	CL	CL	59.021	0.0	0.095	0.0
-2	-1	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-2	-1	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-2	-1	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-2	0	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-2	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-2	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-2	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	-2	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	-2	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	0	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	0	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	-2	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	0	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	0	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-2	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	-2	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	-1	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	0	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	-1	0	1	8	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	0	-1	1	4	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
0	0	-1	1	6	1.00000	6.29229	NA	CL	-52.790	0.0	0.000	0.0
-1	-1	-1	1	3	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	-1	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	-1	1	7	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	-1	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	-1	2	6	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	-1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	0	1	3	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	0	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0

-1	-1	0	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	0	2	6	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	-1	1	1	7	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	-1	1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	-1	1	3	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	0	-1	1	7	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	0	-1	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	-1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	0	1	3	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	0	0	2	4	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	0	1	1	7	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	0	1	2	8	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	1	-1	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	1	-1	2	6	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
-1	1	0	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
-1	1	0	2	6	0.50000	6.89286	CL	CL	48.190	0.0	0.007	0.0
0	-1	-1	1	5	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0
0	-1	-1	1	7	0.50000	6.89286	NA	NA	48.190	0.0	0.000	0.0

WC	WV	WR	WX	WT
-206.286	0.0	29.507	0.0	-176.779

16 NONE 1 APNA 5 A

			WC	WV	WR	WX	WT
0.0	0.80000	5.50000	-211.087	0.0	31.109	0.0	-179.978
0.0	0.80000	5.60000	-207.317	0.0	26.715	0.0	-180.602
0.0	0.80000	5.70000	-203.680	0.0	22.944	0.0	-180.736
0.0	0.80000	5.80000	-200.168	0.0	19.708	0.0	-180.451
0.0	0.80000	5.90000	-196.776	0.0	16.929	0.0	-179.847
0.0	0.80000	6.00000	-193.496	0.0	14.543	0.0	-178.953
0.0	0.85000	5.50000	-211.087	0.0	32.589	0.0	-178.497
0.0	0.85000	5.60000	-207.317	0.0	27.979	0.0	-179.338
0.0	0.85000	5.70000	-203.680	0.0	24.024	0.0	-179.658
0.0	0.85000	5.80000	-200.168	0.0	20.629	0.0	-179.539
0.0	0.85000	5.90000	-196.776	0.0	17.716	0.0	-179.060
0.0	0.85000	6.00000	-193.496	0.0	15.215	0.0	-178.281
0.0	0.90000	5.50000	-211.087	0.0	34.323	0.0	-178.764
0.0	0.90000	5.60000	-207.317	0.0	29.460	0.0	-177.858
0.0	0.90000	5.70000	-203.680	0.0	25.288	0.0	-178.392
0.0	0.90000	5.80000	-200.168	0.0	21.709	0.0	-178.460
0.0	0.90000	5.90000	-196.776	0.0	18.638	0.0	-178.138
0.0	0.90000	6.00000	-193.496	0.0	16.003	0.0	-177.494
0.0	0.95000	5.50000	-211.087	0.0	36.353	0.0	-174.734
0.0	0.95000	5.60000	-207.317	0.0	31.193	0.0	-176.124
0.0	0.95000	5.70000	-203.680	0.0	26.768	0.0	-176.912
0.0	0.95000	5.80000	-200.168	0.0	22.972	0.0	-177.196
0.0	0.95000	5.90000	-196.776	0.0	19.717	0.0	-177.059
0.0	0.95000	6.00000	-193.496	0.0	16.924	0.0	-176.572
0.0	1.00000	5.50000	-211.087	0.0	38.730	0.0	-172.357
0.0	1.00000	5.60000	-207.317	0.0	33.222	0.0	-174.095
0.0	1.00000	5.70000	-203.680	0.0	28.501	0.0	-175.180
0.0	1.00000	5.80000	-200.168	0.0	24.452	0.0	-175.716
0.0	1.00000	5.90000	-196.776	0.0	20.980	0.0	-175.795
0.0	1.00000	6.00000	-193.496	0.0	18.003	0.0	-175.493
0.0	1.05000	5.50000	-211.087	0.0	41.512	0.0	-169.574
0.0	1.05000	5.60000	-207.317	0.0	35.598	0.0	-171.719
0.0	1.05000	5.70000	-203.680	0.0	30.539	0.0	-173.151
0.0	1.05000	5.80000	-200.168	0.0	26.185	0.0	-173.984
0.0	1.05000	5.90000	-196.776	0.0	22.460	0.0	-174.316
0.0	1.05000	6.00000	-193.496	0.0	19.266	0.0	-174.230
0.0	1.10000	5.50000	-211.087	0.0	44.771	0.0	-166.316
0.0	1.10000	5.60000	-207.317	0.0	38.380	0.0	-168.937
0.0	1.10000	5.70000	-203.680	0.0	32.905	0.0	-170.775
0.0	1.10000	5.80000	-200.168	0.0	28.213	0.0	-171.955
0.0	1.10000	5.90000	-196.776	0.0	24.192	0.0	-172.584
0.0	1.10000	6.00000	-193.496	0.0	20.745	0.0	-172.751
0.0	1.15000	5.50000	-211.087	0.0	48.586	0.0	-162.501
0.0	1.15000	5.60000	-207.317	0.0	41.638	0.0	-165.680
0.0	1.15000	5.70000	-203.680	0.0	35.686	0.0	-167.994
0.0	1.15000	5.80000	-200.168	0.0	30.568	0.0	-169.580
0.0	1.15000	5.90000	-196.776	0.0	26.220	0.0	-170.556
0.0	1.15000	6.00000	-193.496	0.0	22.477	0.0	-171.019
0.0	1.20000	5.50000	-211.087	0.0	53.052	0.0	-158.034
0.0	1.20000	5.60000	-207.317	0.0	45.452	0.0	-161.866
0.0	1.20000	5.70000	-203.680	0.0	38.943	0.0	-164.737
0.0	1.20000	5.80000	-200.168	0.0	33.369	0.0	-166.800
0.0	1.20000	5.90000	-196.776	0.0	28.595	0.0	-168.181
0.0	1.20000	6.00000	-193.496	0.0	24.505	0.0	-168.991

NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGY CALCULATION FOR THIS CYCLE

	NT	SEC	AVT
INITIAL	56	0.03	0.0005
COORDINATES	56	0.06	0.0011
SLOW RECIP	1	0.0	0.0
FAST RECIP	55	0.22	0.0040
UNIT CELL	55	0.0	0.0
SLOW DIRECT	1	0.10	0.1000
FAST DIRECT	55	0.66	0.0120
SLOW CONFIG	1	0.0	0.0
FAST CONFIG	55	0.0	0.0

TOTAL TIME (SEC) 1.07

SUMMATION LIMITS FOR MINIMUM TIME
DEL IS PROPORTIONAL TO RELATIVE ERROR OF RESULT
PRQ IS RECOMMENDED QLIM
PRR IS RECOMMENDED RLIM
PRK IS RECOMMENDED VALUE OF CK
PRT IS PREDICTED TOTAL TIME PER CYCLE FOR RECIPROCAL AND DIRECT SUMS

DEL	PRQ	PRR	PRK	PRT
1.0E-2	0.43839	2.81943	0.36532	0.10
1.0E-3	0.55115	3.54462	0.37240	0.20
1.0E-4	0.64403	4.14202	0.37663	0.31
1.0E-5	0.72502	4.66289	0.37959	0.45
1.0E-6	0.79809	5.13278	0.38186	0.60
1.0E-7	0.86910	5.58948	0.38286	0.77

10.2 Benzene, Mode 1 and Mode 3

```
DYNAMIC DIMENSIONS FOR WMIN
  NPCMAX    NAMAX   NKAMAX    NSMAX  NRBMAX  NPXMAX  NCTMAX  NBCMAX
       9       13        2        8       1       0       6      80

    MMAX   NFSMAX   NGSMAX   NPSMAX   NPMAX  NOSMAX   NOMAX   NVMAX
       0       50      700       12      21       6       6       6

                        1          2          3          4          5          6          7          8          9         10
ARRAY                 ACZ        AKE         AM      AMASS         AN         AR         BR        BTR       CHAR       CMBT
DIMEN-             (    9      (   0     ( NVMAX     (   1    ( NVMAX      (   1      (   1    ( NVMAX      (   1      (   1
 SIONS             *NRBMAX)    *   0 )   * NVMAX)   *NKAMAX)  * NVMAX)   *NKAMAX)   *NKAMAX)   *NOSMAX)   * NSMAX)   *NGSMAX)
WORDS                   9          0         36          2         36          2          2         36          8        700
BYTES/WORD              8          8          8          8          8          8          8          8          8          4
HEX ADDRESS      00000000   00000048   00000048   00000158   00000178   00000298   000002A8   000002B8   000003D8   J00004

                       11         12         13         14         15         16         17         18
ARRAY                 CSV         DP        DPC        DPX         DW       DWDQ        DXQ        DYC
DIMEN-             (    1      (   1     (   1       (   1      (   1      (   1     ( NVMAX     (   1
 SIONS            *NGSMAX)   * NPMAX)  *NPCMAX)   *NPXMAX)   * NPMAX)   * NVMAX)   * NAMAX)   * N
WORDS                 700         21          9          0         21          6         78
BYTES/WORD              8          8          8          8          8          8                                       AX)
HEX ADDRESS      00000F08   000024E8   00002590   000025D8   000025D8   00002680                                         1
                                                                                                                         8
                                                                                                          JUD0E0  000003E0
                       21         22         23         24         25
ARRAY                 EPS        ERR       EVAL       EVEC        FMC
DIMEN-             (    1      (   1     (   1      ( NVMAX                                    118        119        120
 SIONS            * NPMAX)   * NVMAX)   * NVMAX)   * NVMAX                                     VM         VN        VSV
WORDS                  21          6          6                                               (   1      (   1      (   1
BYTES/WORD              8          8          8                                  *NGSMAX)   * NVMAX)   * NVMAX)   *NGSMAX)
HEX ADDRESS      00002E30   00002ED8   00002                                        700          6          6        700
                                                                          8            4          8          8          8
                       31                                              0000D678   0000D720   0000E210   0000E240   0000E270
ARRAY                 HMT
DIMEN-             (    1                                     125        126        127        128        129        130
 SIONS             *                                  JV       XC        XYZ       XYZC       XYZO       XYZN       XYZR
WORDS                                                (  1   ( NAMAX     (   3      (   3      (   3      (   3      (   3
BYTES/W                                   AX)      *  MMAX)  * NSMAX)   * NAMAX)   * NAMAX)   * NAMAX)   * NAMAX)   * NAMAX)
HE                                         21           0       104         39         39         39         39         39
                                            8           8         8          8          8          8          8          8
                             F970   0000FA18   0000FAC0   0000FAC0   0000FE00   0000FF38   00010070   000101A8   000102E0

                      131        132        133
                       YC        ZAM         ZC
                  ( NAMAX      (   1    ( NAMAX      (
                  * NSMAX)   * NAMAX)   * NSMAX)     *
WORDS                 104         13        104
BYTES/WORD              8          8          8
HEX ADDRESS      00010418   00010758   000107C0
   8544 8-BYTE STORAGE LOCATIONS HAVE BEEN REQUESTED. THE PROGRAM IS DIMENSIONED FOR   12000
COMMON/S/ AND NST MAY BE DECREASED BY  3456 WORDS. THIS WILL REDUCE THE REGION USED BY  27K BYTES.


TEST PROBLEM 2A. MINIMIZE ENERGY BY NEWTON'S METHOD                                  01-06-81
 MODE    NC   NPC  ILSQ  IWGT  IPLM  IPRT  NSTG  IBPC         ARE         SLIM       CMPR        XDRD        EPSC
    1     2     9     0     0     0     2     4     0   0.100D-03   0.100D-05   0.0         0.200D-02   0.100D 02

NAMPC(I)
     PLC      PLH      BCC      BCH      BHH      CCC      CCH      CHH
      QH

   PC(I)
24.02372  5.70218 87.80210 15.65620  2.79170  3.60000  3.67000  3.74000
 0.15300

  DPC(I)
 0.01000  0.01000  0.01000  0.01000  0.01000  0.01000  0.01000  0.01000
 0.00100

  KPC(I)
       1        1        2        2        2        2        2        2
       1


TEST PROBLEM 2A. MINIMIZE ENERGY BY NEWTON'S METHOD                                  01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

  ISB
   4

  NA   NKA   NS ICENT HXNEG HYNEG HZNEG   NRB   NPX   NRP  ICMB  IVDW  IREP  IMOL   NCT  IRSC  IZAM  IGEM  IRBA ISETA
   7     2    8     2   0.0   0.0   0.0     1     0     8     1     1     2     0     6     2     0     0     0     0

     CK     NQ    NR
0.30000      2     2

QLIM(I)
0.44000  0.51000

RLIM(I)
4.45000  5.20000

   A(I)
7.44000  9.55000  6.92000  0.0      0.0      0.0

NAMS          TRANSFORMED X                        TRANSFORMED Y                        TRANSFORMED Z

         0.0      1.0*X  0.0*Y  0.0*Z     0.0      0.0*X  1.0*Y  0.0*Z     0.0      0.0*X  0.0*Y  1.0*Z
         0.0     -1.0*X  0.0*Y  0.0*Z     0.0      0.0*X -1.0*Y  0.0*Z     0.0      0.0*X  0.0*Y -1.0*Z
         0.5000   1.0*X  0.0*Y  0.0*Z     0.5000   0.0*X -1.0*Y  0.0*Z     0.0      0.0*X  0.0*Y -1.0*Z
         0.5000  -1.0*X  0.0*Y  0.0*Z     0.5000   0.0*X  1.0*Y  0.0*Z     0.0      0.0*X  0.0*Y  1.0*Z
         0.0     -1.0*X  0.0*Y  0.0*Z     0.5000   0.0*X  1.0*Y  0.0*Z     0.5000   0.0*X  0.0*Y -1.0*Z
         0.0      1.0*X  0.0*Y  0.0*Z     0.5000   0.0*X -1.0*Y  0.0*Z     0.5000   0.0*X  0.0*Y  1.0*Z
         0.5000  -1.0*X  0.0*Y  0.0*Z     0.0      0.0*X -1.0*Y  0.0*Z     0.5000   0.0*X  0.0*Y  1.0*Z
         0.5000   1.0*X  0.0*Y  0.0*Z     0.0      0.0*X  1.0*Y  0.0*Z     0.5000   0.0*X  0.0*Y -1.0*Z

 K  NAMK        Q        PL        AR        BR     AMASS
 1  C         0.0       0.0       0.0       0.0       0.0
 2  H         0.0       0.0       0.0       0.0       0.0

 J  NAME    IKA    IRB         X         Y         Z
 1  C1        1      0  -0.05690   0.13870  -0.00540
 2  C2        1      0  -0.13350   0.04600   0.12640
 3  C3        1      0  -0.07740  -0.09250   0.12950
 4  H1        2      0  -0.09862   0.24040  -0.00936
```

5	H2	2	0	-0.23115	0.07965	0.21886
6	H3	2	0	-0.13445	-0.16068	0.22495
7	XTRA	0	0	0.0	0.0	0.0

I	NAME	ISC	JAC	SMC	FMC	IRBC	XC	YC	ZC
1	C1	1	1	1.	1.0	0	-0.05690	0.13870	-0.00540
2	C2	1	2	1.	1.0	0	-0.13350	0.04600	0.12640
3	C3	1	3	1.	1.0	0	-0.07740	-0.09250	0.12950
4	H1	1	4	1.	1.0	0	-0.09862	0.24040	-0.00936
5	H2	1	5	1.	1.0	0	-0.23115	0.07965	0.21886
6	H3	1	6	1.	1.0	0	-0.13445	-0.16068	0.22495
7	XTRA	1	7	2.	1.0	0	0.0	0.0	0.0
8	C1	2	1	1.	1.0	1	0.05690	-0.13870	0.00540
9	C2	2	2	1.	1.0	1	0.13350	-0.04600	-0.12640
10	C3	2	3	1.	1.0	1	0.07740	0.09250	-0.12950
11	H1	2	4	1.	1.0	1	0.09862	-0.24040	0.00936
12	H2	2	5	1.	1.0	1	0.23115	-0.07965	-0.21886
13	H3	2	6	1.	1.0	1	0.13445	0.16068	-0.22495
14	C1	3	1	1.	1.0	2	0.44310	0.36130	0.00540
15	C2	3	2	1.	1.0	2	0.36650	0.45400	-0.12640
16	C3	3	3	1.	1.0	2	0.42260	0.59250	-0.12950
17	H1	3	4	1.	1.0	2	0.40138	0.25960	0.00936
18	H2	3	5	1.	1.0	2	0.26885	0.42035	-0.21886
19	H3	3	6	1.	1.0	2	0.36555	0.66068	-0.22495
20	XTRA	3	7	2.	1.0	2	0.50000	0.50000	0.0
21	C1	4	1	1.	1.0	3	0.55690	0.63870	-0.00540
22	C2	4	2	1.	1.0	3	0.63350	0.54600	0.12640
23	C3	4	3	1.	1.0	3	0.57740	0.40750	0.12950
24	H1	4	4	1.	1.0	3	0.59862	0.74040	-0.00936
25	H2	4	5	1.	1.0	3	0.73115	0.57965	0.21886
26	H3	4	6	1.	1.0	3	0.63445	0.33932	0.22495
27	C1	5	1	1.	1.0	4	0.05690	0.63870	0.50540
28	C2	5	2	1.	1.0	4	0.13350	0.54600	0.37360
29	C3	5	3	1.	1.0	4	0.07740	0.40750	0.37050
30	H1	5	4	1.	1.0	4	0.09862	0.74040	0.50936
31	H2	5	5	1.	1.0	4	0.23115	0.57965	0.28114
32	H3	5	6	1.	1.0	4	0.13445	0.33932	0.27505
33	XTRA	5	7	2.	1.0	4	0.0	0.50000	0.50000
34	C1	6	1	1.	1.0	5	-0.05690	0.36130	0.49460
35	C2	6	2	1.	1.0	5	-0.13350	0.45400	0.62640
36	C3	6	3	1.	1.0	5	-0.07740	0.59250	0.62950
37	H1	6	4	1.	1.0	5	-0.09862	0.25960	0.49064
38	H2	6	5	1.	1.0	5	-0.23115	0.42035	0.71886
39	H3	6	6	1.	1.0	5	-0.13445	0.66068	0.72495
40	C1	7	1	1.	1.0	6	0.55690	-0.13870	0.49460
41	C2	7	2	1.	1.0	6	0.63350	-0.04600	0.62640
42	C3	7	3	1.	1.0	6	0.57740	0.09250	0.62950
43	H1	7	4	1.	1.0	6	0.59862	-0.24040	0.49064
44	H2	7	5	1.	1.0	6	0.73115	-0.07965	0.71886
45	H3	7	6	1.	1.0	6	0.63445	0.16068	0.72495
46	XTRA	7	7	2.	1.0	6	0.50000	0.0	0.50000
47	C1	8	1	1.	1.0	7	0.44310	0.13870	0.50540
48	C2	8	2	1.	1.0	7	0.36650	0.04600	0.37360
49	C3	8	3	1.	1.0	7	0.42260	-0.09250	0.37050
50	H1	8	4	1.	1.0	7	0.40138	0.24040	0.50936
51	H2	8	5	1.	1.0	7	0.26885	0.07965	0.28114
52	H3	8	6	1.	1.0	7	0.36555	-0.16068	0.27505

ABOVE ATOMS USED TO COMPUTE STRUCTURE FACTORS

REVISED ATOM LIST AFTER RELAXING SYMMETRY CONSTRAINTS

J	NAME	IKA	IRB	X	Y	Z
1	C1	1	1	-0.05690	0.13870	-0.00540
2	C2	1	1	-0.13350	0.04600	0.12640
3	C3	1	1	-0.07740	-0.09250	0.12950
4	H1	2	1	-0.09862	0.24040	-0.00936
5	H2	2	1	-0.23115	0.07965	0.21886
6	H3	2	1	-0.13445	-0.16068	0.22495
7	XTRA	0	1	0.0	0.0	0.0
8	C1	1	1	0.05690	-0.13870	0.00540
9	C2	1	1	0.13350	-0.04600	-0.12640
10	C3	1	1	0.07740	0.09250	-0.12950
11	H1	2	1	0.09862	-0.24040	0.00936
12	H2	2	1	0.23115	-0.07965	-0.21886
13	H3	2	1	0.13445	0.16068	-0.22495

I	NAME	ISC	JAC	SMC	FMC	IRBC	XC	YC	ZC
1	C1	1	1	2.	1.0	1	-0.05690	0.13870	-0.00540
2	C2	1	2	2.	1.0	1	-0.13350	0.04600	0.12640
3	C3	1	3	2.	1.0	1	-0.07740	-0.09250	0.12950
4	H1	1	4	2.	1.0	1	-0.09862	0.24040	-0.00936
5	H2	1	5	2.	1.0	1	-0.23115	0.07965	0.21886
6	H3	1	6	2.	1.0	1	-0.13445	-0.16068	0.22495
7	XTRA	1	7	2.	1.0	1	0.0	0.0	0.0
8	C1	1	8	2.	1.0	1	0.05690	-0.13870	0.00540
9	C2	1	9	2.	1.0	1	0.13350	-0.04600	-0.12640
10	C3	1	10	2.	1.0	1	0.07740	0.09250	-0.12950
11	H1	1	11	2.	1.0	1	0.09862	-0.24040	0.00936
12	H2	1	12	2.	1.0	1	0.23115	-0.07965	-0.21886
13	H3	1	13	2.	1.0	1	0.13445	0.15066	-0.22495
14	C1	3	1	2.	1.0	3	0.44310	0.36130	0.00540
15	C2	3	2	2.	1.0	3	0.36650	0.45400	-0.12640
16	C3	3	3	2.	1.0	3	0.42260	0.59250	-0.12950
17	H1	3	4	2.	1.0	3	0.40138	0.25960	0.00936
18	H2	3	5	2.	1.0	3	0.26885	0.42035	-0.21886
19	H3	3	6	2.	1.0	3	0.36555	0.66068	-0.22495
20	XTRA	3	7	2.	1.0	3	0.50000	0.50000	0.0
21	C1	3	8	2.	1.0	3	0.55690	0.63870	-0.00540
22	C2	3	9	2.	1.0	3	0.63350	0.54600	0.12640
23	C3	3	10	2.	1.0	3	0.57740	0.40750	0.12950
24	H1	3	11	2.	1.0	3	0.59862	0.74040	-0.00936
25	H2	3	12	2.	1.0	3	0.73115	0.57965	0.21886
26	H3	3	13	2.	1.0	3	0.63445	0.33932	0.22495
27	C1	5	1	2.	1.0	5	0.05690	0.63870	0.50540
28	C2	5	2	2.	1.0	5	0.13350	0.54500	0.37360
29	C3	5	3	2.	1.0	5	0.07740	0.40750	0.37050
30	H1	5	4	2.	1.0	5	0.09862	0.74040	0.50936
31	H2	5	5	2.	1.0	5	0.23115	0.57965	0.28114
32	H3	5	6	2.	1.0	5	0.13445	0.33932	0.27505
33	XTRA	5	7	2.	1.0	5	0.0	0.50000	0.50000
34	C1	5	8	2.	1.0	5	-0.05690	0.36130	0.49460
35	C2	5	9	2.	1.0	5	-0.13350	0.45400	0.62640
36	C3	5	10	2.	1.0	5	-0.07740	0.59250	0.62950
37	H1	5	11	2.	1.0	5	-0.09862	0.25960	0.49064
38	H2	5	12	2.	1.0	5	-0.23115	0.42035	0.71886
39	H3	5	13	2.	1.0	5	-0.13445	0.66068	0.72495
40	C1	7	1	2.	1.0	7	0.55690	-0.13870	0.49460
41	C2	7	2	2.	1.0	7	0.63350	-0.04600	0.62640
42	C3	7	3	2.	1.0	7	0.57740	0.09250	0.62950
43	H1	7	4	2.	1.0	7	0.59862	-0.24040	0.49064
44	H2	7	5	2.	1.0	7	0.73115	-0.07965	0.71886
45	H3	7	6	2.	1.0	7	0.63445	0.16068	0.72495
46	XTRA	7	7	2.	1.0	7	0.50000	0.0	0.50000
47	C1	7	8	2.	1.0	7	0.44310	0.13870	0.50540
48	C2	7	9	2.	1.0	7	0.36650	0.04600	0.37360
49	C3	7	10	2.	1.0	7	0.42260	-0.09250	0.37050
50	H1	7	11	2.	1.0	7	0.40138	0.24040	0.50936
51	H2	7	12	2.	1.0	7	0.26885	0.07965	0.28114
52	H3	7	13	2.	1.0	7	0.36555	-0.16068	0.27505

ABOVE ATOMS USED TO COMPUTE STRUCTURE FACTORS

ZMC
4.0

I	NAME(I)	ZAM(I)
1	C1	1.0
2	C2	1.0

3	C3	1.0
4	H1	1.0
5	H2	1.0
6	H3	1.0
7	XTRA	1.0
8	C1	1.0
9	C2	1.0
10	C3	1.0
11	H1	1.0
12	H2	1.0
13	H3	1.0

J	IZ(J)	IU(J)	IV(J)	IW(J)	SSR(J)	STR(J)	SXR(J)	SYR(J)	SZR(J)	TR(1,J)	TR(2,J)	TR(3,J)
1	7	0	0	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

IACT	ICT				IDZ				IAZ						ITBR			
1	2	4	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	1	3	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	2	6	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	3	9	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	8	10	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	1	9	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

LBCI	LBCJ																							
1	2	1	4	1	10	2	3	2	5	3	6	3	8	8	9	8	11	9	10	9	12	10	13

KPWS	KPW	WOBS	SIGWO
0	0	0.0	0.0

I	NAMP(I)	P(I)	DP(I)	PMN(I)	PMX(I)	KP(I)	KQ(I)	DKT(KQ)	SP(I)	ISBP(I)
1	PLC	24.023720	0.010000	0.0	0.0	0	0	0.0	0.0	0
2	PLH	5.702180	0.010000	0.0	0.0	0	0	0.0	0.0	0
3	BCC	87.802100	0.010000	0.0	0.0	0	0	0.0	0.0	0
4	BCH	15.656200	0.010000	0.0	0.0	0	0	0.0	0.0	0
5	BHH	2.791700	0.010000	0.0	0.0	0	0	0.0	0.0	0
6	CCC	3.600000	0.010000	0.0	0.0	0	0	0.0	0.0	0
7	CCH	3.670000	0.010000	0.0	0.0	0	0	0.0	0.0	0
8	CHH	3.740000	0.010000	0.0	0.0	0	0	0.0	0.0	0
9	QH	0.153000	0.001000	0.0	0.0	0	0	0.0	0.0	0
10	A	7.440000	0.000010	6.440000	8.440000	1	1	1.000	0.0	4
11	B	9.550000	0.000010	8.550000	10.550000	1	1	1.000	0.0	4
12	C	6.920000	0.000010	5.920000	7.920000	1	1	1.000	0.0	4
13	COSA	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	4
14	COSB	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	4
15	COSG	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	4
16	RX	0.0	0.000010	-0.200000	0.200000	1	1	1.000	0.0	4
17	RY	0.0	0.000010	-0.200000	0.200000	1	1	1.000	0.0	4
18	RZ	0.0	0.000010	-0.200000	0.200000	1	1	1.000	0.0	4
19	TX	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	4
20	TY	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	4
21	TZ	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	4

NO	NV	NOV	LS	IWT
6	6	6	0	0

01-06-81

TEST PROBLEM 2A. MINIMIZE ENERGY BY NEWTON'S METHOD
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

CYCLE 1

CSF	VSF	QMAX	NF
4.471021	-4.840268	0.440000	20
4.475676	-4.842977	0.510000	34

SQK	SPLK	SPPK
-27.992757	-36.108733	6.890180

SGK	SVDW	WR	RMAX	NG	NSRB
21.189748	16.920684	7.004175	4.450000	222	66
21.181217	16.842343	7.093283	5.200000	339	66

GX	GY	GZ	I	J	GM	R	NAMES		CMG	VDW	REP	SRB
0	0	0	1	4	1.00000	1.02000	C1	H1	-7.623	-121.643	0.0	1.0
0	0	0	3	6	1.00000	1.02000	C3	H3	-7.623	-121.643	0.0	1.0
0	0	0	8	11	1.00000	1.02000	C1	H1	-7.623	-121.643	0.0	1.0
0	0	0	10	13	1.00000	1.02000	C3	H3	-7.623	-121.643	0.0	1.0
0	0	0	2	5	1.00000	1.02003	C2	H2	-7.623	-121.617	0.0	1.0
0	0	0	9	12	1.00000	1.02003	C2	H2	-7.623	-121.617	0.0	1.0
0	0	0	2	3	1.00000	1.38713	C2	C3	5.606	-81.016	0.0	1.0
0	0	0	9	10	1.00000	1.38713	C2	C3	5.606	-81.016	0.0	1.0
0	0	0	1	10	1.00000	1.38944	C1	C3	5.596	-80.213	0.0	1.0
0	0	0	3	8	1.00000	1.38944	C3	C1	5.596	-80.213	0.0	1.0
0	0	0	1	2	1.00000	1.39297	C1	C2	5.582	-79.000	0.0	1.0
0	0	0	8	9	1.00000	1.39297	C1	C2	5.582	-79.000	0.0	1.0
0	0	0	2	6	1.00000	2.08830	C2	H3	-3.723	-1.652	0.0	1.0
0	0	0	9	13	1.00000	2.08830	C2	H3	-3.723	-1.652	0.0	1.0
0	0	0	1	13	1.00000	2.09262	C1	H3	-3.716	-1.631	0.0	1.0
0	0	0	6	8	1.00000	2.09262	H3	C1	-3.716	-1.631	0.0	1.0
0	0	0	3	5	1.00000	2.09612	C3	H2	-3.710	-1.615	0.0	1.0
0	0	0	10	12	1.00000	2.09612	C3	H2	-3.710	-1.615	0.0	1.0
0	0	0	2	4	1.00000	2.09681	C2	H1	-3.708	-1.612	0.0	1.0
0	0	0	9	11	1.00000	2.09681	C2	H1	-3.708	-1.612	0.0	1.0
0	0	0	3	11	1.00000	2.09790	C3	H1	-3.706	-1.607	0.0	1.0
0	0	0	4	10	1.00000	2.09790	H1	C3	-3.706	-1.607	0.0	1.0
0	0	0	1	5	1.00000	2.09930	C1	H2	-3.704	-1.600	0.0	1.0
0	0	0	8	12	1.00000	2.09930	C1	H2	-3.704	-1.600	0.0	1.0
0	0	0	1	3	1.00000	2.40204	C1	C3	3.237	-3.005	0.0	1.0
0	0	0	8	10	1.00000	2.40204	C1	C3	3.237	-3.005	0.0	1.0
0	0	0	5	6	1.00000	2.40564	H2	H3	3.232	-0.168	0.0	1.0
0	0	0	12	13	1.00000	2.40564	H2	H3	3.232	-0.168	0.0	1.0
0	0	0	2	10	1.00000	2.40730	C2	C3	3.230	-2.966	0.0	1.0
0	0	0	3	9	1.00000	2.40730	C3	C2	3.230	-2.966	0.0	1.0
0	0	0	4	13	1.00000	2.41086	H1	H3	3.225	-0.166	0.0	1.0
0	0	0	6	11	1.00000	2.41086	H3	H1	3.225	-0.166	0.0	1.0
0	0	0	1	9	1.00000	2.41228	C1	C2	3.223	-2.929	0.0	1.0
0	0	0	2	8	1.00000	2.41228	C2	C1	3.223	-2.929	0.0	1.0
0	0	0	4	5	1.00000	2.41311	H1	H2	3.222	-0.165	0.0	1.0
0	0	0	11	12	1.00000	2.41311	H1	H2	3.222	-0.165	0.0	1.0
-1	-1	0	6	25	1.00000	2.67419	H3	H2	2.908	-0.089	0.127	0.0
-1	0	0	5	26	1.00000	2.67419	H2	H3	2.908	-0.089	0.127	0.0
0	0	-1	4	38	1.00000	2.73179	H1	H2	2.846	-0.078	0.102	0.0
0	0	0	5	37	1.00000	2.73179	H2	H1	2.846	-0.078	0.102	0.0
-1	-1	0	6	24	1.00000	2.73230	H3	H1	2.846	-0.078	0.102	0.0
-1	0	0	4	26	1.00000	2.73230	H1	H3	2.846	-0.078	0.102	0.0
0	0	0	3	10	1.00000	2.76769	C3	C3	2.809	-1.284	0.0	1.0
0	0	0	1	8	1.00000	2.78218	C1	C1	2.795	-1.244	0.0	1.0
0	-1	-1	11	39	1.00000	2.78798	H1	H3	2.789	-0.069	0.083	0.0
0	0	0	4	32	1.00000	2.78798	H1	H3	2.789	-0.069	0.083	0.0
0	0	0	2	9	1.00000	2.78897	C2	C2	2.788	-1.226	0.0	1.0
-1	0	-1	4	45	1.00000	2.81141	H1	H3	2.766	-0.066	0.076	0.0
0	0	0	11	52	1.00000	2.81141	H1	H3	2.766	-0.066	0.076	0.0
-1	0	-1	1	45	1.00000	2.96634	C1	H3	-2.621	-0.201	0.293	0.0
0	0	0	8	52	1.00000	2.96634	C1	H3	-2.621	-0.201	0.293	0.0
-1	-1	0	3	24	1.00000	3.04631	C3	H1	-2.553	-0.171	0.218	0.0
-1	0	0	4	23	1.00000	3.04631	H1	C3	-2.553	-0.171	0.218	0.0
0	-1	-1	8	39	1.00000	3.07634	C1	H3	-2.528	-0.162	0.196	0.0
0	0	0	1	32	1.00000	3.07634	C1	H3	-2.528	-0.162	0.196	0.0
-1	0	-1	3	44	1.00000	3.18100	C3	H2	-2.444	-0.132	0.133	0.0
0	0	0	10	51	1.00000	3.18100	C3	H2	-2.444	-0.132	0.133	0.0

-1	0	0	5	47	1.00000	3.18174	H2	C1	-2.444	-0.132	0.133	0.0
0	0	0	1	51	1.00000	3.18174	C1	H2	-2.444	-0.132	0.133	0.0
-1	0	0	5	48	1.00000	3.19544	H2	C2	-2.433	-0.129	0.126	0.0
0	0	0	2	51	1.00000	3.19544	C2	H2	-2.433	-0.129	0.126	0.0
-1	0	-1	2	44	1.00000	3.22604	C2	H2	-2.410	-0.122	0.113	0.0
0	0	0	9	51	1.00000	3.22604	C2	H2	-2.410	-0.122	0.113	0.0
-1	0	0	5	49	1.00000	3.23114	H2	C3	-2.407	-0.120	0.111	0.0
0	0	0	3	51	1.00000	3.23114	C3	H2	-2.407	-0.120	0.111	0.0
-1	0	-1	1	44	1.00000	3.23663	C1	H2	-2.402	-0.119	0.109	0.0
0	0	0	8	51	1.00000	3.23663	C1	H2	-2.402	-0.119	0.109	0.0
0	0	-1	4	35	1.00000	3.25293	H1	C2	-2.390	-0.116	0.102	0.0
0	0	0	2	37	1.00000	3.25293	C2	H1	-2.390	-0.116	0.102	0.0
0	0	0	1	6	1.00000	3.32387	C1	H3	-2.339	-0.102	0.0	1.0
0	0	0	8	13	1.00000	3.32387	C1	H3	-2.339	-0.102	0.0	1.0
0	0	0	3	4	1.00000	3.32499	C3	H1	-2.339	-0.101	0.0	1.0
0	0	0	10	11	1.00000	3.32499	C3	H1	-2.339	-0.101	0.0	1.0
0	0	0	2	13	1.00000	3.32943	C2	H3	-2.335	-0.101	0.0	1.0
0	0	0	6	9	1.00000	3.32943	H3	C2	-2.335	-0.101	0.0	1.0
0	0	0	3	12	1.00000	3.33109	C3	H2	-2.334	-0.100	0.0	1.0
0	0	0	5	10	1.00000	3.33109	H2	C3	-2.334	-0.100	0.0	1.0
0	0	0	2	11	1.00000	3.33456	C2	H1	-2.332	-0.100	0.0	1.0
0	0	0	4	9	1.00000	3.33456	H1	C2	-2.332	-0.100	0.0	1.0
0	0	0	1	12	1.00000	3.33512	C1	H2	-2.331	-0.100	0.0	1.0

BOND DISTANCES

		IA	JA	DIJ	WD
C1	C2	1	2	1.3930	0.0
C1	H1	1	4	1.0200	0.0
C1	C3	1	10	1.3894	0.0
C2	C3	2	3	1.3871	0.0
C2	H2	2	5	1.0200	0.0
C3	H3	3	6	1.0200	0.0
C3	C1	3	8	1.3894	0.0
C1	C2	8	9	1.3930	0.0
C1	H1	8	11	1.0200	0.0
C2	C3	9	10	1.3871	0.0
C2	H2	9	12	1.0200	0.0
C3	H3	10	13	1.0200	0.0

BOND ANGLES

			IA	JA	KA	AIJK	WA
C2	C1	H1	2	1	4	119.88	0.0
C2	C1	C3	2	1	10	119.81	0.0
H1	C1	C3	4	1	10	120.30	0.0
C1	C2	C3	1	2	3	119.54	0.0
C1	C2	H2	1	2	5	120.12	0.0
C3	C2	H2	3	2	5	120.33	0.0
C2	C3	H3	2	3	6	119.57	0.0
C2	C3	C1	2	3	8	120.64	0.0
H3	C3	C1	6	3	8	119.79	0.0
C3	C1	C2	3	8	9	119.81	0.0
C3	C1	H1	3	8	11	120.30	0.0
C2	C1	H1	9	8	11	119.88	0.0
C1	C2	C3	8	9	10	119.54	0.0
C1	C2	H2	8	9	12	120.12	0.0
C3	C2	H2	10	9	12	120.33	0.0
C1	C3	C2	1	10	9	120.64	0.0
C1	C3	H3	1	10	13	119.79	0.0
C2	C3	H3	9	10	13	119.57	0.0

CONFORMATION ANGLES

				IA	JA	KA	LA	CNF	WCF
H1	C1	C2	C3	4	1	2	3	179.32	0.0
H1	C1	C2	H2	4	1	2	5	-0.00	0.0
C3	C1	C2	C3	10	1	2	3	-1.37	0.0
C3	C1	C2	H2	10	1	2	5	179.31	0.0
C2	C1	C3	C2	2	1	10	9	1.38	0.0
C2	C1	C3	H3	2	1	10	13	-179.31	0.0
H1	C1	C3	C2	4	1	10	9	-179.30	0.0
H1	C1	C3	H3	4	1	10	13	0.00	0.0
C1	C2	C3	H3	1	2	3	6	-179.31	0.0
C1	C2	C3	C1	1	2	3	8	1.38	0.0
H2	C2	C3	H3	5	2	3	6	0.00	0.0
H2	C2	C3	C1	5	2	3	8	-179.30	0.0
C2	C3	C1	C2	2	3	8	9	-1.38	0.0
C2	C3	C1	H1	2	3	8	11	179.30	0.0
H3	C3	C1	C2	6	3	8	9	179.31	0.0
H3	C3	C1	H1	6	3	8	11	-0.00	0.0
C3	C1	C2	C3	3	8	9	10	1.37	0.0
C3	C1	C2	H2	3	8	9	12	-179.31	0.0
H1	C1	C2	C3	11	8	9	10	-179.32	0.0
H1	C1	C2	H2	11	8	9	12	0.00	0.0
C1	C2	C3	C1	8	9	10	1	-1.38	0.0
C1	C2	C3	H3	8	9	10	13	179.31	0.0
H2	C2	C3	C1	12	9	10	1	179.30	0.0
H2	C2	C3	H3	12	9	10	13	-0.00	0.0

WC	WV	WR	WX	WT
-2.336	-17.219	7.093	0.0	-12.462

TEST PROBLEM 2A. MINIMIZE ENERGY BY NEWTON'S METHOD 01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

WOBS	WCALC BEFORE CYCLE 1
0.0	-12.4618

DERIVATIVES BEFORE CYCLE 1

DDW/DP(I)DP(J) FOR I=

J	NAMP(J)	DYC(J)	10 A	11 B	12 C	16 RX	17 RY	18 RZ
10	A	-0.3839	3.8350	1.0349	2.3891	1.8946	-5.3282	5.1128
11	B	-0.5963	1.0349	2.1567	1.1361	2.8062	0.5174	-1.8993
12	C	-0.5161	2.3691	1.1361	3.5939	-3.0774	2.6013	1.6005
16	RX	0.1367	1.8946	2.8062	-3.0774	83.3360	-0.0504	13.8940
17	RY	-0.6006	-5.3282	0.5174	2.6013	-0.0504	39.1510	-8.4989
18	RZ	0.2906	5.1128	-1.8993	1.6005	13.8940	-8.4989	23.6989

RDWS	SDWS
0.111051D 01	0.123323D 01

NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGY CALCULATION FOR THIS CYCLE

	NT	SEC	AVT
INITIAL	28	0.0	0.0
COORDINATES	28	0.06	0.0021
SLOW RECIP	1	0.07	0.0700
FAST RECIP	27	1.71	0.0633
UNIT CELL	15	0.0	0.0
SLOW DIRECT	1	0.32	0.3200
FAST DIRECT	27	1.04	0.0385
SLOW CONFIG	1	0.03	0.0300
FAST CONFIG	27	0.0	0.0

TOTAL TIME (SEC) 3.23

SUMMATION LIMITS FOR MINIMUM TIME
DEL IS PROPORTIONAL TO RELATIVE ERROR OF RESULT
PRQ IS RECOMMENDED QLIM
PRR IS RECOMMENDED RLIM
PRK IS RECOMMENDED VALUE OF CK
PRT IS PREDICTED TOTAL TIME PER CYCLE FOR RECIPROCAL AND DIRECT SUMS

DEL	PRQ	PRR	PRK	PRT
1.0E-2	0.33290	3.71285	0.27742	0.99
1.0E-3	0.41852	4.66784	0.26279	1.97
1.0E-4	0.46906	5.45454	0.28600	3.14
1.0E-5	0.55056	6.14046	0.28825	4.48
1.0E-6	0.60604	6.75926	0.28997	5.97
1.0E-7	0.65997	7.36067	0.29073	7.71

```
                    SAN(I)
                    10  A        11  B        12  C        16  RX       17  RY       18  RZ
                    0.510640     0.680933     0.527497     0.109543     0.159819     0.205417

                   EVEC(I,J)
  J    EVAL(J)     10  A        11  B        12  C        16  RX       17  RY       18  RZ
  1  0.214D 01    -0.660896    -0.296303    -0.467945    -0.157183     0.242572    -0.415814
  2  0.157D 01    -0.021754     0.507740     0.466600    -0.225982     0.493374    -0.479089
  3  0.113D 01    -0.127748     0.394547    -0.242188     0.855316     0.193757    -0.015843
  4  0.934D 00     0.093833     0.440561    -0.301581    -0.128775    -0.682440    -0.473120
  5  0.168D 00    -0.219856     0.546184    -0.348162    -0.405108     0.144143     0.589271
  6  0.617D-01     0.699487    -0.079537    -0.540822    -0.109387     0.416771    -0.161985

                   SAN(I)*EVEC(I,J)
  J    EVAL(J)     10  A        11  B        12  C        16  RX       17  RY       18  RZ
  1  0.214D 01    -0.337480    -0.201762    -0.246839    -0.017218     0.038768    -0.085415
  2  0.157D 01    -0.011109     0.345736     0.246130    -0.024755     0.078850    -0.098413
  3  0.113D 01    -0.065233     0.268660    -0.127754     0.093694     0.030996    -0.003254
  4  0.934D 00     0.047915     0.299992    -0.159083    -0.014106    -0.109067    -0.097187
  5  0.168D 00    -0.112267     0.371915    -0.183654    -0.044377     0.023037     0.121046
  6  0.617D-01     0.357186    -0.054159    -0.285282    -0.011983     0.066608    -0.033275

                          %MAT*BMAT*SAN*EVEC
  J   NAMP(J)   DYC(J)        1          2          3          4          5          6
 10   A        -0.3839    -2.7687    -0.0670    -0.2815     0.1717    -0.0723     0.0845
 11   B        -0.5963    -0.9309     1.1720     0.6519     0.6044     0.1348    -0.0072
 12   C        -0.5161    -1.8977     1.3904    -0.5166    -0.5341    -0.1109    -0.0632
 16   RX        0.1367    -3.0695    -3.2426     8.7847    -1.0982    -0.6214    -0.0616
 17   RY       -0.6006     3.2469     4.8523     1.3640    -3.9891     0.1515     0.1608
 18   RZ        0.2906    -4.3303    -3.6659    -0.0868    -2.1517     0.4820    -0.0486

PARAMETERS AFTER CYCLE  1
  I    NAMP       OLD P       CHANGE       NEW P        ERR
 10    A        7.440000   -0.054042    7.385958   2.446508
 11    B        9.550000   -0.308500    9.241500   1.250818
 12    C        6.920000    0.036751    6.956751   1.808869
 16    RX       0.0         0.018533    0.018533   0.025089
 17    RY       0.0        -0.026348   -0.026348   0.103647
 18    RZ       0.0        -0.023601   -0.023601   0.138643


TEST PROBLEM 2A. MINIMIZE ENERGY BY NEWTON'S METHOD                                    01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

CYCLE  2

      WC        WV        WR        WX        WT
   -2.480   -18.795     8.731     0.0      -12.545

TEST PROBLEM 2A. MINIMIZE ENERGY BY NEWTON'S METHOD                                    01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

      WOBS       WCALC BEFORE CYCLE  2
     0.0       -12.5445

DERIVATIVES BEFORE CYCLE  2
                      DDW/DP(I)DP(J) FOR I=
  J   NAMP(J)   DYC(J)    10  A       11  B       12  C       16  RX      17  RY      18  RZ
 10   A        0.0809     4.7457      1.5652      2.5881      2.6514     -7.2697      6.2370
 11   B        0.1602     1.5652      3.2909      1.9977      2.8943      1.4934     -3.3440
 12   C        0.1530     2.5881      1.9977      4.5370     -4.2327      5.5350      1.1577
 16   RX       0.0089     2.6514      2.8943     -4.2327     95.6958     -0.8017     20.6461
 17   RY       0.2626    -7.2697      1.4934      5.5350     -0.8017     56.0556    -10.2936
 18   RZ      -0.1549     6.2370     -3.3440      1.1577     20.6461    -10.2936     31.4228

          RDWS          SDWS
   0.385504D 00   0.148613D 00

PARAMETERS AFTER CYCLE  2
  I    NAMP       OLD P       CHANGE       NEW P        ERR
 10    A        7.385958    0.005352    7.391309   0.734726
 11    B        9.241500    0.038753    9.280253   0.505158
 12    C        6.956751    0.009379    6.966130   0.568261
 16    RX       0.018533   -0.000618    0.017915   0.010377
 17    RY      -0.026348    0.003156   -0.023192   0.030654
 18    RZ      -0.023601   -0.000773   -0.024373   0.056802


TEST PROBLEM 2A. MINIMIZE ENERGY BY NEWTON'S METHOD                                    01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

CYCLE  3

          CSF          VSF          QMAX          NF
     4.316946    -4.570555     0.440000          19
     4.323045    -4.573151     0.510000          32

          SQK         SPLK         SPPK
   -27.992757   -37.155395     6.890180

          SGK         SVDW           WR          RMAX          NG        NSRB
    21.209902    16.425523     8.308982      4.450000         228          66
    21.207870    16.336318     8.414729      5.200000         356          66

 GX GY GZ  I  J       GM          R   NAMES        CMB       VDW       REP       SRB
  0  0  0  1  4   1.00000    1.02000   C1   H1    -7.623  -121.643     0.0       1.0
  0  0  0  3  6   1.00000    1.02000   C3   H3    -7.623  -121.643     0.0       1.0
  0  0  0  8 11   1.00000    1.02000   C1   H1    -7.623  -121.643     0.0       1.0
  0  0  0 10 13   1.00000    1.02000   C3   H3    -7.623  -121.643     0.0       1.0
  0  0  0  2  5   1.00000    1.02003   C2   H2    -7.623  -121.617     0.0       1.0
  0  0  0  9 12   1.00000    1.02003   C2   H2    -7.623  -121.617     0.0       1.0
  0  0  0  2  3   1.00000    1.38713   C2   C3     5.606   -81.016     0.0       1.0
  0  0  0  9 10   1.00000    1.38713   C2   C3     5.606   -81.016     0.0       1.0
  0  0  0  1 10   1.00000    1.38944   C1   C3     5.596   -80.213     0.0       1.0
  0  0  0  3  8   1.00000    1.38944   C3   C1     5.596   -80.213     0.0       1.0
  0  0  0  1  2   1.00000    1.39297   C1   C2     5.582   -79.000     0.0       1.0
  0  0  0  8  9   1.00000    1.39297   C1   C2     5.582   -79.000     0.0       1.0
  0  0  0  2  6   1.00000    2.08830   C2   H3    -3.723    -1.652     0.0       1.0
  0  0  0  9 13   1.00000    2.08830   C2   H3    -3.723    -1.652     0.0       1.0
  0  0  0  1 13   1.00000    2.09262   C1   H3    -3.716    -1.631     0.0       1.0
  0  0  0  6  8   1.00000    2.09262   H3   C1    -3.716    -1.631     0.0       1.0
  0  0  0  3  5   1.00000    2.09612   C3   H2    -3.710    -1.615     0.0       1.0
  0  0  0 10 12   1.00000    2.09612   C3   H2    -3.710    -1.615     0.0       1.0
  0  0  0  2  4   1.00000    2.09681   C2   H1    -3.708    -1.612     0.0       1.0
  0  0  0  9 11   1.00000    2.09681   C2   H1    -3.708    -1.612     0.0       1.0
  0  0  0  3 11   1.00000    2.09790   C3   H1    -3.706    -1.607     0.0       1.0
  0  0  0  4 10   1.00000    2.09790   H1   C3    -3.706    -1.607     0.0       1.0
  0  0  0  1  5   1.00000    2.09930   C1   H2    -3.704    -1.600     0.0       1.0
  0  0  0  8 12   1.00000    2.09930   C1   H2    -3.704    -1.600     0.0       1.0
  0  0  0  1  3   1.00000    2.40204   C1   C3     3.237    -3.305     0.0       1.0
  0  0  0  8 10   1.00000    2.40204   C1   C3     3.237    -3.305     0.0       1.0
  0  0  0  5  6   1.00000    2.40564   H2   H3     3.232    -0.168     0.0       1.0
  0  0  0 12 13   1.00000    2.40564   H2   H3     3.232    -0.168     0.0       1.0
  0  0  0  2 10   1.00000    2.40730   C2   C3     3.230    -2.966     0.0       1.0
  0  0  0  3  9   1.00000    2.40730   C3   C2     3.230    -2.966     0.0       1.0
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0	0	0	4	13	1.00000	2.41086	H1	H3	3.225	-0.166	0.0	1.0
0	0	0	6	11	1.00000	2.41086	H3	H1	3.225	-0.166	0.0	1.0
0	0	0	1	9	1.00000	2.41226	C1	C2	3.223	-2.929	0.0	1.0
0	0	0	2	8	1.00000	2.41226	C2	C1	3.223	-2.929	0.0	1.0
0	0	0	4	5	1.00000	2.41311	H1	H2	3.222	-0.165	0.0	1.0
0	0	0	11	12	1.00000	2.41311	H1	H2	3.222	-0.165	0.0	1.0
-1	-1	0	6	25	1.00000	2.59447	H3	H2	2.997	-0.107	0.171	0.0
-1	0	0	5	25	1.00000	2.59447	H2	H3	2.997	-0.107	0.171	0.0
0	0	-1	4	38	1.00000	2.62425	H1	H2	2.963	-0.100	0.153	0.0
0	0	0	5	37	1.00000	2.62425	H2	H1	2.963	-0.100	0.153	0.0
-1	-1	0	6	24	1.00000	2.73554	H3	H1	2.842	-0.078	0.101	0.0
-1	0	0	4	26	1.00000	2.73554	H1	H3	2.842	-0.078	0.101	0.0
0	-1	-1	11	39	1.00000	2.74063	H1	H3	2.837	-0.077	0.099	0.0
0	0	0	4	32	1.00000	2.74063	H1	H3	2.837	-0.077	0.099	0.0
0	0	0	5	10	1.00000	2.76769	C3	C3	2.809	-1.284	0.0	1.0
-1	0	-1	4	45	1.00000	2.76829	H1	H3	2.809	-0.072	0.089	0.0
0	0	0	11	32	1.00000	2.76829	H1	H3	2.809	-0.072	0.089	0.0
0	0	0	1	8	1.00000	2.78218	C1	C1	2.795	-1.244	0.0	1.0
0	0	0	2	9	1.00000	2.78897	C2	C2	2.788	-1.226	0.0	1.0
-1	0	-1	1	45	1.00000	2.95398	C1	H3	-2.632	-0.206	0.307	0.0
0	0	0	8	52	1.00000	2.95398	C1	H3	-2.632	-0.206	0.307	0.0
-1	-1	0	3	24	1.00000	2.97495	C3	H1	-2.614	-0.198	0.284	0.0
-1	0	0	4	33	1.00000	2.97495	H1	C3	-2.614	-0.198	0.284	0.0
0	-1	-1	8	39	1.00000	2.97671	C1	H3	-2.612	-0.197	0.282	0.0
0	0	0	1	32	1.00000	2.97671	C1	H3	-2.612	-0.197	0.282	0.0
0	0	-1	4	39	1.00000	3.16996	H1	C2	-2.453	-0.135	0.139	0.0
0	0	0	2	37	1.00000	3.16996	C2	H1	-2.453	-0.135	0.139	0.0
-1	0	0	5	49	1.00000	3.17209	H2	C3	-2.451	-0.134	0.138	0.0
0	0	0	3	51	1.00000	3.17209	C3	H2	-2.451	-0.134	0.138	0.0
-1	0	0	5	48	1.00000	3.17279	H2	C2	-2.451	-0.134	0.137	0.0
0	0	0	2	51	1.00000	3.17279	C2	H2	-2.451	-0.134	0.137	0.0
-1	0	-1	1	44	1.00000	3.19025	C1	H2	-2.437	-0.130	0.129	0.0
0	0	0	8	51	1.00000	3.19025	C1	H2	-2.437	-0.130	0.129	0.0
-1	0	0	5	47	1.00000	3.20884	H2	C1	-2.423	-0.125	0.120	0.0
0	0	0	1	51	1.00000	3.20884	C1	H2	-2.423	-0.125	0.120	0.0
-1	0	-1	3	44	1.00000	3.22055	C3	H2	-2.414	-0.123	0.115	0.0
0	0	0	10	51	1.00000	3.22055	C3	H2	-2.414	-0.123	0.115	0.0
-1	0	-1	2	44	1.00000	3.22903	C2	H2	-2.408	-0.121	0.112	0.0
0	0	0	9	51	1.00000	3.22903	C2	H2	-2.408	-0.121	0.112	0.0
-1	-1	0	6	22	1.00000	3.29904	H3	C2	-2.357	-0.106	0.086	0.0
-1	0	0	2	26	1.00000	3.29904	C2	H3	-2.357	-0.106	0.086	0.0
0	-1	0	3	30	1.00000	3.31124	C3	H1	-2.348	-0.104	0.083	0.0
0	0	-1	10	37	1.00000	3.31124	C3	H1	-2.348	-0.104	0.083	0.0
0	0	0	1	6	1.00000	3.32387	C1	H3	-2.339	-0.102	0.0	1.0
0	0	0	8	13	1.00000	3.32387	C1	H3	-2.339	-0.102	0.0	1.0
0	0	0	3	4	1.00000	3.32499	C3	H1	-2.339	-0.101	0.0	1.0
0	0	0	10	11	1.00000	3.32499	C3	H1	-2.339	-0.101	0.0	1.0
0	0	0	2	13	1.00000	3.32943	C2	H3	-2.335	-0.101	0.0	1.0
0	0	0	6	9	1.00000	3.32943	H3	C2	-2.335	-0.101	0.0	1.0
0	0	0	3	12	1.00000	3.33109	C3	H2	-2.334	-0.100	0.0	1.0

BOND DISTANCES

		IA	JA	DIJ	WD
C1	C2	1	2	1.3930	0.0
C1	H1	1	4	1.0200	0.0
C1	C3	1	10	1.3894	0.0
C2	C3	2	3	1.3871	0.0
C2	H2	2	5	1.0200	0.0
C3	H3	3	6	1.0200	0.0
C3	C1	3	8	1.3894	0.0
C1	C2	8	9	1.3930	0.0
C1	H1	8	11	1.0200	0.0
C2	C3	9	10	1.3871	0.0
C2	H2	9	12	1.0200	0.0
C3	H3	10	13	1.0200	0.0

BOND ANGLES

			IA	JA	KA	AIJK	WA
C2	C1	H1	2	1	4	119.88	0.0
C2	C1	C3	2	1	10	119.81	0.0
H1	C1	C3	4	1	10	120.30	0.0
C1	C2	C3	1	2	3	119.54	0.0
C1	C2	H2	1	2	5	120.12	0.0
C3	C2	H2	3	2	5	120.33	0.0
C2	C3	H3	2	3	6	119.57	0.0
C2	C3	C1	2	3	8	120.64	0.0
H3	C3	C1	6	3	8	119.79	0.0
C3	C1	C2	3	8	9	119.81	0.0
C3	C1	H1	3	8	11	120.30	0.0
C2	C1	H1	9	8	11	119.88	0.0
C1	C2	C3	8	9	10	119.54	0.0
C1	C2	H2	8	9	12	120.12	0.0
C3	C2	H2	10	9	12	120.33	0.0
C1	C3	C2	1	10	9	120.64	0.0
C1	C3	H3	1	10	13	119.79	0.0
C2	C3	H3	9	10	13	119.57	0.0

CONFORMATION ANGLES

				IA	JA	KA	LA	CNF	WCF
H1	C1	C2	C3	4	1	2	3	179.32	0.0
H1	C1	C2	H2	4	1	2	5	-0.00	0.0
C3	C1	C2	C3	10	1	2	3	-1.37	0.0
C3	C1	C2	H2	10	1	2	5	179.31	0.0
C2	C1	C3	C2	2	1	10	9	1.38	0.0
C2	C1	C3	H3	2	1	10	13	-179.31	0.0
H1	C1	C3	C2	4	1	10	9	-179.30	0.0
H1	C1	C3	H3	4	1	10	13	0.00	0.0
C1	C2	C3	H3	1	2	3	6	-179.31	0.0
C1	C2	C3	C1	1	2	3	8	1.36	0.0
H2	C2	C3	H3	5	2	3	6	0.00	0.0
H2	C2	C3	C1	5	2	3	8	-179.30	0.0
C2	C3	C1	C2	2	3	8	9	-1.36	0.0
C2	C3	C1	H1	2	3	8	11	179.30	0.0
H3	C3	C1	C2	6	3	8	9	179.31	0.0
H3	C3	C1	H1	6	3	8	11	-0.00	0.0
C3	C1	C2	C3	3	8	9	10	1.37	0.0
C3	C1	C2	H2	3	8	9	12	-179.31	0.0
H1	C1	C2	C3	11	8	9	10	-179.32	0.0
H1	C1	C2	H2	11	8	9	12	0.00	0.0
C1	C2	C3	C1	8	9	10	1	-1.38	0.0
C1	C2	C3	H3	8	9	10	13	179.31	0.0
H2	C2	C3	C1	12	9	10	1	179.30	0.0
H2	C2	C3	H3	12	9	10	13	-0.00	0.0

WC	WV	WR	WX	WT
-2.452	-16.502	8.415	0.0	-12.549

TEST PROBLEM 2A. MINIMIZE ENERGY BY NEWTON'S METHOD 01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

WOBS	WCALC BEFORE CYCLE 3
0.0	-12.5492

DERIVATIVES BEFORE CYCLE 3

J	NAMP(J)	DYC(J)
10	A	0.0013
11	B	0.0060
12	C	0.0055
16	RX	-0.0099
17	RY	0.0131
18	RZ	-0.0123

NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGY CALCULATION FOR THIS CYCLE

	NT	SEC	AVT
INITIAL	13	0.0	0.0
COORDINATES	13	0.02	0.0015
SLEW RECIP	1	0.06	0.0600

```
FAST RECIP      12      0.72    0.0600
UNIT CELL        8      0.0     0.0
SLOW DIRECT      1      0.33    0.3300
FAST DIRECT     12      0.49    0.0408
SLOW CONFIG      1      0.02    0.0200
FAST CONFIG     12      0.0     0.0

TOTAL TIME (SEC)        1.64

SUMMATION LIMITS FOR MINIMUM TIME
   DEL IS PROPORTIONAL TO RELATIVE ERROR OF RESULT
   PRQ IS RECOMMENDED QLIM
   PRR IS RECOMMENDED RLIM
   PRK IS RECOMMENDED VALUE OF CK
   PRT IS PREDICTED TOTAL TIME PER CYCLE FOR RECIPROCAL AND DIRECT SUMS

   DEL       PRQ       PRR       PRK       PRT
1.0E-2  0.35108   3.52052   0.29257      0.51
1.0E-3  0.44139   4.4260A   0.29923      1.01
1.0E-4  0.51578   5.17199   0.30162      1.61
1.0E-5  0.58064   5.82239   0.30400      2.30
1.0E-6  0.63915   6.40913   0.30581      3.07
1.0E-7  0.69602   6.97939   0.30662      3.97

  J  NAME    IKA    IRB          X          Y          Z
  1  C1       1      1   -0.06180   0.14148  -0.00736
  2  C2       1      1   -0.13309   0.04645   0.12769
  3  C3       1      1   -0.07215  -0.09487   0.13278
  4  H1       2      1   -0.10711   0.24522  -0.01275
  5  H2       2      1   -0.23043   0.08043   0.22109
  6  H3       2      1   -0.12532  -0.16480   0.23064
  7  XTRA     0      1    0.0       0.0       0.0
  8  C1       1      1    0.06180  -0.14148   0.00736
  9  C2       1      1    0.13309  -0.04645  -0.12769
 10  C3       1      1    0.07215   0.09487  -0.13278
 11  H1       2      1    0.10711  -0.24522   0.01275
 12  H2       2      1    0.23043  -0.08043  -0.22109
 13  H3       2      1    0.12532   0.16480  -0.23064


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TEST PROBLEM 2A. MINIMIZE ENERGY BY NEWTON'S METHOD                    01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

  MODE    NC    NPC  ILSQ  IWGT  IPLM  IPRT  NSTG  IBPC        ARE        SLIM        CMPR        XDRD        EPSC
     1     2      9     0     0     0     2     4     0   0.100D-03   0.100D-05   0.0         0.200D-02   0.100D 02

    PLC       PLH       BCC       BCH       BHH       CCC       CCH       CHH
    QH
24.02372   5.70218 87.80210 15.65620  2.79170  3.60000  3.67000  3.74000
 0.15300

    NA    NKA     NS ICENT HXNEG HYNEG HZNEG    NRB    NPX    NRP   ICMB   IVDW   IREP   IMOL    NCT   IRSC   IZAM   IGEM   IRBA  ISETA
    13      2      8     2   0.0   0.0   0.0      1      0      8      1      1      2      0      6      2      0      0      0      0

    NO     NV    NOV     LS    IWT
     6      6      6      0      0

                    PARAMETERS AFTER EACH CYCLE
  J  NAMP    DKT      INITIAL        1          2
 10  A      1.000    7.440000   7.385958   7.391309
 11  B      1.000    9.550000   9.241500   9.280253
 12  C      1.000    6.920000   6.956751   6.966130
 16  RX     1.000    0.0        0.018533   0.017915
 17  RY     1.000    0.0       -0.026348  -0.023192
 18  RZ     1.000    0.0       -0.023601  -0.024373

             NVU                        6          6

             RDWS 0.1111D 01 0.3855D 00

             W       -12.4618   -12.5445   -12.5492

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DYNAMIC DIMENSIONS FOR BMIN

  NPCMAX   NAMAX  NKAMAX   NSMAX  NRBMAX  NPXMAX  NCTMAX  NBCMAX
       9      13       2       8       1       0       1       1

    MMAX  NFSMAX  NGSMAX  NPSMAX   NPMAX  NOSMAX   NOMAX   NVMAX
       0      50     700      12      21       6       6       6

                    1          2          3          4          5          6          7          8          9         10
ARRAY             ACZ        AKE         AM       AMASS         AN         AR         BR        BTR       CHAR       CMBT
DIMEN-          (   9      (   0      ( NVMAX    (   1      ( NVMAX    (   1      (   1      ( NVMAX    (   1      (   1
 SIONS          *NRBMAX)   *   0  )   * NVMAX)   *NKAMAX)   * NVMAX)   *NKAMAX)   *NKAMAX)   *NOSMAX)   * NSMAX)   *NGSMAX)
WORDS                9          0         36          2         36          2          2         36          8        70
BYTES/WORD           8          8          8          8          8          8          8          8          8
HEX ADDRESS   00000000   00000048   00000048   00000158   00000178   00000298   000002A8   000002B8   0000030

                   11         12         13         14         15         16         17         18
ARRAY             CSV         DP        DPC        DPX         DW       DWDQ        DXQ        DY
DIMEN-          (   1      (   1      (   1      (   1      (   1      (   1      ( NVMAX
 SIONS          *NGSMAX)   * NPMAX)   *NPCMAX)   *NPXMAX)   * NPMAX)   * NVMAX)   * NAMA
WORDS              700         21          9          0         21          6                                                  8
BYTES/WORD           8          8          8          8          8          8                                                 8
HEX ADDRESS   00000F08   000024E8   00002590   000025D8   000025D8   0000                                                 000CFF8

                   21         22         23         24                                                                  119        120
ARRAY             EPS        ERR       EVAL       EVEC                                                                     VN        VSV
DIMEN-          (   1      (   1      (   1      ( NVMA                                                              (   1      (   1
 SIONS          * NPMAX)   * NVMAX)   * NVMAX)   *                                                              * NVMAX)   * NVMAX)   *NGSMAX)
WORDS               21          6          6                                                                 4          6          6        700
BYTES/WORD           8          8                                                                            8          8          8          8
HEX ADDRESS   00002E30   00002ED8                                                                   00000338   0000DE28   0000DE58   0000DE88

                   31                                                                            126        127        128        129        130
ARRAY             HMT                                                                           XYZ       XYZC       XYZD       XYZN       XYZR
DIMEN-          (                                                                          ( NAMAX    (   3      (   3      (   3      (   3
 SIONS                                                                                     * NSMAX)   * NAMAX)   * NAMAX)   * NAMAX)   * NAMAX)
WORDS                                                                                        104         39         39         39         39
BYTES/WORD                                                                                     8          8          8          8          8
                                                                                     0F630   0000F5D8   0000F6D8   0000FA18   0000FB50   0000FC88   0000FDC0   0000FEF8

                                                                                    132        133
                                                                                   ZAM         ZC
                                                                                 (   1      ( NAMAX    (
                                                                                 NSMAX)   * NAMAX)   * NSMAX)   *
                                                                                   104         13        104
                                                                                     8          8          8
                                                                                00010030   00010370   000103D8

    8419 8-BYTE STORAGE LOCATIONS HAVE BEEN REQUESTED. THE PROGRAM IS DIMENSIONED FOR   12000

COMMON/SX AND NST MAY BE DECREASED BY  3581 WORDS. THIS WILL REDUCE THE REGION USED BY  27K BYTES.
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TEST PROBLEM 28. MINIMIZE ENERGY BY MODIFIED ROSENBROCK SEARCH                    01-06-81

  MODE     NC    NPC   ILSO   IWGT   IPLM   IPRT   NSTG   IBPC          ARE          SLIM          CMPR          XORD          EPSC
     3      2      9      0      0      0      2      4      0    0.100D-03    0.100D-05     0.0           0.200D-02     0.100D 02

 NAMPC(I)
    PLC       PLH       BCC       BCH       BHH       CCC       CCH       CHH
    OH

   PC(I)
 24.02372  5.70218 87.80210 15.65620  2.79170  3.60000  3.67000  3.74000
  0.15300

   DPC(I)
  0.01000  0.01000  0.01000  0.01000  0.01000  0.01000  0.01000  0.01000
  0.00100

   KPC(I)
      1
      1        1        2        2        2        2        2        2
```

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TEST PROBLEM 29. MINIMIZE ENERGY BY MODIFIED ROSENBROCK SEARCH                    01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

   ISB
    4

    NA    NKA     NS  ICENT  HXNEG  HYNEG  HZNEG    NRB    NPX    NRP   ICMB   IVDW   IREP   IMOL    NCT   IRSC   IZAM   IGEM   IRBA  ISETA
     7      2      8      2    0.0    0.0    0.0      1      0      8      1      1      2      0      0      2      0      0      0      0

     CK     NQ     NR
  0.29000    2      2

  GLIM(I)
  0.42000  0.49000

  FLIM(I)
  4.65000  5.43000

    A(I)
  7.44000  9.55000  6.92000  0.0       0.0       0.0
```

NAMS	TRANSFORMED X				TRANSFORMED Y				TRANSFORMED Z			
	0.0	1.0*X	0.0*Y	0.0*Z	0.0	0.0*X	1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	1.0*Z
	0.0	-1.0*X	0.0*Y	0.0*Z	0.0	0.0*X	-1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	-1.0*Z
	0.5000	1.0*X	0.0*Y	0.0*Z	0.5000	0.0*X	-1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	-1.0*Z
	0.5000	-1.0*X	0.0*Y	0.0*Z	0.5000	0.0*X	1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	1.0*Z
	0.0	-1.0*X	0.0*Y	0.0*Z	0.5000	0.0*X	1.0*Y	0.0*Z	0.5000	0.0*X	0.0*Y	-1.0*Z
	0.0	1.0*X	0.0*Y	0.0*Z	0.5000	0.0*X	-1.0*Y	0.0*Z	0.5000	0.0*X	0.0*Y	1.0*Z
	0.5000	-1.0*X	0.0*Y	0.0*Z	0.0	0.0*X	-1.0*Y	0.0*Z	0.5000	0.0*X	0.0*Y	1.0*Z
	0.5000	1.0*X	0.0*Y	0.0*Z	0.0	0.0*X	1.0*Y	0.0*Z	0.5000	0.0*X	0.0*Y	-1.0*Z

K	NAMK	Q	PL	AR	BR	AMASS
1	C	0.0	0.0	0.0	0.0	0.0
2	H	0.0	0.0	0.0	0.0	0.0

J	NAME	IKA	IRB	X	Y	Z
1	C1	1	0	-0.05690	0.13870	-0.00540
2	C2	1	0	-0.13350	0.04600	0.12640
3	C3	1	0	-0.07740	-0.09250	0.12950
4	H1	2	0	-0.09862	0.24040	-0.00936
5	H2	2	0	-0.23115	0.07965	0.21886
6	H3	2	0	-0.13445	-0.16068	0.22495
7	XTRA	0	0	0.0	0.0	0.0

I	NAME	ISC	JAC	SMC	FMC	IRBC	XC	YC	ZC
1	C1	1	1	1.	1.0	0	-0.05690	0.13870	-0.00540
2	C2	1	2	1.	1.0	0	-0.13350	0.04600	0.12640
3	C3	1	3	1.	1.0	0	-0.07740	-0.09250	0.12950
4	H1	1	4	1.	1.0	0	-0.09862	0.24040	-0.00936
5	H2	1	5	1.	1.0	0	-0.23115	0.07965	0.21886
6	H3	1	6	1.	1.0	0	-0.13445	-0.16068	0.22495
7	XTRA	1	7	2.	1.0	0	0.0	0.0	0.0
8	C1	2	1	1.	1.0	1	0.05690	-0.13870	0.00540
9	C2	2	2	1.	1.0	1	0.13350	-0.04600	-0.12640
10	C3	2	3	1.	1.0	1	0.07740	0.09250	-0.12950
11	H1	2	4	1.	1.0	1	0.09862	-0.24040	0.00936
12	H2	2	5	1.	1.0	1	0.23115	-0.07965	-0.21886
13	H3	2	6	1.	1.0	1	0.13445	0.16068	-0.22495
14	C1	3	1	1.	1.0	2	0.44310	0.36130	0.00540
15	C2	3	2	1.	1.0	2	0.36650	0.45400	-0.12640
16	C3	3	3	1.	1.0	2	0.42260	0.59250	-0.12950
17	H1	3	4	1.	1.0	2	0.40138	0.25960	0.00936
18	H2	3	5	1.	1.0	2	0.26885	0.42035	-0.21886
19	H3	3	6	1.	1.0	2	0.36555	0.66068	-0.22495
20	XTRA	3	7	2.	1.0	2	0.50000	0.50000	0.0
21	C1	4	1	1.	1.0	3	0.55690	0.63870	-0.00540
22	C2	4	2	1.	1.0	3	0.63350	0.54600	0.12640
23	C3	4	3	1.	1.0	3	0.57740	0.40750	0.12950
24	H1	4	4	1.	1.0	3	0.59862	0.74040	-0.00936
25	H2	4	5	1.	1.0	3	0.73115	0.57965	0.21886
26	H3	4	6	1.	1.0	3	0.63445	0.33932	0.22495
27	C1	5	1	1.	1.0	4	0.05690	0.63870	0.50540
28	C2	5	2	1.	1.0	4	0.13350	0.54600	0.37360
29	C3	5	3	1.	1.0	4	0.07740	0.40750	0.37050
30	H1	5	4	1.	1.0	4	0.09862	0.74040	0.50936
31	H2	5	5	1.	1.0	4	0.23115	0.57965	0.28114
32	H3	5	6	1.	1.0	4	0.13445	0.33932	0.27505
33	XTRA	5	7	2.	1.0	4	0.0	0.50000	0.50000
34	C1	6	1	1.	1.0	5	-0.05690	0.36130	0.49460
35	C2	6	2	1.	1.0	5	-0.13350	0.45400	0.62640
36	C3	6	3	1.	1.0	5	-0.07740	0.59250	0.62950
37	H1	6	4	1.	1.0	5	-0.09862	0.25960	0.49064
38	H2	6	5	1.	1.0	5	-0.23115	0.42035	0.71886
39	H3	6	6	1.	1.0	5	-0.13445	0.66068	0.72495
40	C1	7	1	1.	1.0	6	0.55690	-0.13870	0.49460
41	C2	7	2	1.	1.0	6	0.63350	-0.04600	0.62640
42	C3	7	3	1.	1.0	6	0.57740	0.09250	0.62950
43	H1	7	4	1.	1.0	6	0.59862	-0.24040	0.49064
44	H2	7	5	1.	1.0	6	0.73115	-0.07965	0.71886
45	H3	7	6	1.	1.0	6	0.63445	0.16068	0.72495
46	XTRA	7	7	2.	1.0	6	0.50000	0.0	0.50000
47	C1	8	1	1.	1.0	7	0.44310	0.13870	0.50540
48	C2	8	2	1.	1.0	7	0.36650	0.04600	0.37360
49	C3	8	3	1.	1.0	7	0.42260	-0.09250	0.37050
50	H1	8	4	1.	1.0	7	0.40138	0.24040	0.50936
51	H2	8	5	1.	1.0	7	0.26885	0.07965	0.28114
52	H3	8	6	1.	1.0	7	0.36555	-0.16068	0.27505

ABOVE ATOMS USED TO COMPUTE STRUCTURE FACTORS

REVISED ATOM LIST AFTER RELAXING SYMMETRY CONSTRAINTS

J	NAME	IKA	IRB	X	Y	Z
1	C1	1	1	-0.05690	0.13870	-0.00540
2	C2	1	1	-0.13350	0.04600	0.12640
3	C3	1	1	-0.07740	-0.09250	0.12950
4	H1	2	1	-0.09862	0.24040	-0.00936
5	H2	2	1	-0.23115	0.07965	0.21886
6	H3	2	1	-0.13445	-0.16068	0.22495
7	XTRA	0	1	0.0	0.0	0.0

8	C1	1	1	0.05690	-0.13870	0.00540
9	C2	1	1	0.13350	-0.04600	-0.12640
10	C3	1	1	0.07740	0.09250	-0.12950
11	H1	2	1	0.09862	-0.24040	0.00936
12	H2	2	1	0.23115	-0.07965	-0.21886
13	H3	2	1	0.13445	0.16068	-0.22495

I	NAME	ISC	JAC	SMC	FMC	IRBC	XC	YC	ZC
1	C1	1	1	2.	1.0	1	-0.05690	0.13870	-0.00540
2	C2	1	2	2.	1.0	1	-0.13350	0.04600	0.12640
3	C3	1	3	2.	1.0	1	-0.07740	-0.09250	0.12950
4	H1	1	4	2.	1.0	1	-0.09862	0.24040	-0.00936
5	H2	1	5	2.	1.0	1	-0.23115	0.07965	0.21886
6	H3	1	6	2.	1.0	1	-0.13445	-0.16068	0.22495
7	XTRA	1	7	2.	1.0	1	0.0	0.0	0.0
8	C1	1	8	2.	1.0	1	0.05690	-0.13870	0.00540
9	C2	1	9	2.	1.0	1	0.13350	-0.04600	-0.12640
10	C3	1	10	2.	1.0	1	0.07740	0.09250	-0.12950
11	H1	1	11	2.	1.0	1	0.09862	-0.24040	0.00936
12	H2	1	12	2.	1.0	1	0.23115	-0.07965	-0.21886
13	H3	1	13	2.	1.0	1	0.13445	0.16068	-0.22495
14	C1	3	1	2.	1.0	3	0.44310	0.36130	0.00540
15	C2	3	2	2.	1.0	3	0.36650	0.45400	-0.12640
16	C3	3	3	2.	1.0	3	0.42260	0.59250	-0.12950
17	H1	3	4	2.	1.0	3	0.40138	0.25960	0.00936
18	H2	3	5	2.	1.0	3	0.26885	0.42035	-0.21886
19	H3	3	6	2.	1.0	3	0.36555	0.66068	-0.22495
20	XTRA	3	7	2.	1.0	3	0.50000	0.50000	0.0
21	C1	3	8	2.	1.0	3	0.55690	0.63870	-0.00540
22	C2	3	9	2.	1.0	3	0.63350	0.54600	0.12640
23	C3	3	10	2.	1.0	3	0.57740	0.40750	0.12950
24	H1	3	11	2.	1.0	3	0.59862	0.74040	-0.00936
25	H2	3	12	2.	1.0	3	0.73115	0.57965	0.21886
26	H3	3	13	2.	1.0	3	0.63445	0.33932	0.22495
27	C1	5	1	2.	1.0	5	0.05690	0.63870	0.50540
28	C2	5	2	2.	1.0	5	0.13350	0.54600	0.37360
29	C3	5	3	2.	1.0	5	0.07740	0.40750	0.37050
30	H1	5	4	2.	1.0	5	0.09862	0.74040	0.50936
31	H2	5	5	2.	1.0	5	0.23115	0.57965	0.28114
32	H3	5	6	2.	1.0	5	0.13445	0.33932	0.27505
33	XTRA	5	7	2.	1.0	5	0.0	0.50000	0.56000
34	C1	5	8	2.	1.0	5	-0.05690	0.36130	0.49460
35	C2	5	9	2.	1.0	5	-0.13350	0.45400	0.62640
36	C3	5	10	2.	1.0	5	-0.07740	0.59250	0.62950
37	H1	5	11	2.	1.0	5	-0.09862	0.25960	0.49064
38	H2	5	12	2.	1.0	5	-0.23115	0.42035	0.71886
39	H3	5	13	2.	1.0	5	-0.13445	0.66068	0.72495
40	C1	7	1	2.	1.0	7	0.55690	-0.13870	0.49460
41	C2	7	2	2.	1.0	7	0.63350	-0.04600	0.62640
42	C3	7	3	2.	1.0	7	0.57740	0.09250	0.62950
43	H1	7	4	2.	1.0	7	0.59862	-0.24040	0.49064
44	H2	7	5	2.	1.0	7	0.73115	-0.07965	0.71886
45	H3	7	6	2.	1.0	7	0.63445	0.16068	0.72495
46	XTRA	7	7	2.	1.0	7	0.50000	0.0	0.50000
47	C1	7	8	2.	1.0	7	0.44310	0.13870	0.50540
48	C2	7	9	2.	1.0	7	0.36650	0.04600	0.37360
49	C3	7	10	2.	1.0	7	0.42260	-0.09250	0.37050
50	H1	7	11	2.	1.0	7	0.40138	0.24040	0.50936
51	H2	7	12	2.	1.0	7	0.26885	0.07965	0.28114
52	H3	7	13	2.	1.0	7	0.36555	-0.16068	0.27505

ABOVE ATOMS USED TO COMPUTE STRUCTURE FACTORS

ZMC
4.0

I	NAME(I)	ZAM(I)
1	C1	1.0
2	C2	1.0
3	C3	1.0
4	H1	1.0
5	H2	1.0
6	H3	1.0
7	XTRA	1.0
8	C1	1.0
9	C2	1.0
10	C3	1.0
11	H1	1.0
12	H2	1.0
13	H3	1.0

J	IZ(J)	IU(J)	IV(J)	IW(J)	SSR(J)	STR(J)	SXR(J)	SYR(J)	SZR(J)	TR(1,J)	TR(2,J)	TR(3,J)
1	7	0	0	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

KPWS	KPW	WOBS	SIGWO
0	0	0.0	0.0

I	NAME(I)	P(I)	DP(I)	PMN(I)	PMX(I)	KP(I)	KO(I)	DKT(KO)	SP(I)	ISBP(I)
1	PLC	24.023720	0.010000	0.0	0.0	0	0	0.0	0.0	0
2	PLH	5.702180	0.010000	0.0	0.0	0	0	0.0	0.0	0
3	BCC	87.802100	0.010000	0.0	0.0	0	0	0.0	0.0	0
4	BCH	15.656200	0.010000	0.0	0.0	0	0	0.0	0.0	0
5	BHH	2.791700	0.010000	0.0	0.0	0	0	0.0	0.0	0
6	CCC	3.600000	0.010000	0.0	0.0	0	0	0.0	0.0	0
7	CCH	3.670000	0.010000	0.0	0.0	0	0	0.0	0.0	0
8	CHH	3.740000	0.010000	0.0	0.0	0	0	0.0	0.0	0
9	QH	0.153000	0.001000	0.0	0.0	0	0	0.0	0.0	0
10	A	7.440000	0.000010	6.440000	8.440000	1	1	1.000	0.0	4
11	B	9.550000	0.000010	8.550000	10.550000	1	1	1.000	0.0	4
12	C	6.920000	0.000010	5.920000	7.920000	1	1	1.000	0.0	4
13	COSA	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	4
14	COSB	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	4
15	COSG	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	4
16	RX	0.0	0.000010	-0.200000	0.200000	1	1	1.000	0.0	4
17	RY	0.0	0.000010	-0.200000	0.200000	1	1	1.000	0.0	4
18	RZ	0.0	0.000010	-0.200000	0.200000	1	1	1.000	0.0	4
19	TX	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	4
20	TY	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	4
21	TZ	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	4

NG	NV	NOV	LS	IWT
6	6	6	0	0

TEST PROBLEM 2B. MINIMIZE ENERGY BY MODIFIED ROSENBROCK SEARCH 01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

CYCLE 1

CSF	VSF	QMAX	NF
3.931619	-3.668453	0.420000	19
3.935609	-3.669434	0.490000	28

SOK	SPLK	SPPK
-27.059665	-32.616885	5.622002

SGK	SVDW	WR	RMAX	NG	NSRB
20.785827	13.519360	7.039483	4.650000	244	66
20.788421	13.439722	7.102872	5.430000	408	66

GX	GY	GZ	I	J	GM	R	NAMES		CMB	VDW	REP	SRB
0	0	0	1	4	1.00000	1.02000	C1	H1	-7.623	-121.643	0.0	1.0
0	0	0	3	6	1.00000	1.02000	C3	H3	-7.623	-121.643	0.0	1.0

0	0	0	8	11	1.00000	1.02000	C1	H1	-7.623	-121.643	0.0	1.0
0	0	0	10	13	1.00000	1.02000	C3	H3	-7.623	-121.643	0.0	1.0
0	0	0	2	5	1.00000	1.02003	C2	H2	-7.623	-121.617	0.0	1.0
0	0	0	9	12	1.00000	1.02003	C2	H2	-7.623	-121.617	0.0	1.0
0	0	0	2	3	1.00000	1.36713	C2	C3	5.606	-81.016	0.0	1.0
0	0	0	9	10	1.00000	1.36713	C2	C3	5.606	-81.016	0.0	1.0
0	0	0	1	10	1.00000	1.38944	C1	C3	5.596	-80.213	0.0	1.0
0	0	0	3	8	1.00000	1.38944	C3	C1	5.596	-80.213	0.0	1.0
0	0	0	1	2	1.00000	1.39297	C1	C2	5.582	-79.000	0.0	1.0
0	0	0	8	9	1.00000	1.39297	C1	C2	5.582	-79.000	0.0	1.0
0	0	0	2	6	1.00000	2.08830	C2	H3	-3.723	-1.652	0.0	1.0
0	0	0	9	13	1.00000	2.08830	C2	H3	-3.723	-1.652	0.0	1.0
0	0	0	1	13	1.00000	2.09262	C1	H3	-3.716	-1.631	0.0	1.0
0	0	0	6	8	1.00000	2.09262	H3	C1	-3.716	-1.631	0.0	1.0
0	0	0	3	5	1.00000	2.09612	C3	H2	-3.710	-1.615	0.0	1.0
0	0	0	10	12	1.00000	2.09612	C3	H2	-3.710	-1.615	0.0	1.0
0	0	0	2	4	1.00000	2.09681	C2	H1	-3.708	-1.612	0.0	1.0
0	0	0	9	11	1.00000	2.09681	C2	H1	-3.708	-1.612	0.0	1.0
0	0	0	3	11	1.00000	2.09790	C3	H1	-3.706	-1.607	0.0	1.0
0	0	0	4	10	1.00000	2.09790	H1	C3	-3.706	-1.607	0.0	1.0
0	0	0	1	5	1.00000	2.09930	C1	H2	-3.704	-1.600	0.0	1.0
0	0	0	8	12	1.00000	2.09930	C1	H2	-3.704	-1.600	0.0	1.0
0	0	0	1	3	1.00000	2.40204	C1	C3	3.237	-3.005	0.0	1.0
0	0	0	8	10	1.00000	2.40204	C1	C3	3.237	-3.005	0.0	1.0
0	0	0	5	6	1.00000	2.40564	H2	H3	3.232	-0.168	0.0	1.0
0	0	0	12	13	1.00000	2.40564	H2	H3	3.232	-0.168	0.0	1.0
0	0	0	2	10	1.00000	2.40730	C2	C3	3.230	-2.966	0.0	1.0
0	0	0	3	9	1.00000	2.40730	C3	C2	3.230	-2.966	0.0	1.0
0	0	0	4	13	1.00000	2.41086	H1	H3	3.225	-0.166	0.0	1.0
0	0	0	6	11	1.00000	2.41086	H3	H1	3.225	-0.166	0.0	1.0
0	0	0	1	9	1.00000	2.41228	C1	C2	3.223	-2.929	0.0	1.0
0	0	0	2	8	1.00000	2.41228	C2	C1	3.223	-2.929	0.0	1.0
0	0	0	4	5	1.00000	2.41311	H1	H2	3.222	-0.165	0.0	1.0
0	0	0	11	12	1.00000	2.41311	H1	H2	3.222	-0.165	0.0	1.0
-1	-1	0	6	25	1.00000	2.67419	H3	H2	2.908	-0.089	0.127	0.0
-1	0	0	5	26	1.00000	2.67419	H2	H3	2.908	-0.089	0.127	0.0
0	0	-1	4	36	1.00000	2.73179	H1	H2	2.846	-0.078	0.102	0.0
0	0	0	5	37	1.00000	2.73179	H2	H1	2.846	-0.078	0.102	0.0
-1	-1	0	6	24	1.00000	2.73230	H3	H1	2.846	-0.078	0.102	0.0
-1	0	0	4	26	1.00000	2.73230	H1	H3	2.846	-0.078	0.102	0.0
0	0	0	3	10	1.00000	2.76769	C3	C3	2.809	-1.284	0.0	1.0
0	0	0	1	8	1.00000	2.78216	C1	C1	2.795	-1.244	0.0	1.0
0	-1	-1	11	39	1.00000	2.78798	H1	H3	2.789	-0.069	0.083	0.0
0	0	0	4	32	1.00000	2.78798	H1	H3	2.789	-0.069	0.083	0.0
0	0	0	2	9	1.00000	2.78897	C2	C2	2.788	-1.236	0.0	1.0
-1	0	-1	4	45	1.00000	2.81141	H1	H3	2.766	-0.066	0.076	0.0
0	0	0	11	52	1.00000	2.81141	H1	H3	2.766	-0.066	0.076	0.0
-1	0	-1	1	45	1.00000	2.96634	C1	H3	-2.621	-0.201	0.293	0.0
0	0	0	8	52	1.00000	2.96634	C1	H3	-2.621	-0.201	0.293	0.0
-1	-1	0	3	24	1.00000	3.04831	C3	H1	-2.553	-0.171	0.218	0.0
-1	0	0	4	23	1.00000	3.04831	H1	C3	-2.553	-0.171	0.218	0.0
0	-1	-1	8	39	1.00000	3.07634	C1	H3	-2.528	-0.162	0.196	0.0
0	0	0	1	32	1.00000	3.07634	C1	H3	-2.528	-0.162	0.196	0.0
-1	0	-1	3	44	1.00000	3.18100	C3	H2	-2.444	-0.132	0.133	0.0
0	0	0	10	51	1.00000	3.18100	C3	H2	-2.444	-0.132	0.133	0.0
-1	0	0	5	47	1.00000	3.18174	H2	C1	-2.444	-0.132	0.133	0.0
0	0	0	1	51	1.00000	3.18174	C1	H2	-2.444	-0.132	0.133	0.0
-1	0	0	5	48	1.00000	3.19544	H2	C2	-2.433	-0.129	0.126	0.0
0	0	0	2	51	1.00000	3.19544	C2	H2	-2.433	-0.129	0.126	0.0
-1	0	-1	2	44	1.00000	3.22604	C2	H2	-2.410	-0.122	0.113	0.0
0	0	0	9	51	1.00000	3.22604	C2	H2	-2.410	-0.122	0.113	0.0
-1	0	0	5	49	1.00000	3.23114	H2	C3	-2.407	-0.120	0.111	0.0
0	0	0	3	51	1.00000	3.23114	C3	H2	-2.407	-0.120	0.111	0.0
-1	0	-1	1	44	1.00000	3.23663	C1	H2	-2.402	-0.119	0.109	0.0
0	0	0	8	51	1.00000	3.23663	C1	H2	-2.402	-0.119	0.109	0.0
0	0	-1	4	35	1.00000	3.25293	H1	C2	-2.399	-0.116	0.102	0.0
0	0	0	2	37	1.00000	3.25293	C2	H1	-2.399	-0.116	0.102	0.0
0	0	0	1	6	1.00000	3.32387	C1	H3	-2.339	-0.102	0.0	1.0
0	0	0	8	13	1.00000	3.32387	C1	H3	-2.339	-0.102	0.0	1.0
0	0	0	3	4	1.00000	3.32499	C3	H1	-2.339	-0.101	0.0	1.0
0	0	0	10	11	1.00000	3.32499	C3	H1	-2.339	-0.101	0.0	1.0
0	0	0	2	13	1.00000	3.32943	C2	H3	-2.335	-0.101	0.0	1.0
0	0	0	6	9	1.00000	3.32943	H3	C2	-2.335	-0.101	0.0	1.0
0	0	0	3	12	1.00000	3.33109	C3	H2	-2.334	-0.100	0.0	1.0
0	0	0	5	10	1.00000	3.33109	H2	C3	-2.334	-0.100	0.0	1.0
0	0	0	2	11	1.00000	3.33456	C2	H1	-2.332	-0.100	0.0	1.0
0	0	0	4	9	1.00000	3.33456	H1	C2	-2.332	-0.100	0.0	1.0
0	0	0	1	12	1.00000	3.33512	C1	H2	-2.331	-0.100	0.0	1.0

WC	WV	WR	WX	WT
-2.336	-17.225	7.103	0.0	-12.457

TEST PROBLEM 28. MINIMIZE ENERGY BY MODIFIED ROSENBROCK SEARCH 01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

WOBS	WCALC BEFORE CYCLE 1
0.0	-12.4574

SEARCH FOR MINIMUM ENERGY

I	EPS(I)	P(I)	WTR
10	0.1000000D-03	7.440100	-12.457319
10	-0.5000000D-04	7.439950	-12.457376
11	0.1000000D-03	9.550100	-12.457317
11	-0.5000000D-04	9.549950	-12.457405
12	0.1000000D-03	6.920100	-12.457354
12	-0.5000000D-04	6.919950	-12.457431
16	0.1000000D-03	0.000100	-12.457445
16	0.3000000D-03	0.000400	-12.457482
16	0.9000000D-03	0.001300	-12.457547
16	0.2700000D-02	0.004000	-12.457338
17	0.1000000D-03	0.000100	-12.457487
17	-0.5000000D-04	-0.000050	-12.457577
18	0.1000000D-03	0.000100	-12.457606
18	0.3000000D-03	0.000400	-12.457692
18	0.9000000D-03	0.001300	-12.457936
18	0.2700000D-02	0.004000	-12.458554
18	0.8100000D-02	0.012100	-12.459426
18	0.2430000D-01	0.036400	-12.454221
*	0.2500000D 00		-12.459355
*	-0.1250000D 00		-12.459375
*	0.8250000D-01		-12.459430
10	-0.5000000D-04	7.439897	-12.459452
10	-0.1500000D-03	7.439747	-12.459519
10	-0.4500000D-03	7.439297	-12.459718
10	-0.1350000D-02	7.437947	-12.460313
10	-0.4050000D-02	7.433897	-12.462055
10	-0.1215000D-01	7.421747	-12.466907
10	-0.3645000D-01	7.385297	-12.477991
10	-0.1093500D 00	7.275947	-12.477117
11	-0.5000000D-04	9.549897	-12.478016
11	-0.1500000D-03	9.549747	-12.478093
11	-0.4500000D-03	9.549297	-12.478324
11	-0.1350000D-02	9.547947	-12.479013
11	-0.4050000D-02	9.543897	-12.481053
11	-0.1215000D-01	9.531747	-12.486946
11	-0.3645000D-01	9.495297	-12.502493
11	-0.1093500D 00	9.385947	-12.528316
11	-0.3280500D 00	9.057897	-12.366892
12	-0.5000000D-04	6.919897	-12.528324
12	-0.1500000D-03	6.919747	-12.528349
12	-0.4500000D-03	6.919297	-12.528425
12	-0.1350000D-02	6.917947	-12.528645
12	-0.4050000D-02	6.913897	-12.529261
12	-0.1215000D-01	6.901747	-12.530685
12	-0.3645000D-01	6.865297	-12.531047
12	-0.1093500D 00	6.755947	-12.494081
16	0.9000000D-03	0.002281	-12.531202

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 16    0.2700000D-02          0.004981        -12.531182
 17   -0.5000000D-04         -0.000103        -12.531229
 17   -0.1500000D-03         -0.000253        -12.531307
 17   -0.4500000D-03         -0.000703        -12.531536
 17   -0.1350000D-02         -0.002053        -12.532162
 17   -0.4050000D-02         -0.006103        -12.533486
 17   -0.1215000D-01         -0.018253        -12.532332
 18    0.8100000D-02          0.020956        -12.531838
 18   -0.4050000D-02          0.008806        -12.533715
  *    0.2500000D 00                          -12.525457
  *   -0.1250000D 00                          -12.533448
  *    0.6250000D-01                          -12.532771
  *   -0.3125000D-01                          -12.533915
 10   -0.3645000D-01          7.350555        -12.527490
 10    0.1822500D-01          7.405230        -12.534771
 11   -0.1093500D 00          9.281722        -12.521381
 11    0.5467750D-01          9.445747        -12.527653
 11   -0.2733375D-01          9.363734        -12.535014
 12   -0.3645000D-01          6.830555        -12.528952
 12    0.1822500D-01          6.885230        -12.535742
 16    0.9000000D-03          0.003151        -12.535957
 16    0.2700000D-02          0.005851        -12.536135
 16    0.8100000D-02          0.013951        -12.532471
 17   -0.4050000D-02         -0.009964        -12.536534
 17   -0.1215000D-01         -0.022114        -12.532484
 18   -0.4050000D-02          0.004859        -12.537555
 18   -0.1215000D-01         -0.007291        -12.538054
 18   -0.3645000D-01         -0.043741        -12.512184
  *    0.2500000D 00                          -12.538559
  *    0.7500000D 00                          -12.538645
  *    0.2250000D 01                          -12.525305
 10    0.1822250D-01          7.443388        -12.537886
 10   -0.9112250D-02          7.416050        -12.538462
 10    0.4556250D-02          7.429719        -12.538595
 10   -0.2278125D-02          7.422885        -12.538635
 10    0.1139062D-02          7.426302        -12.538642
 10   -0.5695310D-03          7.424593        -12.538645
 11   -0.2733750D-01          9.314185        -12.540217
 11   -0.8201250D-01          9.232172        -12.530972
 12    0.1822500D-01          6.923388        -12.540389
 12    0.5467750D-01          6.978063        -12.532432
 16    0.2700000D-02          0.012120        -12.541213
 16    0.8100000D-02          0.020220        -12.539611
 17   -0.4050000D-02         -0.017875        -12.541144
 17    0.2025000D-02         -0.011800        -12.540925
 17   -0.1012500D-02         -0.014837        -12.541277
 18   -0.1215000D-01         -0.035538        -12.537427
 18    0.6075000D-02         -0.017313        -12.541453

PARAMETERS AFTER CYCLE  1
  I     NAMP      OLD P       CHANGE       NEW P
 10     A       7.440000   -0.014837    7.425163
 11     B       9.550000   -0.235815    9.314185
 12     C       6.920000    0.003388    6.923388
 16     RX      0.0         0.012120    0.012120
 17     RY      0.0        -0.014837   -0.014837
 18     RZ      0.0        -0.017313   -0.017313

NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGY CALCULATION FOR THIS CYCLE
                 NT      SEC      AVT
INITIAL          97      0.03     0.0003
COORDINATES      97      0.19     0.0020
SLOW RECIP        1      0.05     0.0500
FAST RECIP       96      4.99     0.0520
UNIT CELL        61      0.0      0.0
SLOW DIRECT       1      0.34     0.3400
FAST DIRECT      96      4.46     0.0465
SLOW CONFIG       1      0.0      0.0
FAST CONFIG      96      0.01     0.0001

TOTAL TIME (SEC)      10.07

SUMMATION LIMITS FOR MINIMUM TIME
   DEL  IS PROPORTIONAL TO RELATIVE ERROR OF RESULT
   PRQ  IS RECOMMENDED QLIM
   PRR  IS RECOMMENDED RLIM
   PRK  IS RECOMMENDED VALUE OF CK
   PRT  IS PREDICTED TOTAL TIME PER CYCLE FOR RECIPROCAL AND DIRECT SUMS

   DEL       PRQ       PRR       PRK       PRT
1.0E-2   0.33126   3.73116   0.27605     3.11
1.0E-3   0.41647   4.69086   0.28140     6.19
1.0E-4   0.48666   5.48144   0.28460     9.88
1.0E-5   0.54786   6.17075   0.28684    14.09
1.0E-6   0.60307   6.79259   0.28855    18.79
1.0E-7   0.65673   7.39698   0.28931    24.27


TEST PROBLEM 28. MINIMIZE ENERGY BY MODIFIED ROSENBROCK SEARCH                01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

CYCLE  2

      WC        WV        WR        WX        WT
   -2.442   -18.404     8.304     0.0     -12.542

TEST PROBLEM 28. MINIMIZE ENERGY BY MODIFIED ROSENBROCK SEARCH                01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

      WOBS        WCALC BEFORE CYCLE  2
    0.0        -12.5423

PARAMETERS AFTER CYCLE  2
  I     NAMP      OLD P       CHANGE       NEW P
 10     A       7.425163   -0.025620    7.399542
 11     B       9.314185   -0.031930    9.282255
 12     C       6.923388    0.037197    6.960585
 16     RX      0.012120    0.005443    0.017563
 17     RY     -0.014837   -0.006815   -0.021652
 18     RZ     -0.017313   -0.007517   -0.024830


TEST PROBLEM 28. MINIMIZE ENERGY BY MODIFIED ROSENBROCK SEARCH                01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

CYCLE  3

          CSF          VSF          OMAX          NF
     3.784069    -3.455749      0.420000          17
     3.789477    -3.457902      0.490000          28

          SQK          SPLK          SPPK
   -27.059665   -33.544459      5.622002
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SGK	SVDW	WR	RMAX	NG	NSRB
20.804611	12.987590	8.326287	4.650000	246	66
20.810386	12.997322	8.398326	5.430000	424	66

GX	GY	GZ	I	J	GM	R	NAMES		CMB	VDW	REP	SRB
0	0	0	1	4	1.00000	1.02000	C1	H1	-7.623	-121.643	0.0	1.0
0	0	0	3	6	1.00000	1.02000	C3	H3	-7.623	-121.643	0.0	1.0
0	0	0	8	11	1.00000	1.02000	C1	H1	-7.623	-121.643	0.0	1.0
0	0	0	10	13	1.00000	1.02000	C3	H3	-7.623	-121.643	0.0	1.0
0	0	0	2	5	1.00000	1.02003	C2	H2	-7.623	-121.617	0.0	1.0
0	0	0	9	12	1.00000	1.02003	C2	H2	-7.623	-121.617	0.0	1.0
0	0	0	2	3	1.00000	1.38713	C2	C3	5.606	-81.016	0.0	1.0
0	0	0	9	10	1.00000	1.38713	C2	C3	5.606	-81.016	0.0	1.0
0	0	0	1	10	1.00000	1.38944	C1	C3	5.596	-80.213	0.0	1.0
0	0	0	3	8	1.00000	1.38944	C3	C1	5.596	-80.213	0.0	1.0
0	0	0	1	2	1.00000	1.39297	C1	C2	5.582	-79.000	0.0	1.0
0	0	0	8	9	1.00000	1.39297	C1	C2	5.582	-79.000	0.0	1.0
0	0	0	2	6	1.00000	2.08830	C2	H3	-3.723	-1.652	0.0	1.0
0	0	0	9	13	1.00000	2.08830	C2	H3	-3.723	-1.652	0.0	1.0
0	0	0	1	13	1.00000	2.09262	C1	H3	-3.716	-1.631	0.0	1.0
0	0	0	6	8	1.00000	2.09262	H3	C1	-3.716	-1.631	0.0	1.0
0	0	0	3	5	1.00000	2.09612	C3	H2	-3.710	-1.615	0.0	1.0
0	0	0	10	12	1.00000	2.09612	C3	H2	-3.710	-1.615	0.0	1.0
0	0	0	2	4	1.00000	2.09681	C2	H1	-3.708	-1.612	0.0	1.0
0	0	0	9	11	1.00000	2.09681	C2	H1	-3.708	-1.612	0.0	1.0
0	0	0	3	11	1.00000	2.09790	C3	H1	-3.706	-1.607	0.0	1.0
0	0	0	4	10	1.00000	2.09790	H1	C3	-3.706	-1.607	0.0	1.0
0	0	0	1	5	1.00000	2.09930	C1	H2	-3.704	-1.600	0.0	1.0
0	0	0	8	12	1.00000	2.09930	C1	H2	-3.704	-1.600	0.0	1.0
0	0	0	1	3	1.00000	2.40204	C1	C3	3.237	-3.005	0.0	1.0
0	0	0	8	10	1.00000	2.40204	C1	C3	3.237	-3.005	0.0	1.0
0	0	0	5	6	1.00000	2.40564	H2	H3	3.232	-0.168	0.0	1.0
0	0	0	12	13	1.00000	2.40564	H2	H3	3.232	-0.168	0.0	1.0
0	0	0	2	10	1.00000	2.40730	C2	C3	3.230	-2.966	0.0	1.0
0	0	0	3	9	1.00000	2.40730	C3	C2	3.230	-2.966	0.0	1.0
0	0	0	4	13	1.00000	2.41086	H1	H3	3.225	-0.166	0.0	1.0
0	0	0	6	11	1.00000	2.41086	H3	H1	3.225	-0.166	0.0	1.0
0	0	0	1	9	1.00000	2.41228	C1	C2	3.223	-2.929	0.0	1.0
0	0	0	2	8	1.00000	2.41228	C2	C1	3.223	-2.929	0.0	1.0
0	0	0	4	5	1.00000	2.41311	H1	H2	3.222	-0.165	0.0	1.0
0	0	0	11	12	1.00000	2.41311	H1	H2	3.222	-0.165	0.0	1.0
-1	-1	0	6	25	1.00000	2.59554	H3	H2	2.996	-0.106	0.170	0.0
-1	0	0	5	26	1.00000	2.59554	H2	H3	2.996	-0.106	0.170	0.0
0	0	-1	4	38	1.00000	2.62599	H1	H2	2.961	-0.099	0.152	0.0
0	0	0	5	37	1.00000	2.62599	H2	H1	2.961	-0.099	0.152	0.0
-1	-1	0	6	24	1.00000	2.73564	H3	H1	2.842	-0.078	0.101	0.0
-1	0	0	4	26	1.00000	2.73564	H1	H3	2.842	-0.078	0.101	0.0
0	-1	-1	11	39	1.00000	2.74207	H1	H3	2.836	-0.076	0.098	0.0
0	0	0	4	32	1.00000	2.74207	H1	H3	2.836	-0.076	0.098	0.0
0	0	0	3	10	1.00000	2.76769	C3	C3	2.809	-1.284	0.0	1.0
-1	0	-1	4	45	1.00000	2.76827	H1	H3	2.809	-0.072	0.089	0.0
0	0	0	11	52	1.00000	2.76827	H1	H3	2.809	-0.072	0.089	0.0
0	0	0	1	8	1.00000	2.78218	C1	C1	2.795	-1.244	0.0	1.0
0	0	0	2	9	1.00000	2.78897	C2	C2	2.788	-1.226	0.0	1.0
-1	0	-1	1	45	1.00000	2.95492	C1	H3	-2.631	-0.206	0.305	0.0
0	0	0	8	52	1.00000	2.95492	C1	H3	-2.631	-0.206	0.305	0.0
-1	-1	0	3	24	1.00000	2.97679	C3	H1	-2.612	-0.197	0.282	0.0
-1	0	0	4	23	1.00000	2.97679	H1	C3	-2.612	-0.197	0.282	0.0
0	-1	-1	8	39	1.00000	2.97748	C1	H3	-2.612	-0.197	0.281	0.0
0	0	0	1	32	1.00000	2.97748	C1	H3	-2.612	-0.197	0.281	0.0
0	0	-1	4	35	1.00000	3.16990	H1	C2	-2.453	-0.135	0.139	0.0
0	0	0	2	37	1.00000	3.16990	C2	H1	-2.453	-0.135	0.139	0.0
-1	0	0	5	49	1.00000	3.17387	H2	C3	-2.450	-0.134	0.137	0.0
0	0	0	3	51	1.00000	3.17387	C3	H2	-2.450	-0.134	0.137	0.0
-1	0	0	5	48	1.00000	3.17582	H2	C2	-2.448	-0.134	0.136	0.0
0	0	0	2	51	1.00000	3.17582	C2	H2	-2.448	-0.134	0.136	0.0
-1	0	-1	1	44	1.00000	3.18931	C1	H2	-2.438	-0.130	0.129	0.0
0	0	0	8	51	1.00000	3.18931	C1	H2	-2.438	-0.130	0.129	0.0
-1	0	0	5	47	1.00000	3.21036	H2	C1	-2.422	-0.125	0.120	0.0
0	0	0	1	51	1.00000	3.21036	C1	H2	-2.422	-0.125	0.120	0.0
-1	0	-1	3	44	1.00000	3.21938	C3	H2	-2.415	-0.123	0.116	0.0
0	0	0	10	51	1.00000	3.21938	C3	H2	-2.415	-0.123	0.116	0.0
-1	0	-1	2	44	1.00000	3.22663	C2	H2	-2.410	-0.121	0.113	0.0
0	0	0	9	51	1.00000	3.22663	C2	H2	-2.410	-0.121	0.113	0.0
-1	-1	0	6	22	1.00000	3.29993	H3	C2	-2.356	-0.106	0.086	0.0
-1	0	0	2	26	1.00000	3.29993	C2	H3	-2.356	-0.106	0.086	0.0
0	-1	0	3	30	1.00000	3.31129	C3	H1	-2.348	-0.104	0.083	0.0
0	0	-1	10	37	1.00000	3.31129	C3	H1	-2.348	-0.104	0.083	0.0
0	0	0	1	6	1.00000	3.32387	C1	H3	-2.339	-0.102	0.0	1.0
0	0	0	8	13	1.00000	3.32387	C1	H3	-2.339	-0.102	0.0	1.0
0	0	0	3	4	1.00000	3.32499	C3	H1	-2.339	-0.101	0.0	1.0
0	0	0	10	11	1.00000	3.32499	C3	H1	-2.339	-0.101	0.0	1.0
0	0	0	2	13	1.00000	3.32943	C2	H3	-2.335	-0.101	0.0	1.0
0	0	0	6	9	1.00000	3.32943	H3	C2	-2.335	-0.101	0.0	1.0
0	0	0	3	12	1.00000	3.33109	C3	H2	-2.334	-0.100	0.0	1.0

WC	WV	WR	WX	WT
-2.460	-18.483	8.398	0.0	-12.545

TEST PROBLEM 28. MINIMIZE ENERGY BY MODIFIED ROSENBROCK SEARCH 01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

WOBS	WCALC BEFORE CYCLE 3
0.0	-12.5445

J	NAME	IKA	IRB	X	Y	Z
1	C1	1	1	-0.06180	0.14143	-0.00739
2	C2	1	1	-0.13315	0.04635	0.12760
3	C3	1	1	-0.07220	-0.09492	0.13271
4	H1	2	1	-0.10711	0.24513	-0.01281
5	H2	2	1	-0.23054	0.08026	0.22093
6	H3	2	1	-0.12542	-0.16488	0.23053
7	XTRA	0	1	0.0	0.0	0.0
8	C1	1	1	0.06180	-0.14143	0.00739
9	C2	1	1	0.13315	-0.04635	-0.12760
10	C3	1	1	0.07220	0.09492	-0.13271
11	H1	2	1	0.10711	-0.24513	0.01281
12	H2	2	1	0.23054	-0.08026	-0.22093
13	H3	2	1	0.12542	0.16488	-0.23053

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TEST PROBLEM 28. MINIMIZE ENERGY BY MODIFIED ROSENBROCK SEARCH 01-06-81
BENZENE. POTENTIAL OF WILLIAMS AND STARR (1977). C-H BOND SHORTENED.

MODE	NC	NPC	ILSQ	IWGT	IPLM	IPRT	NSTG	IBPC	ARE	SLIM	CMPR	XDRD	EPSC
3	2	9	0	0	0	2	4	0	0.100D-03	0.100D-05	0.0	0.200D-02	0.100D 02

PLC	PLH	BCC	BCH	BHH	CCC	CCH	CHH
QH							
24.02372	5.70218	87.80210	15.65620	2.79170	3.60000	3.67000	3.74000
0.15300							

NA	NKA	NS	ICENT	HXNEG	HYNEG	HZNEG	NRB	NPX	NRP	ICMB	IVDW	IREP	IMOL	NCT	IRSC	IZAM	IGEM	IRBA	ISETA
13	2	8	2	0.0	0.0	0.0	1	0	8	1	1	2	0	0	2	0	0	0	0

ND	NV	NOV	LS	IWT
6	6	6	0	0

```
                    PARAMETERS AFTER EACH CYCLE
 J  NAMP    DKT     INITIAL      1          2
10  A      1.000   7.440000   7.425163   7.399542
11  B      1.000   9.550000   9.314185   9.282255
12  C      1.000   6.920000   6.923388   6.960585
16  RX     1.000   0.0        0.012120   0.017563
17  RY     1.000   0.0       -0.014837  -0.021652
18  RZ     1.000   0.0       -0.017313  -0.024830

            W     -12.4574   -12.5423   -12.5445
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10.3 Ethane and Propane, Mode 0 and Mode 4

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DYNAMIC DIMENSIONS FOR WMIN

  NPCMAX   NAMAX  NKAMAX   NSMAX  NRBMAX  NPXMAX  NCTMAX  NBCMAX
      17       8       2      12       8       0       3      10

    MMAX   NFSMAX  NGSMAX  NPSMAX   NPMAX  NOSMAX   NOMAX   NVMAX
      46       0      30      30      50      24      24      24

                     1          2          3          4          5          6          7          8          9         10
ARRAY              ACZ        AKE         AM       AMASS         AN         AR         BR        BTR       CHAR       CMBT
DIMEN-           (   9      (   0      ( NVMAX    (   1      ( NVMAX    (   1      (   1      ( NVMAX    (   1      (   1
 SIONS           *NRBMAX)   *   0   )  * NVMAX)   *NKAMAX)   * NVMAX)   *NKAMAX)   *NKAMAX)   *NGSMAX)   * NSMAX)   *NGSMAX)
WORDS                72          0        576          2        576          2          2        576         12         30
BYTES/WORD            8          8          8          8          8          8          8          8          8
HEX ADDRESS    00000000   00000240   00000240   00001440   00001450   00002650   00002660   00002670   00003870

                    11         12         13         14         15         16         17         18
ARRAY              CSV         DP        DPC        DPX         DW       DWDQ        DXQ        DYC
DIMEN-           (   1      (   1      (   1      (   1      (   1      (   1      ( NVMAX    (
 SIONS           *NGSMAX)   * NPMAX)   *NPCMAX)   *NPXMAX)   * NPMAX)   * NVMAX)   * NAMAX)
WORDS                30         50         17          0         50         24
BYTES/WORD            8          8          8          8          8          8                                                  8
HEX ADDRESS    00003948   00003A38   00003BC8   00003C50   00003C50   00003DF0                                          00009F08

                    21         22         23         24         25                                                   119        120
ARRAY              EPS        ERR       EVAL       EVEC                                                                 VN        VSV
DIMEN-           (   1      (   1      (   1      ( NVMAX                                                   (   1      (   1      (   1
 SIONS           * NPMAX)   * NVMAX)   * NVMAX)   * NVMAX                                                 * NVMAX)   * NVMAX)   *NGSMAX)
WORDS                50         24         24                                                                30         24         24         30
BYTES/WORD            8          8                                                                           4          8          8          8
HEX ADDRESS    00005160   000052F0   0000                                                            0000C698   0000C710   0000C7D0   0000C890

                    31                                                                                   125        126        127        128        129        130
ARRAY              HMT                                                                                   XC        XYZ       XYZC       XYZD       XYZN       XYZR
DIMEN-           (   1                                                                              ( NAMAX    (   3      (   3      (   3      (   3      (   3
 SIONS           *                                                                                  * NSMAX)   * NAMAX)   * NAMAX)   * NAMAX)   * NAMAX)   * NAMAX)
WORDS                                                                                                  46         96         24         24         24         24         24
BYTES/W                                                                                                 8          8          8          8          8          8          8
HE                                                                                            0000DD10   0000DEA0   0000E010   0000E310   0000E300   0000E490   0000E550   0000E610

                                                                  132        133
                                                                 ZAM         ZC
                                                            NAMAX    (   1      ( NAMAX    (
                                                          * NSMAX)   * NAMAX)   * NSMAX)   *
                                                                 96         8         96
 ES/WORD                                                          8         8          8
HEX ADDRESS                                               0000E6D0   0000E9D0   0000EA10

    7586 8-BYTE STORAGE LOCATIONS HAVE BEEN REQUESTED. THE PROGRAM IS DIMENSIONED FOR   12000
COMMON/S/ AND NST MAY BE DECREASED BY  4414 WORDS. THIS WILL REDUCE THE REGION USED BY  34K BYTES.
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TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES          01-06-81

  MODE     NC    NPC   ILSQ   IWGT   IPLM   IPRT   NSTG   IBPC          ARE          SLIM          CMPR          XDRD          EPSC
     0      1     17      0      0      0      2      4      0    0.100D-01    0.100D-05     0.0          0.200D-02    0.100D 02

 NAMPC(I)
    ARC       ARH       BRC       BRH       PLC       PLH       TBR       DCC
    KCC       DCH       KCH       ACCC      KCCC      ACCH      KCCH      AHCH
    KHCH

   PC(I)
 1.71100  1.23400  0.14070  0.14590 22.64000  4.94000  0.28167  1.40000
 4.26800  1.00000  6.35100102.00000  0.01169109.50000  0.01673110.00000
 0.01799

  DPC(I)
 0.00100  0.00100  0.00010  0.00010  0.01000  0.01000  0.00100  0.00100
 0.00100  0.00100  0.00100  0.10000  0.00010  0.10000  0.00010  0.10000
 0.00010

  KPC(I)
       2        2        2        2        1        1        3        3
       3        3        3        3        3        3        3        3
       3
```

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TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES          01-06-81
ETHANE. TOTALLY SYMMETRIC

   ISB
     1

    NA    NKA     NS ICENT HXNEG HYNEG HZNEG    NRB    NPX    NRP  ICMB   IVDW   IREP   IMOL    NCT   IRSC   IZAM   IGEM   IRBA ISETA
     2      2      6     2   1.0    1.0    0.0      2      0     10      0      1      1      1      2      0      2      0      1      0

      CK     NQ     NR
 0.0          1      1

 QLIM(I)
 0.0

 RLIM(I)
10.00000

    A(I)
 1.00000  1.00000  1.00000  0.0       0.0      -0.50000
```

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NAMS          TRANSFORMED X                          TRANSFORMED Y                          TRANSFORMED Z

          0.0      1.0*X   0.0*Y   0.0*Z        0.0      0.0*X   0.0*Y   0.0*Z        0.0      0.0*X   0.0*Y   1.0*Z
          0.0      0.0*X   0.0*Y   0.0*Z        0.0      1.0*X   0.0*Y   0.0*Z        0.0      0.0*X   0.0*Y   1.0*Z
          0.0     -1.0*X   0.0*Y   0.0*Z        0.0     -1.0*X   0.0*Y   0.0*Z        0.0      0.0*X   0.0*Y   1.0*Z
          0.0     -1.0*X   0.0*Y   0.0*Z        0.0      0.0*X   0.0*Y   0.0*Z        0.0      0.0*X   0.0*Y  -1.0*Z
          0.0      0.0*X   0.0*Y   0.0*Z        0.0     -1.0*X   0.0*Y   0.0*Z        0.0      0.0*X   0.0*Y  -1.0*Z
          0.0      1.0*X   0.0*Y   0.0*Z        0.0      1.0*X   0.0*Y   0.0*Z        0.0      0.0*X   0.0*Y  -1.0*Z

  K  NAMK          Q        PL        AR        BR      AMASS
  1  C        0.0      0.0       0.0       0.0     12.00390
  2  H        0.0      0.0       0.0       0.0      1.00810

  J  NAME    IKA   IRB          X         Y         Z
  1  C         1     1      0.0       0.0      0.76700
  2  H         2     2      1.02162   0.0      1.16110

  I  NAME    ISC   JAC   SMC   FMC   IRBC        XC        YC        ZC
  1  C         1     1    3.    1.0     1   0.0       0.0       0.76700
  2  H         1     2    1.    1.0     2   1.02162   0.0       1.16110
  3  H         2     2    1.    1.0     4   0.0       1.02162   1.16110
  4  H         3     2    1.    1.0     6  -1.02162  -1.02162   1.16110
  5  C         4     1    3.    1.0     7   0.0       0.0      -0.76700
  6  H         4     2    1.    1.0     8  -1.02162   0.0      -1.16110
  7  H         5     2    1.    1.0    10   0.0      -1.02162  -1.16110
  8  H         6     2    1.    1.0    12   1.02162   1.02162  -1.16110
ABOVE ATOMS USED TO COMPUTE STRUCTURE FACTORS

   ZNC
   1.0

  I  NAME(I)   ZAM(I)
  1    C         2.0
  2    H         6.0

  J IZ(J) IU(J) IV(J) IW(J)   SSR(J)   STR(J)   SXR(J)   SYR(J)   SZR(J)   TR(1,J)  TR(2,J)  TR(3,J)
  1    1    0    0    0    0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
  2    2    0    0    0    0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0

IACT    ICT                  IDZ                  IAZ                  ITBR
   1      5    2    3    4      8   10   10   10     14   14   14   16   16   16     -1    0    0    0
   5      1    6    7    8      8   10   10   10     14   14   14   16   16   16     -1    0    0    0

LBCI LBCJ
   1    5     1    2     1    3     1    4     5    6     5    7     5    8

  KPWS   KPW     WOBS     SIGWO
     0     0     0.0       0.0
```

```
TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES          01-06-81
PROPANE. TOTALLY SYMMETRIC

   ISB
    2

    NA    NKA     NS ICENT HXNEG HYNEG HZNEG    NRB    NPX    NRP   ICMB   IVDW   IREP   IMDL    NCT   IRSC   IZAN   IGEN   IRBA ISETA
     5      2      4     2   1.0    1.0    0.0      5      0     10      0      1      1      1      3      0      0      0      1      0

       CK     NQ     NR
  0.0          1      1

  QLIM(I)
  0.0

  RLIM(I)
 10.00000

     A(I)
 1.00000  1.00000  1.00000  0.0       0.0       0.0

NAMS          TRANSFORMED X                          TRANSFORMED Y                          TRANSFORMED Z

          0.0      1.0*X   0.0*Y   0.0*Z        0.0      0.0*X   1.0*Y   0.0*Z        0.0      0.0*X   0.0*Y   1.0*Z
          0.0      1.0*X   0.0*Y   0.0*Z        0.0      0.0*X  -1.0*Y   0.0*Z        0.0      0.0*X   0.0*Y   1.0*Z
          0.0     -1.0*X   0.0*Y   0.0*Z        0.0      0.0*X   1.0*Y   0.0*Z        0.0      0.0*X   0.0*Y   1.0*Z
          0.0     -1.0*X   0.0*Y   0.0*Z        0.0      0.0*X  -1.0*Y   0.0*Z        0.0      0.0*X   0.0*Y   1.0*Z

  K  NAMK          Q        PL        AR        BR      AMASS
  1  C        0.0      0.0       0.0       0.0     12.00390
  2  H        0.0      0.0       0.0       0.0      1.00810

  J  NAME    IKA   IRB          X         Y         Z
  1  C1        1     1      0.0       0.0       0.0
  2  C2        1     2      1.26808   0.0      -0.84891
  3  H1        2     3      0.0       0.87588   0.65883
  4  H21       2     4      2.16177   0.0      -0.22315
  5  H22       2     5      1.31300   0.88090  -1.49101

  I  NAME    ISC   JAC   SMC   FMC   IRBC        XC        YC        ZC
  1  C1        1     1    4.    1.0     1   0.0       0.0       0.0
  2  C2        1     2    2.    1.0     2   1.26808   0.0      -0.84891
  3  H1        1     3    2.    1.0     3   0.0       0.87588   0.65883
  4  H21       1     4    2.    1.0     4   2.16177   0.0      -0.22315
  5  H22       1     5    1.    1.0     5   1.31300   0.88090  -1.49101
  6  H1        2     3    2.    1.0     8   0.0      -0.87588   0.65883
  7  H22       2     5    1.    1.0    10   1.31300  -0.88090  -1.49101
  8  C2        3     2    2.    1.0    12  -1.26808   0.0      -0.84891
  9  H21       3     4    2.    1.0    14  -2.16177   0.0      -0.22315
 10  H22       3     5    1.    1.0    15  -1.31300   0.88090  -1.49101
 11  H22       4     5    1.    1.0    20  -1.31300  -0.88090  -1.49101
ABOVE ATOMS USED TO COMPUTE STRUCTURE FACTORS

   ZNC
   1.0

  I  NAME(I)   ZAM(I)
  1    C1        1.0
  2    C2        2.0
  3    H1        2.0
  4    H21       2.0
  5    H22       4.0

  J IZ(J) IU(J) IV(J) IW(J)   SSR(J)   STR(J)   SXR(J)   SYR(J)   SZR(J)   TR(1,J)  TR(2,J)  TR(3,J)
  1    1    0    0    0    0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
  2    2    0    0    0    0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
  3    3    0    0    0    0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
  4    4    0    0    0    0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
  5    5    0    0    0    0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0

IACT    ICT                  IDZ                  IAZ                  ITBR
   1      2    8    3    6      8    8   10   10     12   14   14   14   14   16     -1   -1    0    0
   2      1    4    5    7      8   10   10   10     14   14   14   16   16   16     -1    0    0    0
   8      1    9   10   11      8   10   10   10     14   14   14   16   16   16     -1    0    0    0

LBCI LBCJ
   1    2     1    8     1    3     1    6     2    4     2    5     2    7     8    9     8   10     3   11

  KPWS   KPW     WOBS     SIGWO
     0     0     0.0       0.0
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TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES 01-06-81

I	NAMP(I)	P(I)	DP(I)	PMN(I)	PMX(I)	KP(I)	KQ(I)	DKT(KQ)	SP(I)	ISBP(I)
1	ARC	1.711000	0.001000	0.0	0.0	0	0	0.0	0.0	0
2	ARH	1.234000	0.001000	0.0	0.0	0	0	0.0	0.0	0
3	BRC	0.140700	0.000100	0.0	0.0	0	0	0.0	0.0	0
4	BRH	0.145900	0.000100	0.0	0.0	0	0	0.0	0.0	0
5	PLC	22.640000	0.010000	0.0	0.0	0	0	0.0	0.0	0
6	PLH	4.940000	0.010000	0.0	0.0	0	0	0.0	0.0	0
7	TBR	0.281667	0.001000	0.0	0.0	0	0	0.0	0.0	0
8	DCC	1.400000	0.001000	0.0	0.0	0	1	1.000	0.0	0
9	KCC	4.268000	0.001000	0.0	0.0	0	0	0.0	0.0	0
10	DCH	1.000000	0.001000	0.0	0.0	0	1	1.000	0.0	0
11	KCH	6.351000	0.001000	0.0	0.0	0	0	0.0	0.0	0
12	ACCC	102.000000	0.100000	0.0	0.0	0	1	1.000	0.0	0
13	KCCC	0.011690	0.000100	0.0	0.0	0	0	0.0	0.0	0
14	ACCH	109.500000	0.100000	0.0	0.0	0	0	0.0	0.0	0
15	KCCH	0.016730	0.000100	0.0	0.0	0	0	0.0	0.0	0
16	AHCH	110.000000	0.100000	0.0	0.0	0	1	1.000	0.0	0
17	KHCH	0.017990	0.000100	0.0	0.0	0	0	0.0	0.0	0
18	A	1.000000	0.000010	0.0	2.000000	0	0	0.0	0.0	1
19	B	1.000000	0.000010	0.0	2.000000	0	0	0.0	0.0	1
20	C	1.000000	0.000010	0.0	2.000000	0	0	0.0	0.0	1
21	COSA	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	1
22	COSB	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	1
23	COSG	-0.500000	0.000010	-0.700000	-0.300000	0	0	0.0	0.0	1
24	TX	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	1
25	TY	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	1
26	TZ	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	1
27	TX	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	1
28	TY	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	1
29	TZ	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	1
30	A	1.000000	0.000010	0.0	2.000000	0	0	0.0	0.0	2
31	B	1.000000	0.000010	0.0	2.000000	0	0	0.0	0.0	2
32	C	1.000000	0.000010	0.0	2.000000	0	0	0.0	0.0	2
33	COSA	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	2
34	COSB	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	2
35	COSG	0.0	0.000010	-0.200000	0.200000	0	0	0.0	0.0	2
36	TX	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	2
37	TY	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	2
38	TZ	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	2
39	TX	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	2
40	TY	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	2
41	TZ	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	2
42	TX	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	2
43	TY	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	2
44	TZ	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	2
45	TX	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	2
46	TY	0.0	0.000010	-0.500000	0.500000	0	0	0.0	0.0	2
47	TZ	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	2
48	TX	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	2
49	TY	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	2
50	TZ	0.0	0.000010	-0.500000	0.500000	1	0	0.0	0.0	2

ND	NV	NOV	LS	IWT
13	4	0	1	0

TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES 01-06-81
ETHANE. TOTALLY SYMMETRIC

CYCLE 1

SGK	SVDW	WR	RMAX	NG	NSRB
0.0	-11.619650	45.300624	10.000000	8	0

GX	GY	GZ	I	J	GM	R	NAMES		CMB	VDW	REP	SRB
0	0	0	2	3	3.00000	1.76950	H	H	0.0	-0.795	3.197	0.0
0	0	0	2	4	3.00000	1.76950	H	H	0.0	-0.795	3.197	0.0
0	0	0	1	6	2.00000	2.18203	C	H	0.0	-1.036	4.106	0.0
0	0	0	1	7	2.00000	2.18203	C	H	0.0	-1.036	4.106	0.0
0	0	0	1	8	2.00000	2.18203	C	H	0.0	-1.036	4.106	0.0
0	0	0	2	7	3.00000	2.53699	H	H	0.0	-0.092	0.230	0.0
0	0	0	2	8	3.00000	2.53699	H	H	0.0	-0.092	0.230	0.0
0	0	0	2	6	3.00000	3.09313	H	H	0.0	-0.028	0.034	0.0

BOND DISTANCES

		IA	JA	DIJ	WD
C	C	1	5	1.5340	3.8318
C	H	1	2	1.0950	2.8658
C	H	1	3	1.0950	2.8658
C	H	1	4	1.0950	2.8658
C	H	5	6	1.0950	2.8658
C	H	5	7	1.0950	2.8658
C	H	5	8	1.0950	2.8658

BOND ANGLES

			IA	JA	KA	AIJK	WA
C	C	H	5	1	2	111.09	0.0213
C	C	H	5	1	3	111.09	0.0213
C	C	H	5	1	4	111.09	0.0213
H	C	H	2	1	3	107.80	0.0435
H	C	H	2	1	4	107.80	0.0435
H	C	H	3	1	4	107.80	0.0435
C	C	H	1	5	6	111.09	0.0213
C	C	H	1	5	7	111.09	0.0213
C	C	H	1	5	8	111.09	0.0213
H	C	H	6	5	7	107.80	0.0435
H	C	H	6	5	8	107.80	0.0435
H	C	H	7	5	8	107.80	0.0435

CONFORMATION ANGLES

				IA	JA	KA	LA	CNF	WCF
H	C	C	H	2	1	5	6	180.00	0.0000
H	C	C	H	2	1	5	7	60.00	0.0000
H	C	C	H	2	1	5	8	-60.00	0.0000
H	C	C	H	3	1	5	6	-60.00	0.0000
H	C	C	H	3	1	5	7	180.00	0.0000
H	C	C	H	3	1	5	8	60.00	0.0000
H	C	C	H	4	1	5	6	60.00	0.0000
H	C	C	H	4	1	5	7	-60.00	0.0000
H	C	C	H	4	1	5	8	180.00	0.0000

WC	WV	WR	WX	WT
0.0	-11.620	45.301	21.415	55.096

TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES 01-06-81
ETHANE. TOTALLY SYMMETRIC

WOBS	WCALC BEFORE CYCLE 1
0.0	55.0965

DERIVATIVES BEFORE CYCLE 1

J	NAMP(J)	DYC(J)	DDW/DP(I)DP(J) FOR I= 8 DCC	10 DCH	12 ACCC	16 AHCH
26	TZ	96.8350	-853.6000	1371.4544	0.0	-5.5752
27	TX	-210.2888	0.0	-3555.2440	0.0	-2.1507
29	TZ	-82.9369	0.0	-1371.4847	0.0	5.5752

RDWS	SDWS
0.245921D 03	0.604769D 05

NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGY CALCULATION FOR THIS CYCLE

	NT	SEC	AVT
INITIAL	23	0.0	0.0
COORDINATES	10	0.01	0.0010
SLOW RECIP	0	0.0	0.0
FAST RECIP	0	0.0	0.0
UNIT CELL	0	0.0	0.0
SLOW DIRECT	1	0.01	0.0100
FAST DIRECT	9	0.0	0.0
SLOW CONFIG	1	0.01	0.0100
FAST CONFIG	22	0.10	0.0045

TOTAL TIME (SEC) 0.13

TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES 01-06-81
PROPANE. TOTALLY SYMMETRIC

CYCLE 1

SGK	SVDW	WR	RMAX	NG	NSRB
0.0	-20.677452	77.608281	10.000000	27	0

GX	GY	GZ	I	J	GM	R	NAMES		CMS	VDW	REP	SRB
0	0	0	3	6	1.00000	1.75176	H1	H1	0.0	-0.845	3.397	0.0
0	0	0	4	5	2.00000	1.76178	H21	H22	0.0	-0.816	3.282	0.0
0	0	0	4	7	2.00000	1.76178	H21	H22	0.0	-0.816	3.282	0.0
0	0	0	5	7	2.00000	1.76180	H22	H22	0.0	-0.816	3.282	0.0
0	0	0	2	3	2.00000	2.15603	C2	H1	0.0	-1.113	4.496	0.0
0	0	0	2	6	2.00000	2.15603	C2	H1	0.0	-1.113	4.496	0.0
0	0	0	1	4	1.00000	2.17326	C1	H21	0.0	-1.062	4.234	0.0
0	0	0	1	9	1.00000	2.17326	C1	H21	0.0	-1.062	4.234	0.0
0	0	0	1	5	1.00000	2.17326	C1	H22	0.0	-1.062	4.234	0.0
0	0	0	1	7	1.00000	2.17326	C1	H22	0.0	-1.062	4.234	0.0
0	0	0	1	10	1.00000	2.17326	C1	H22	0.0	-1.062	4.234	0.0
0	0	0	1	11	1.00000	2.17326	C1	H22	0.0	-1.062	4.234	0.0
0	0	0	3	4	2.00000	2.49365	H1	H21	0.0	-0.101	0.267	0.0
0	0	0	3	9	2.00000	2.49365	H1	H21	0.0	-0.101	0.267	0.0
0	0	0	3	5	2.00000	2.51909	H1	H22	0.0	-0.095	0.245	0.0
0	0	0	3	10	2.00000	2.51909	H1	H22	0.0	-0.095	0.245	0.0
0	0	0	2	8	1.00000	2.53616	C2	C2	0.0	-1.926	6.553	0.0
0	0	0	5	10	2.00000	2.62600	H22	H22	0.0	-0.074	0.170	0.0
0	0	0	2	10	2.00000	2.80183	C2	H22	0.0	-0.231	0.472	0.0
0	0	0	2	11	2.00000	2.80183	C2	H22	0.0	-0.231	0.472	0.0
0	0	0	3	7	2.00000	3.07117	H1	H22	0.0	-0.029	0.037	0.0
0	0	0	3	11	2.00000	3.07117	H1	H22	0.0	-0.029	0.037	0.0
0	0	0	5	11	2.00000	3.16225	H22	H22	0.0	-0.024	0.027	0.0
0	0	0	2	9	2.00000	3.48647	C2	H21	0.0	-0.062	0.043	0.0
0	0	0	4	10	2.00000	3.80230	H21	H22	0.0	-0.008	0.003	0.0
0	0	0	4	11	2.00000	3.80230	H21	H22	0.0	-0.008	0.003	0.0
0	0	0	4	9	1.00000	4.32354	H21	H21	0.0	-0.004	0.001	0.0

BOND DISTANCES

		IA	JA	DIJ	WD
C1	C2	1	2	1.5260	3.3879
C1	C2	1	8	1.5260	3.3879
C1	H1	1	3	1.0960	2.9267
C1	H1	1	6	1.0960	2.9267
C2	H21	2	4	1.0910	2.6290
C2	H22	2	5	1.0910	2.6300
C2	H22	2	7	1.0910	2.6300
C2	H21	8	9	1.0910	2.6290
C2	H22	8	10	1.0910	2.6300
C2	H22	8	11	1.0910	2.6300

BOND ANGLES

			IA	JA	KA	AIJK	WA
C2	C1	C2	2	1	8	112.40	0.6322
C2	C1	H1	2	1	3	109.54	0.0000
C2	C1	H1	2	1	6	109.54	0.0000
C2	C1	H1	8	1	3	109.54	0.0000
C2	C1	H1	8	1	6	109.54	0.0000
H1	C1	H1	3	1	6	106.10	0.1368
C1	C2	H21	1	2	4	111.20	0.0242
C1	C2	H22	1	2	5	111.20	0.0242
C1	C2	H22	1	2	7	111.20	0.0242
H21	C2	H22	4	2	5	107.69	0.0481
H21	C2	H22	4	2	7	107.69	0.0481
H22	C2	H22	5	2	7	107.69	0.0480
C1	C2	H21	1	8	9	111.20	0.0242
C1	C2	H22	1	8	10	111.20	0.0242
C1	C2	H22	1	8	11	111.20	0.0242
H21	C2	H22	9	8	10	107.69	0.0481
H21	C2	H22	9	8	11	107.69	0.0481
H22	C2	H22	10	8	11	107.69	0.0480

CONFORMATION ANGLES

				IA	JA	KA	LA	CNF	WCF
C2	C1	C2	H21	8	1	2	4	180.00	0.0000
C2	C1	C2	H22	8	1	2	5	60.00	0.0000
C2	C1	C2	H22	8	1	2	7	-60.00	0.0000
H1	C1	C2	H21	3	1	2	4	57.99	0.0008
H1	C1	C2	H22	3	1	2	5	-62.01	0.0008
H1	C1	C2	H22	3	1	2	7	177.99	0.0008
H1	C1	C2	H21	6	1	2	4	-57.99	0.0008
H1	C1	C2	H22	6	1	2	5	-177.99	0.0008
H1	C1	C2	H22	6	1	2	7	62.01	0.0008
C2	C1	C2	H21	2	1	8	9	180.00	0.0000
C2	C1	C2	H22	2	1	8	10	-60.00	0.0000
C2	C1	C2	H22	2	1	8	11	60.00	0.0000
H1	C1	C2	H21	3	1	8	9	-57.99	0.0008
H1	C1	C2	H22	3	1	8	10	62.01	0.0008
H1	C1	C2	H22	3	1	8	11	-177.99	0.0008
H1	C1	C2	H21	6	1	8	9	57.99	0.0008
H1	C1	C2	H22	6	1	8	10	177.99	0.0008
H1	C1	C2	H22	6	1	8	11	-62.01	0.0008

WC	WV	WR	WX	WT
0.0	-20.677	77.608	29.619	86.550

TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES 01-06-81
PROPANE. TOTALLY SYMMETRIC

WOBS	WCALC BEFORE CYCLE 1
0.0	86.5496

DERIVATIVES BEFORE CYCLE 1

DDW/DP(I)DP(J) FOR I=

J	NAMP(J)	DYC(J)	8 DCC	10 DCH	12 ACCC	16 AHCH
38	TZ	62.3063	-474.8576	763.5397	0.7295	-1.5032
39	TX	98.8410	-709.3281	1145.0739	-0.4883	-4.6624
41	TZ	-63.8117	474.8537	-766.5863	-0.7295	3.1213
43	TY	-53.6605	0.0	-1015.0930	0.0	-1.1307
44	TZ	-41.1278	0.0	-763.5471	0.0	1.5032
45	TX	-56.7885	0.0	-1040.4935	0.0	1.1506
47	TZ	-39.0350	0.0	-728.5541	0.0	-1.6432
48	TX	-3.1328	0.0	-104.6075	0.0	3.5119
49	TY	-110.1700	0.0	-2051.1729	0.0	-1.2564
50	TZ	81.4682	-0.0000	1495.1173	0.0	-1.4781

RDWS	SDWS
0.214014D 03	0.458019D 05

NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGY CALCULATION FOR THIS CYCLE

	NT	SEC	AVT
INITIAL	65	0.01	0.0002
COORDINATES	31	0.08	0.0026
SLOW RECIP	0	0.0	0.0
FAST RECIP	0	0.0	0.0
UNIT CELL	0	0.0	0.0
SLOW DIRECT	1	0.02	0.0200
FAST DIRECT	30	0.05	0.0017
SLOW CONFIG	1	0.03	0.0300
FAST CONFIG	64	0.43	0.0067

TOTAL TIME (SEC) 0.62

TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES 01-06-81

CYCLE 1

RDWST	SDWST	SIGMA
0.326004D 03	0.105279D 06	0.108668D 03

SAN(I)	8 DCC	10 DCH	12 ACCC	16 AHCH
	0.000771	0.000187	0.876145	0.089734

J	EVAL(J)	EVEC(I,J) 8 DCC	10 DCH	12 ACCC	16 AHCH
1	0.201D 01	-0.639035	0.432201	0.238196	-0.590003
2	0.954D 00	0.042950	-0.150624	0.960308	0.230813
3	0.774D 00	-0.211690	-0.879449	-0.026196	-0.425525
4	0.264D 00	-0.738225	-0.130708	-0.142789	0.646182

J	EVAL(J)	SAN(I)*EVEC(I,J) 8 DCC	10 DCH	12 ACCC	16 AHCH
1	0.201D 01	-0.000493	0.000081	0.208685	-0.052943
2	0.954D 00	0.000033	-0.000028	0.841369	0.020712
3	0.774D 00	-0.000163	-0.000165	-0.022951	-0.038184
4	0.264D 00	-0.000569	-0.000024	-0.125104	0.057984

J	NAMP(J)	DYC(J)	WMAT*BMAT*SAN*EVEC 1	2	3	4
26	TZ	96.8350	0.8266	-0.1824	0.1265	0.1290
27	TX	-210.2888	-0.1736	0.0557	0.6671	-0.0378
29	TZ	-82.9369	-0.4061	0.1541	0.0128	0.3568
38	TZ	62.3063	0.5275	0.5454	-0.0075	0.0731
39	TX	98.8410	0.5870	-0.5632	0.1166	0.1664
41	TZ	-63.6117	-0.6134	-0.5118	-0.0538	0.0208
43	TY	-53.6806	-0.0222	0.0052	0.2102	-0.0407
44	TZ	-41.1278	-0.1413	0.0527	0.0682	0.1058
45	TX	-56.7685	-0.1451	0.0532	0.1273	0.0922
47	TZ	-39.0350	0.0281	-0.0135	0.1826	-0.0775
48	TX	-3.1328	-0.1944	0.0757	-0.1169	0.2062
49	TY	-110.1700	-0.0994	0.0318	0.3855	-0.0327
50	TZ	81.4682	0.1992	-0.0727	-0.1896	-0.1223

PARAMETERS AFTER CYCLE 1 I	NAMP	OLD P	CHANGE	NEW P	ERR
8	DCC	1.400000	-0.034140	1.365860	0.127765
10	DCH	1.000000	0.057144	1.057144	0.022089
12	ACCC	102.000000	-0.078466	101.921534	98.599658
16	AHCH	110.000000	-0.030182	109.969818	13.939990

TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES 01-06-81
ETHANE, TOTALLY SYMMETRIC

CYCLE 2

SGK	SVDW	WR	RMAX	NG	NSRB
0.0	-11.619650	45.300624	10.000000	8	0

GX	GY	GZ	I	J	GM	R	NAMES		CMB	VDW	REP	SRB
0	0	0	2	3	3.00000	1.76950	H	H	0.0	-0.795	3.197	0.0
0	0	0	2	4	3.00000	1.76950	H	H	0.0	-0.795	3.197	0.0
0	0	0	1	6	2.00000	2.18203	C	H	0.0	-1.036	4.106	0.0
0	0	0	1	7	2.00000	2.18203	C	H	0.0	-1.036	4.106	0.0
0	0	0	1	8	2.00000	2.18203	C	H	0.0	-1.036	4.106	0.0
0	0	0	2	7	3.00000	2.53699	H	H	0.0	-0.092	0.230	0.0
0	0	0	2	8	3.00000	2.53699	H	H	0.0	-0.092	0.230	0.0
0	0	0	2	6	3.00000	3.09313	H	H	0.0	-0.028	0.034	0.0

BOND DISTANCES

		IA	JA	DIJ	WD
C	C	1	5	1.5340	6.0330
C	H	1	2	1.0950	0.4550
C	H	1	3	1.0950	0.4550
C	H	1	4	1.0950	0.4550
C	H	5	6	1.0950	0.4550
C	H	5	7	1.0950	0.4550
C	H	5	8	1.0950	0.4550

BOND ANGLES

			IA	JA	KA	AIJK	WA
C	C	H	5	1	2	111.09	0.0213
C	C	H	5	1	3	111.09	0.0213
C	C	H	5	1	4	111.09	0.0213
H	C	H	2	1	3	107.80	0.0423
H	C	H	2	1	4	107.80	0.0423
H	C	H	3	1	4	107.80	0.0423
C	C	H	1	5	6	111.09	0.0213
C	C	H	1	5	7	111.09	0.0213
C	C	H	1	5	8	111.09	0.0213
H	C	H	6	5	7	107.80	0.0423
H	C	H	6	5	8	107.80	0.0423
H	C	H	7	5	8	107.80	0.0423

CONFORMATION ANGLES

				IA	JA	KA	LA	CNF	WCF
H	C	C	H	2	1	5	6	180.00	0.0000
H	C	C	H	2	1	5	7	60.00	0.0000
H	C	C	H	2	1	5	8	-60.00	0.0000
H	C	C	H	3	1	5	6	-60.00	0.0000
H	C	C	H	3	1	5	7	180.00	0.0000
H	C	C	H	3	1	5	8	60.00	0.0000
H	C	C	H	4	1	5	6	60.00	0.0000
H	C	C	H	4	1	5	7	-60.00	0.0000
H	C	C	H	4	1	5	8	180.00	0.0000

WC	WV	WR	WX	WT
0.0	-11.620	45.301	9.145	42.826

TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES 01-06-81
ETHANE, TOTALLY SYMMETRIC

WOBS	WCALC BEFORE CYCLE 2
0.0	42.8260

DERIVATIVES BEFORE CYCLE 2

J	NAMP(J)	DYC(J)
26	TZ	-10.8457
27	TX	-7.1937
28	TZ	-4.3976

NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGY CALCULATION FOR THIS CYCLE

	NT	SEC	AVT
INITIAL	7	0.0	0.0
COORDINATES	7	0.0	0.0
SLOW RECIP	0	0.0	0.0
FAST RECIP	0	0.0	0.0
UNIT CELL	0	0.0	0.0
SLOW DIRECT	1	0.0	0.0
FAST DIRECT	6	0.0	0.0
SLOW CONFIG	1	0.02	0.0200
FAST CONFIG	6	0.03	0.0050

TOTAL TIME (SEC) 0.05

J	NAME	IKA	IRB	X	Y	Z
1	C	1	1	0.0	0.0	0.76700
2	H	2	2	1.02162	0.0	1.16110

TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES 01-06-81
PROPANE, TOTALLY SYMMETRIC

CYCLE 2

SGK	SVDW	WR	RMAX	NG	NSRB
0.0	-20.677452	77.608281	10.000000	27	0

GX	GY	GZ	I	J	GN	R	NAMES		CMB	VDW	REP	SRB
0	0	0	3	6	1.00000	1.75176	H1	H1	0.0	-0.845	3.397	0.0
0	0	0	4	5	2.00000	1.76178	H21	H22	0.0	-0.816	3.282	0.0
0	0	0	4	7	2.00000	1.76178	H21	H22	0.0	-0.816	3.282	0.0
0	0	0	5	7	2.00000	1.76180	H22	H22	0.0	-0.816	3.282	0.0
0	0	0	2	3	2.00000	2.15603	C2	H1	0.0	-1.113	4.496	0.0
0	0	0	2	6	2.00000	2.15603	C2	H1	0.0	-1.113	4.496	0.0
0	0	0	1	4	1.00000	2.17326	C1	H21	0.0	-1.062	4.234	0.0
0	0	0	1	9	1.00000	2.17326	C1	H21	0.0	-1.062	4.234	0.0
0	0	0	1	5	1.00000	2.17326	C1	H22	0.0	-1.062	4.234	0.0
0	0	0	1	7	1.00000	2.17326	C1	H22	0.0	-1.062	4.234	0.0
0	0	0	1	10	1.00000	2.17326	C1	H22	0.0	-1.062	4.234	0.0
0	0	0	1	11	1.00000	2.17326	C1	H22	0.0	-1.062	4.234	0.0
0	0	0	3	4	2.00000	2.49365	H1	H21	0.0	-0.101	0.267	0.0
0	0	0	3	9	2.00000	2.49365	H1	H21	0.0	-0.101	0.267	0.0
0	0	0	3	5	2.00000	2.51909	H1	H22	0.0	-0.095	0.245	0.0
0	0	0	3	10	2.00000	2.51909	H1	H22	0.0	-0.095	0.245	0.0
0	0	0	2	8	1.00000	2.53616	C2	C2	0.0	-1.926	6.553	0.0
0	0	0	5	10	2.00000	2.62600	H22	H22	0.0	-0.074	0.170	0.0
0	0	0	2	10	2.00000	2.80183	C2	H22	0.0	-0.231	0.472	0.0
0	0	0	2	11	2.00000	2.80183	C2	H22	0.0	-0.231	0.472	0.0
0	0	0	3	7	2.00000	3.07117	H1	H22	0.0	-0.029	0.037	0.0
0	0	0	3	11	2.00000	3.07117	H1	H22	0.0	-0.029	0.037	0.0
0	0	0	5	11	2.00000	3.16235	H22	H22	0.0	-0.024	0.027	0.0
0	0	0	2	9	2.00000	3.48647	C2	H21	0.0	-0.062	0.043	0.0
0	0	0	4	10	2.00000	3.80230	H21	H22	0.0	-0.008	0.003	0.0
0	0	0	4	11	2.00000	3.80230	H21	H22	0.0	-0.008	0.003	0.0
0	0	0	4	9	1.00000	4.32354	H21	H21	0.0	-0.004	0.001	0.0

BOND DISTANCES

		IA	JA	DIJ	WD
C1	C2	1	2	1.5260	5.4726
C1	C2	1	8	1.5260	5.4726
C1	H1	1	3	1.0980	0.4795
C1	H1	1	6	1.0980	0.4795
C2	H21	2	4	1.0910	0.3636
C2	H22	2	5	1.0910	0.3641
C2	H22	2	7	1.0910	0.3641
C2	H21	8	9	1.0910	0.3636
C2	H22	8	10	1.0910	0.3641
C2	H22	8	11	1.0910	0.3641

BOND ANGLES

			IA	JA	KA	AIJK	WA
C2	C1	C2	2	1	8	112.40	0.6417
C2	C1	H1	2	1	3	109.54	0.0000
C2	C1	H1	2	1	6	109.54	0.0000
C2	C1	H1	8	1	3	109.54	0.0000
C2	C1	H1	8	1	6	109.54	0.0000
H1	C1	H1	3	1	6	106.10	0.1347
C1	C2	H21	1	2	4	111.20	0.0242
C1	C2	H22	1	2	5	111.20	0.0242
C1	C2	H22	1	2	7	111.20	0.0242
H21	C2	H22	4	2	5	107.69	0.0468
H21	C2	H22	4	2	7	107.69	0.0468
H22	C2	H22	5	2	7	107.69	0.0468
C1	C2	H21	1	8	9	111.20	0.0242
C1	C2	H22	1	8	10	111.20	0.0242
C1	C2	H22	1	8	11	111.20	0.0242
H21	C2	H22	9	8	10	107.69	0.0468
H21	C2	H22	9	8	11	107.69	0.0468
H22	C2	H22	10	8	11	107.69	0.0468

CONFORMATION ANGLES

				IA	JA	KA	LA	CNF	WCF
C2	C1	C2	H21	8	1	2	4	180.00	0.0000
C2	C1	C2	H22	8	1	2	5	60.00	0.0000
C2	C1	C2	H22	8	1	2	7	-60.00	0.0000
H1	C1	C2	H21	3	1	2	4	57.99	0.0008
H1	C1	C2	H22	3	1	2	5	-62.01	0.0008
H1	C1	C2	H22	3	1	2	7	177.99	0.0008
H1	C1	C2	H21	6	1	2	4	-57.99	0.0008
H1	C1	C2	H22	6	1	2	5	-177.99	0.0008
H1	C1	C2	H22	6	1	2	7	62.01	0.0008
C2	C1	C2	H21	2	1	8	9	180.00	0.0000
C2	C1	C2	H22	2	1	8	10	-60.00	0.0000
C2	C1	C2	H22	2	1	8	11	60.00	0.0000
H1	C1	C2	H21	3	1	8	9	-57.99	0.0008
H1	C1	C2	H22	3	1	8	10	62.01	0.0008
H1	C1	C2	H22	3	1	8	11	-177.99	0.0008
H1	C1	C2	H21	6	1	8	9	57.99	0.0008
H1	C1	C2	H22	6	1	8	10	177.99	0.0008
H1	C1	C2	H22	6	1	8	11	-62.01	0.0008

WC	WV	WR	WX	WT
0.0	-20.677	77.608	15.300	72.231

TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES 01-06-81
PROPANE, TOTALLY SYMMETRIC

WOBS	WCALC BEFORE CYCLE 2
0.0	72.2307

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DERIVATIVES BEFORE CYCLE  2
  J  NAMP(J)  DYC(J)
 38  TZ        2.4751
 39  TX        9.0112
 41  TZ       -3.5583
 43  TY        4.2914
 44  TZ        2.5493
 45  TX        2.7239
 47  TZ        2.5475
 48  TX        2.9502
 49  TY        7.0036
 50  TZ       -4.0136

NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGY CALCULATION FOR THIS CYCLE
                NT       SEC      AVT
INITIAL         21      0.02    0.0010
COORDINATES     21      0.05    0.0024
SLOW RECIP       0      0.0     0.0
FAST RECIP       0      0.0     0.0
UNIT CELL        0      0.0     0.0
SLOW DIRECT      1      0.02    0.0200
FAST DIRECT     20      0.01    0.0005
SLOW CONFIG      1      0.02    0.0200
FAST CONFIG     20      0.10    0.0050

TOTAL TIME (SEC)        0.22

  J  NAME    IKA    IRB          X          Y          Z
  1  C1       1      1      0.0        0.0        0.0
  2  C2       1      2      1.26808    0.0       -0.84891
  3  H1       2      3      0.0        0.87588    0.65883
  4  H21      2      4      2.16177    0.0       -0.22315
  5  H22      2      5      1.31300    0.88090   -1.49101

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TEST PROBLEM 3A. ADJUST ENERGY PARAMETERS FOR ETHANE, PROPANE MOLECULES          01-06-81

  MODE     NC     NPC   ILSQ   IWGT   IPLM   IPRT   NSTG   IBPC        ARE        SLIN       CMPR       XDRD       EPSC
    0      1      17     0      0      0      2      4      0   0.100D-01  0.100D-05   0.0       0.200D-02  0.100D 02

     ARC       ARH       BRC       BRH       PLC       PLH       IBR       DCC
     KCC       DCH       KCH       ACCC      KCCC      ACCH      KCCH      AHCH
    KHCH
  1.71100   1.23400   0.14070   0.14590  22.64000   4.94000   0.28167   1.36586
  4.26800   1.05714   6.35100101.92153   0.01169109.50000   0.01673109.96982
  0.01799

    NO     NV    NOV     LS    IWT
    13     4      0      1      0

                    PARAMETERS AFTER EACH CYCLE
  J  NAMP    DKT      INITIAL        1
  8  DCC    1.000    1.400000    1.365860
 10  DCH    1.000    1.000000    1.057144
 12  ACCC   1.000  102.000000  101.921534
 16  AHCH   1.000  110.000000  109.969818

             NVU                        4

             RDWS 0.3260D 03

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DYNAMIC DIMENSIONS FOR WMIN
  NPCMAX    NAMAX   NKAMAX    NSMAX   NRBMAX   NPXMAX   NCTMAX   NBCMAX
      17        8        2       12        8        0        3       10

    MMAX   NFSMAX   NGSMAX   NPSMAX    NPMAX   NOSMAX    NDMAX    NVMAX
      46        0       30       30       50       24       24       24

                       1         2         3         4         5         6         7         8         9        10
ARRAY                ACZ       AKE        AM     AMASS        AN        AR        BR       BTR      CHAR      CMBT
DIMEN-             (   9     (   0     ( NVMAX   (   1     ( NVMAX   (   1     (   1     ( NVMAX   (   1     (   1
 SIONS             *NRBMAX)  *   0   ) * NVMAX)  *NKAMAX)  * NVMAX)  *NKAMAX)  *NKAMAX)  *NDSMAX)  * NSMAX)  *NGSMAX)
WORDS                 72         0       576         2       576         2         2       576        12        30
BYTES/WORD             8         8         8         8         8         8         8         8         8
HEX ADDRESS     00000000  00000240  00000240  00001440  00001450  00002650  00002660  00002670  00003870  00

                      11        12        13        14        15        16        17        18
ARRAY                CSV        DP       DPC       DPX        DW       DWDQ       DXQ       DYC
DIMEN-             (   1     (   1     (   1     (   1     (   1     (   1     ( NVMAX   (
 SIONS             *NGSMAX)  * NPMAX)  *NPCMAX)  *NPXMAX)  * NPMAX)  * NVMAX)  * NAMAX)
WORDS                 30        50        17         0        50        24
BYTES/WORD             8         8         8         8         8         8                                          8
HEX ADDRESS     00003948  00003A38  00003BC8  00003C50  00003C50  00003D                                   00009F08

                      21        22        23        24        25                                       119       120
ARRAY                EPS       ERR      EVAL      EVEC                                                 VN       VSV
DIMEN-             (   1     (   1     (   1     ( NVMAX                                          (   1     (   1
 SIONS             * NPMAX)  * NVMAX)  * NVMAX)  * NV                                           * NVMAX)  * NVMAX)  *NGSMAX)
WORDS                 50        24        24                                                 30        24        24        30
BYTES/WORD             8         8                                                             4         8         8         8
HEX ADDRESS     00005160  000052F0  000                                                   0008  0000C698  0000C710  0000C7D0  0000C890

                      31                                                                  126       127       128       129       130
ARRAY                HMT                                                                 XC       XYZ      XYZC      XYZD      XYZN      XYZR
DIMEN-             (                                                                 ( NAMAX   (   3     (   3     (   3     (   3     (   3
 SIONS                                                                          MMAX)  * NSMAX)  * NAMAX)  * NAMAX)  * NAMAX)  * NAMAX)  * NAMAX)
WORDS                                                                              46        96        24        24        24        24        24
BYTES/                                                                              8         8         8         8         8         8         8
                                                                            0000DD10  0000DEA0  0000E010  0000E310  0000E3D0  0000E490  0000E550  0000E610

                                                                                 132       133
                                                                                ZAM        ZC
                                                                            NAMAX   (   1     ( NAMAX   (
                                                                          * NSMAX)  * NAMAX)  * NSMAX)  *
                                                                               96         8        96
                                                                                8         8         8
    S/WORD
HEX ADDRESS                                                                 0000E6D0  0000E9D0  0000EA10

    7586 8-BYTE STORAGE LOCATIONS HAVE BEEN REQUESTED. THE PROGRAM IS DIMENSIONED FOR   12000
COMMON/G/ AND NST MAY BE DECREASED BY  4414 WORDS. THIS WILL REDUCE THE REGION USED BY  34K BYTES.
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TEST PROBLEM 38. MINIMIZE ENERGY AND CALCULATE FREQUENCIES OF MOLECULES          01-06-81

 MODE    NC    NPC  ILSQ  IWGT  IPLM  IPRT  NSTG  IBPC          ARE          SLIM          CMPR          XDRD          EPSC
    4     1     17     0     0     0     3     4     1   0.100D-01   0.100D-05   0.0           0.200D-02   0.100D 02

 NAMPC(I)
    ARC       ARH       BRC       BRH       PLC       PLH       TBR       DCC
    KCC       DCH       KCH       ACCC      KCCC      ACCH      KCCH      AHCH
    KHCH

  PC(I)
 1.71100   1.23400   0.14070   0.14590  22.64000   4.94000   0.28167   1.36586
 4.26800   1.05714   6.35100101.92153   0.01169109.50000   0.01673109.96982
 0.01799

  DPC(I)
 0.00100   0.00010   0.00010   0.01000   0.01000   0.00100   0.00100
 0.00100   0.00100   0.00100   0.10000   0.00010   0.10000   0.00010   0.10000
 0.00010

  KPC(I)
       2         2         2         1         1         3         3
       3         3         3         3         3         3         3
       3
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TEST PROBLEM 38. MINIMIZE ENERGY AND CALCULATE FREQUENCIES OF MOLECULES          01-06-81
ETHANE. NO SYMMETRY RESTRICTIONS. PARALLEL CARTESIAN SYSTEMS.

  ISB
   1

   NA    NKA     NS ICENT HXNEG HYNEG HZNEG    NRB    NPX    NRP  ICMB  IVDW  IREP  IMOL   NCT  IRSC  IZAM  IGEM  IRBA ISETA
    2      2     12     1   1.0   1.0   0.0      8      0     10     0     1     1     1     2     6     0     0     1     0

      CK      NQ      NR
 0.0           1       1

 QLIM(I)
 0.0

 RLIM(I)
10.00000

    A(I)
 1.00000   1.00000   1.00000   0.0       0.0      -0.50000
```

NAMS	TRANSFORMED X				TRANSFORMED Y				TRANSFORMED Z			
E	0.0	1.0*X	0.0*Y	0.0*Z	0.0	0.0*X	1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	1.0*Z
C3	0.0	0.0*X	-1.0*Y	0.0*Z	0.0	1.0*X	-1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	1.0*Z
C3	0.0	-1.0*X	1.0*Y	0.0*Z	0.0	-1.0*X	0.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	1.0*Z
C2	0.0	-1.0*X	1.0*Y	0.0*Z	0.0	0.0*X	1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	-1.0*Z
C2	0.0	0.0*X	-1.0*Y	0.0*Z	0.0	-1.0*X	0.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	-1.0*Z
C2	0.0	1.0*X	0.0*Y	0.0*Z	0.0	1.0*X	-1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	-1.0*Z
I	0.0	-1.0*X	0.0*Y	0.0*Z	0.0	0.0*X	-1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	-1.0*Z
S6	0.0	0.0*X	1.0*Y	0.0*Z	0.0	-1.0*X	1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	-1.0*Z
S6	0.0	1.0*X	-1.0*Y	0.0*Z	0.0	1.0*X	0.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	-1.0*Z
M	0.0	1.0*X	-1.0*Y	0.0*Z	0.0	0.0*X	-1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	1.0*Z
M	0.0	0.0*X	1.0*Y	0.0*Z	0.0	1.0*X	0.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	1.0*Z
M	0.0	-1.0*X	0.0*Y	0.0*Z	0.0	-1.0*X	1.0*Y	0.0*Z	0.0	0.0*X	0.0*Y	1.0*Z

```
  K  NAMK          Q          PL          AR          BR       AMASS
  1  C        0.0        0.0        0.0        0.0      12.00390
  2  H        0.0        0.0        0.0        0.0       1.00810

  J  NAME    IKA    IRB          X          Y          Z
  1  C         1      0        0.0        0.0        0.76700
  2  H         2      0    1.02162        0.0        1.16110

  I  NAME    ISC    JAC    SMC    FMC   IRBC         XC         YC         ZC
  1  C         1      1     6.     0.5      0        0.0        0.0    0.76700
  2  H         1      2     2.     0.5      0    1.02162        0.0    1.16110
  3  H         2      2     2.     0.5      8        0.0    1.02162    1.16110
  4  H         3      2     2.     0.5     16   -1.02162   -1.02162    1.16110
  5  C         4      1     6.     0.5     24        0.0        0.0   -0.76700
  6  H         4      2     2.     0.5     24   -1.02162        0.0   -1.16110
  7  H         5      2     2.     0.5     32        0.0   -1.02162   -1.16110
  8  H         6      2     2.     0.5     40    1.02162    1.02162   -1.16110
ABOVE ATOMS USED TO COMPUTE STRUCTURE FACTORS

REVISED ATOM LIST AFTER RELAXING SYMMETRY CONSTRAINTS
  J  NAME    IKA    IRB          X          Y          Z
  1  C         1      1        0.0        0.0        0.76700
  2  H         2      2    1.02162        0.0        1.16110
  3  H         2      3        0.0    1.02162        1.16110
  4  H         2      4   -1.02162   -1.02162        1.16110
  5  C         1      5        0.0        0.0       -0.76700
  6  H         2      6   -1.02162        0.0       -1.16110
  7  H         2      7        0.0   -1.02162       -1.16110
  8  H         2      8    1.02162    1.02162       -1.16110

  I  NAME    ISC    JAC    SMC    FMC   IRBC         XC         YC         ZC
  1  C         1      1    12.     0.5      1        0.0        0.0    0.76700
  2  H         1      2    12.     0.5      2    1.02162        0.0    1.16110
  3  H         1      3    12.     0.5      3        0.0    1.02162    1.16110
  4  H         1      4    12.     0.5      4   -1.02162   -1.02162    1.16110
  5  C         1      5    12.     0.5      5        0.0        0.0   -0.76700
  6  H         1      6    12.     0.5      6   -1.02162        0.0   -1.16110
  7  H         1      7    12.     0.5      7        0.0   -1.02162   -1.16110
  8  H         1      8    12.     0.5      8    1.02162    1.02162   -1.16110
ABOVE ATOMS USED TO COMPUTE STRUCTURE FACTORS

   ZMC
   1.0

  I  NAME(I)    ZAM(I)
  1    C          1.0
  2    H          1.0
  3    H          1.0
  4    H          1.0
  5    C          1.0
  6    H          1.0
  7    H          1.0
  8    H          1.0

  J  IZ(J)  IU(J)  IV(J)  IW(J)   SSR(J)    STR(J)    SXR(J)    SYR(J)    SZR(J)   TR(1,J)   TR(2,J)   TR(3,J)
  1     1       0       0       0     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
  2     2       0       0       0     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
  3     3       0       0       0     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
  4     4       0       0       0     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
  5     5       0       0       0     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
  6     6       0       0       0     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
  7     7       0       0       0     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
  8     8       0       0       0     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0

IACT    ICT                   IDZ                   IAZ                   ITBR
  1      5    2    3    4      8   10   10   10      14   14   14   16   16   16      -1    0    0    0
  5      1    6    7    8      8   10   10   10      14   14   14   15   16   16      -1    0    0    0
```

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LBCI LBCJ
   1   5      1   2      1   3      1   4      5   6      5   7      5   8

  KPWS    KPW      WOBS     SIGWO
     0      0       0.0       0.0

  I   NAMP(I)        P(I)        DP(I)       PMN(I)       PMX(I)   KP(I)   KQ(I)   DKT(KQ)       SP(I)   ISBP(I)
  1      ARC      1.711000    0.001000      0.0          0.0         0       0      0.0          0.0         0
  2      ARH      1.234000    0.001000      0.0          0.0         0       0      0.0          0.0         0
  3      BRC      0.140700    0.000100      0.0          0.0         0       0      0.0          0.0         0
  4      BRH      0.145900    0.000100      0.0          0.0         0       0      0.0          0.0         0
  5      PLC     22.640000    0.010000      0.0          0.0         0       0      0.0          0.0         0
  6      PLH      4.940000    0.010000      0.0          0.0         0       0      0.0          0.0         0
  7      TBR      0.281667    0.001000      0.0          0.0         0       0      0.0          0.0         0
  8      DCC      1.365860    0.001000      0.0          0.0         0       0      0.0          0.0         0
  9      KCC      4.258000    0.001000      0.0          0.0         0       0      0.0          0.0         0
 10      DCH      1.057144    0.001000      0.0          0.0         0       0      0.0          0.0         0
 11      KCH      6.351000    0.001000      0.0          0.0         0       0      0.0          0.0         0
 12     ACCC    101.921534    0.100000      0.0          0.0         0       0      0.0          0.0         0
 13     KCCC      0.011690    0.000100      0.0          0.0         0       0      0.0          0.0         0
 14     ACCH    109.500000    0.100000      0.0          0.0         0       0      0.0          0.0         0
 15     KCCH      0.016730    0.000100      0.0          0.0         0       0      0.0          0.0         0
 16     AHCH    109.969918    0.100000      0.0          0.0         0       0      0.0          0.0         0
 17     KHCH      0.017990    0.000100      0.0          0.0         0       0      0.0          0.0         0
 18      A        1.000000    0.000010      0.0          2.000000    0       0      0.0          0.0         1
 19      B        1.000000    0.000010      0.0          2.000000    0       0      0.0          0.0         1
 20      C        1.000000    0.000010      0.0          2.000000    0       0      0.0          0.0         1
 21     COSA      0.0         0.000010     -0.200000     0.200000    0       0      0.0          0.0         1
 22     COSB      0.0         0.000010     -0.200000     0.200000    0       0      0.0          0.0         1
 23     COSG     -0.500000    0.000010     -0.700000    -0.300000    0       0      0.0          0.0         1
 24      TX       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 25      TY       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 26      TZ       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 27      TX       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 28      TY       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 29      TZ       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 30      TX       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 31      TY       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 32      TZ       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 33      TX       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 34      TY       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 35      TZ       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 36      TX       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 37      TY       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 38      TZ       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 39      TX       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 40      TY       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 41      TZ       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 42      TX       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 43      TY       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 44      TZ       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 45      TX       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 46      TY       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1
 47      TZ       0.0         0.000010     -0.500000     0.500000    1       1      1.000        0.0         1

    NO     NV    NOV     LS    IWT
    24     24     24      0      0


TEST PROBLEM 3D. MINIMIZE ENERGY AND CALCULATE FREQUENCIES OF MOLECULES          01-06-81
ETHANE. NO SYMMETRY RESTRICTIONS. PARALLEL CARTESIAN SYSTEMS.

CYCLE  1

          SGK            SVDW            WR            RMAX            NG            NSRB
          0.0        -11.619650      45.300624      10.000000        21               0

 GX GY GZ  I  J        GM         R    NAMES        CMB       VDW       REP       SRB
  0  0  0  2  3   1.00000   1.76950   H     H       0.0      -0.795     3.197      0.0
  0  0  0  2  4   1.00000   1.76950   H     H       0.0      -0.795     3.197      0.0
  0  0  0  3  4   1.00000   1.76950   H     H       0.0      -0.795     3.197      0.0
  0  0  0  6  7   1.00000   1.76950   H     H       0.0      -0.795     3.197      0.0
  0  0  0  6  8   1.00000   1.76950   H     H       0.0      -0.795     3.197      0.0
  0  0  0  7  8   1.00000   1.76950   H     H       0.0      -0.795     3.197      0.0
  0  0  0  1  6   1.00000   2.18203   C     H       0.0      -1.036     4.106      0.0
  0  0  0  1  7   1.00000   2.18203   C     H       0.0      -1.036     4.106      0.0
  0  0  0  1  8   1.00000   2.18203   C     H       0.0      -1.036     4.106      0.0
  0  0  0  2  5   1.00000   2.18203   H     C       0.0      -1.036     4.106      0.0
  0  0  0  3  5   1.00000   2.18203   H     C       0.0      -1.036     4.106      0.0
  0  0  0  4  5   1.00000   2.18203   H     C       0.0      -1.036     4.106      0.0
  0  0  0  2  7   1.00000   2.53699   H     H       0.0      -0.092     0.230      0.0
  0  0  0  2  8   1.00000   2.53699   H     H       0.0      -0.092     0.230      0.0
  0  0  0  3  6   1.00000   2.53699   H     H       0.0      -0.092     0.230      0.0
  0  0  0  3  8   1.00000   2.53699   H     H       0.0      -0.092     0.230      0.0
  0  0  0  4  6   1.00000   2.53699   H     H       0.0      -0.092     0.230      0.0
  0  0  0  4  7   1.00000   2.53699   H     H       0.0      -0.092     0.230      0.0
  0  0  0  2  6   1.00000   3.09313   H     H       0.0      -0.028     0.034      0.0
  0  0  0  3  7   1.00000   3.09313   H     H       0.0      -0.028     0.034      0.0
  0  0  0  4  8   1.00000   3.09313   H     H       0.0      -0.028     0.034      0.0

BOND DISTANCES
                                IA  JA          DIJ       WD
C     C                          1   5       1.5340   6.0330
C     H                          1   2       1.0950   0.4550
C     H                          1   3       1.0950   0.4550
C     H                          1   4       1.0950   0.4550
C     H                          5   6       1.0950   0.4550
C     H                          5   7       1.0950   0.4550
C     H                          5   8       1.0950   0.4550

BOND ANGLES
                                IA  JA  KA      AIJK       WA
C     C     H                    5   1   2    111.09   0.0213
C     C     H                    5   1   3    111.09   0.0213
C     C     H                    5   1   4    111.09   0.0213
H     C     H                    2   1   3    107.80   0.0423
H     C     H                    2   1   4    107.80   0.0423
H     C     H                    3   1   4    107.80   0.0423
C     C     H                    1   5   6    111.09   0.0213
C     C     H                    1   5   7    111.09   0.0213
C     C     H                    1   5   8    111.09   0.0213
H     C     H                    6   5   7    107.80   0.0423
H     C     H                    6   5   8    107.80   0.0423
H     C     H                    7   5   8    107.80   0.0423

CONFORMATION ANGLES
                                IA  JA  KA  LA      CNF       WCF
H     C     C     H              2   1   5   6   180.00    0.0000
H     C     C     H              2   1   5   7    60.00    0.0000
H     C     C     H              2   1   5   8   -60.00    0.0000
H     C     C     H              3   1   5   6   -60.00    0.0000
H     C     C     H              3   1   5   7   180.00    0.0000
H     C     C     H              3   1   5   8    60.00    0.0000
H     C     C     H              4   1   5   6    60.00    0.0000
H     C     C     H              4   1   5   7   -60.00    0.0000
H     C     C     H              4   1   5   8   180.00    0.0000

      WC        WV        WR        WX        WT
     0.0    -11.620    45.301     9.145    42.826

TEST PROBLEM 3B. MINIMIZE ENERGY AND CALCULATE FREQUENCIES OF MOLECULES          01-06-81
ETHANE. NO SYMMETRY RESTRICTIONS. PARALLEL CARTESIAN SYSTEMS.
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      WOBS        WCALC BEFORE CYCLE  1
 0.0          42.8260

DERIVATIVES BEFORE CYCLE  1
                    DOW/DP(I)OP(J) FOR I=
 J  NAMP(J)  DYC(J)   24  TX      25  TY      26  TZ      27  TX      28  TY      29  TZ      30  TX      31  TY      32  TZ
                      33  TX      34  TY      35  TZ      36  TX      37  TY      38  TZ      39  TX      40  TY      41  TZ
                      42  TX      43  TY      44  TZ      45  TX      46  TY      47  TZ
24  TX      -0.0000  1158.7196   -0.0708    0.0027  -564.0379   -0.0023  -187.4641  -230.4699  192.5852   93.7308
                    -230.4699  -192.6532   93.7309  -151.9540   -0.0867   -0.0007    6.9205   -0.0000  -42.5812
                       5.5314   -0.8021   24.7906    5.5314    0.7361   24.7906
25  TY      -0.0000   -0.0708  1156.7548    0.0027    0.0021  -119.2599   -0.0002  192.5861  -452.8763  -162.3485
                    -192.6497  -452.8764  162.3465   -0.0850  -151.9540   -0.0007   -0.0000    5.0886   -0.0000
                      -0.8022    6.4296  -42.9386    0.7359    6.4296   42.9387
26  TZ      -5.4229   0.0027    0.0027  1089.8347  -168.3474   -0.0003  -190.2702   84.1743  -145.7933  -190.2702
                      84.1743  145.7948  -190.2702    0.0007    0.0007  -426.8000  -19.0752    0.0001  -30.7409
                       9.5376  -16.5195  -30.7409    9.5375   16.5195  -30.7409
27  TX      -1.1990  -564.0379   0.0021  -168.3474  610.1532    0.0020  196.6381  -26.5938   11.5432   -5.1022
                     -26.5938  -11.5433   -5.1022    6.9205    0.0001  -19.0756   -0.1106    0.0      -0.1490
                       0.1313   -0.1639   -0.4301    0.1313    0.1639   -0.4301
28  TY      0.0000   -0.0023  -119.2599   -0.0003    0.0020   97.7896    0.0007   48.6746    8.1727   19.8093
                     -48.6742    8.1726  -19.8095    0.0       5.0886   -0.0001    0.0001    1.2349    0.0000
                      -1.2156   -0.6651   -0.7450    1.2156   -0.6651    0.7451
29  TZ      -0.7329  -187.4641   -0.0002  -190.2702  198.6381    0.0007  188.6318   19.7066    5.4860   17.8943
                      19.7066   -5.4861   17.8943   -49.5806    0.0      -30.7410   -0.1490    0.0      -0.1489
                      -0.4301   -0.7450   -1.7297   -0.4301    0.7451   -1.7297
30  TX      0.5995  -230.4699  192.5861   84.1743  -26.5938   48.6746   19.7066  225.8957  -221.9154  -99.3195
                      25.5558  -18.5656  -14.6044    5.5312   -0.8020    9.5378    0.1313   -1.2156   -0.4301
                       0.8986    0.5827    0.0745   -1.0634    0.5259    0.8604
31  TY      -1.0383  192.5852  -452.8763  -145.7933  11.5432    8.1727    5.4860  -221.9154  482.0952  172.0261
                      18.5653  -43.9772  -14.3232   -0.6020    6.4296  -16.5199   -0.1639   -0.6652   -0.7450
                       0.5827    0.2258   -0.1290   -0.5258    0.5295    0.0001
32  TZ      -0.7329   93.7308  -162.3465  -190.2702  -5.1022   19.8093  17.8943  -99.3195  172.0261  188.8315
                     -14.6043   14.3235   17.8943   24.7902  -42.9381  -30.7410   -0.4302   -0.7451   -1.7297
                       0.0745   -0.1290   -0.1489    0.8603    0.0001   -1.7297
33  TX      0.5995  -230.4699  -192.6497   84.1743  -26.5938  -48.6742   19.7066   25.5558   18.5653  -14.6045
                     225.8958  221.8518  -99.3195    5.5311    0.7363    9.5378    0.1312    1.2157   -0.4302
                      -1.0634   -0.5258    0.8603    0.8985   -0.6486    0.0745
34  TY      1.0383  -192.6532  -452.8764  145.7948  -11.5433   8.1726   -5.4861  -18.5656  -43.9772   14.3235
                     221.8518  482.0952  -172.0276   0.7361    6.4296   16.5201    0.1639   -0.6652    0.7450
                       0.5259    0.5296    0.0000   -0.5486    0.2258    0.1290
35  TZ      -0.7329   93.7309  162.3465  -190.2702  -5.1022  -19.8095  17.6943  -14.6044  -14.3232   17.8943
                     -99.3195  -172.0276  188.8315  24.7902   42.9379  -30.7410   -0.4301    0.7451   -1.7296
                       0.8603    0.0001   -1.7296    0.0745    0.1291   -0.1488
36  TX      0.0000  -151.9540   -0.0850    0.0007   6.9205    0.0      -49.5806    5.5312   -0.8020   24.7902
                       5.5311    0.7361   24.7902  1158.7195   -0.0608   -0.0028  -564.0379    0.0022  -187.4593
                     -230.4696  192.5861   93.7307  -230.4696  -192.6531   93.7307
37  TY      0.0000   -0.0867  -151.9540    0.0007    0.0001    5.0886    0.0      -0.8020    6.4296  -42.9381
                       0.7363    6.4296   42.9379   -0.0608  1158.7549   -0.0028   -0.0021  -119.2600    0.0002
                     192.5863  -452.8765  -162.3446  -192.6536  -452.8763  162.3465
38  TZ      5.4229   -0.0007   -0.0007  -426.8000  -19.0756   -0.0001  -30.7410    9.5378  -16.5199  -30.7410
                       9.5378   16.5201  -30.7410   -0.0028   -0.0028  1089.8347  -168.3510    0.0002  -190.2712
                      84.1748  -145.7960  -190.2712   84.1748  145.7944  -190.2712
39  TX      1.1990    6.9205   -0.0000  -19.0752   -0.1109    0.0003   -0.1490    0.1313   -0.1639   -0.4302
                       0.1312    0.1639   -0.4301  -564.0379   -0.0021  -168.3510  610.1532   -0.0020  198.6388
                     -26.5940   11.5437   -5.1024  -26.5940  -11.5435   -5.1024
40  TY      -0.0000  -0.0000    5.0888    0.0001    0.0       1.2349    0.0      -1.2156   -0.6652   -0.7451
                       1.2157   -0.6652    0.7451    0.0022  -119.2600    0.0002   -0.0020   97.7895   -0.0006
                      48.6735    8.1726   19.8093  -48.6737    8.1727  -19.8095
41  TZ      0.7329  -49.5812   -0.0000  -30.7409   -0.1490    0.0000   -0.1489   -0.4301   -0.7450   -1.7297
                      -0.4302    0.7450   -1.7296  -187.4593   0.0002  -190.2712  198.6388   -0.0006  188.8315
                      19.7069    5.4863   17.8938   19.7069   -5.4860   17.6938
42  TX      -0.5995   5.5314   -0.8022    9.5376    0.1313   -1.2156   -0.4301    0.8986    0.5827   0.0745
                      -1.0634    0.5259    0.8603  -230.4696  192.5853   84.1748  -26.5940   48.6735   19.7069
                     225.8958  -221.9187  -99.3188   25.5559  -18.5649  -14.6043
43  TY      1.0383   -0.8021    6.4296  -16.5195   -0.1639   -0.6651   -0.7450    0.5827    0.2258   -0.1290
                      -0.5258    0.5296    0.0001  192.5861  -452.8765  -145.7960  11.5437    8.1726    5.4863
                     -221.9187  482.0952  172.0260  18.5652  -43.9772  -14.3237
44  TZ      0.7329   24.7906   -42.9386  -30.7409   -0.4301   -0.7450   -1.7297    0.0745   -0.1290   -0.1489
                       0.8603    0.0000   -1.7296   93.7307  -162.3446  -190.2712  -5.1024   19.8099   17.8938
                     -99.3188  172.0260  188.8315  -14.6044   14.3235   17.8938
45  TX      -0.5995   5.5314    0.7359    9.5375    0.1313    1.2156   -0.4301   -1.0634   -0.5258    0.8603
                       0.8985   -0.6486    0.0745  -230.4696  -192.6536   84.1748  -26.5940  -48.6737   19.7069
                      25.5559   18.5652  -14.6044  225.8958  221.8507  -99.3188
46  TY      -1.0383   0.7361    6.4296   16.5195    0.1639   -0.6651    0.7451    0.5259    0.5295    0.0001
                      -0.6486    0.2258    0.1291  -192.6501  -452.8763  145.7944  -11.5435   8.1727   -5.4860
                     -18.5649  -43.9772   14.3235  221.8507  482.0952  -172.0240
47  TZ      0.7329   24.7906   42.9387  -30.7409   -0.4301    0.7451   -1.7297    0.8604    0.0001   -1.7297
                       0.0745    0.1290   -0.1488   93.7307  162.3465  -190.2712  -5.1024  -19.8095   17.6938
                     -14.6043  -14.3237   17.8938  -99.3188  -172.0240  188.8315

          ROWS          SOWS
 0.840514D 01   0.7056320 02

NUMBER OF PASSES AND TIME SPENT ON VARIOUS PARTS OF ENERGY CALCULATION FOR THIS CYCLE
                NT      SEC      AVT
INITIAL        325     0.08     0.0002
COORDINATES    325     1.39     0.0043
SLOW RECIP       0     0.0      0.0
FAST RECIP       0     0.0      0.0
UNIT CELL        0     0.0      0.0
SLOW DIRECT      1     0.02     0.0200
FAST DIRECT    324     0.14     0.0004
SLOW CONFIG      1     0.01     0.0100
FAST CONFIG    324     0.67     0.0021

TOTAL TIME (SEC)       2.31

                    EVEC(I,J)
 J     EVAL(J)      24  TX      25  TY      26  TZ      27  TX      28  TY      29  TZ      30  TX      31  TY      32  TZ
                    33  TX      34  TY      35  TZ      36  TX      37  TY      38  TZ      39  TX      40  TY      41  TZ
                    42  TX      43  TY      44  TZ      45  TX      46  TY      47  TZ
 1  0.280D 01        0.290197  -0.005263  -0.182511  -0.080502   0.000520  -0.087900  -0.265644   0.240261   0.251447
                    -0.259248  -0.232203   0.244914   0.290159  -0.005283  -0.182489  -0.080490   0.000527  -0.057894
                    -0.265626   0.240251   0.251432  -0.259202  -0.232255   0.244872
 2  0.280D 01       -0.004165  -0.370582   0.002611   0.001161   0.037526   0.000836  -0.219505   0.275039   0.226166
                     0.227016   0.262417  -0.233272  -0.004148  -0.370854   0.002598   0.001158   0.037525   0.000835
                    -0.219505   0.275684   0.226165   0.229983   0.262380  -0.233242
 3  0.278D 01        0.299247  -0.000015  -0.216479  -0.077723  -0.000000  -0.028807  -0.264126   0.234890   0.231095
                    -0.264110  -0.234871   0.231079  -0.299282  -0.000010   0.216503   0.077731  -0.000001   0.028812
                     0.264145  -0.234904  -0.231112   0.264156   0.234915  -0.231122
 4  0.275D 01       -0.000006   0.391539   0.000004   0.000003  -0.043698   0.000002   0.224756  -0.285777  -0.200502
                    -0.224742  -0.285766   0.200489  -0.000012  -0.391566   0.000007   0.000004   0.043703   0.000003
                    -0.224756   0.285783  -0.200502   0.224776   0.285800  -0.000006
 5  0.224D 01       -0.237409  -0.000001  -0.329731   0.381530   0.000006   0.365300   0.013775   0.037389   0.102813
                     0.013773  -0.037389   0.102812   0.297133  -0.000001   0.329466  -0.381137   0.000006  -0.364880
                    -0.013787  -0.037328  -0.102700  -0.013789   0.037329  -0.102702
 6  0.224D 01       -0.273833   0.000028  -0.262335   0.391632  -0.000004   0.414758  -0.011696   0.058149   0.107806
                    -0.011695   0.058143   0.107826  -0.274132   0.000031  -0.262689   0.392019  -0.000018   0.415127
                    -0.011683   0.058185   0.107910  -0.011677  -0.058180   0.107925
 7  0.139D 01        0.000003  -0.175550   0.000004  -0.000002   0.561508  -0.000005   0.237783  -0.016951   0.054839
                    -0.237785  -0.016954  -0.054843   0.000003   0.175437   0.000004  -0.000002  -0.591065  -0.000005
                    -0.237610   0.016940  -0.054781   0.237608   0.016938   0.054778
 8  0.138D 01        0.000034  -0.147554  -0.000035  -0.000007   0.594872   0.000017   0.233768  -0.019712   0.083446
                    -0.233767  -0.019653  -0.083367   0.000029  -0.147662  -0.000050  -0.000006   0.595314   0.000023
                     0.233959  -0.019731   0.083492  -0.233939  -0.019663  -0.083407
 9  0.106D 01        0.073665  -0.000003  -0.504446  -0.334335   0.000005  -0.047435   0.186619  -0.163901   0.036728
                     0.186612   0.163898   0.036776  -0.073868  -0.000003   0.504445   0.334337   0.000005   0.047434
                    -0.186615   0.163902  -0.036729  -0.186622  -0.163905  -0.036732
10  0.834D 00        0.042204  -0.000082  -0.257981  -0.357060  -0.000093   0.131940   0.245444  -0.153810   0.243906
                     0.245467   0.153721   0.243901   0.042207  -0.000076  -0.257972  -0.357056  -0.000097   0.131945
                     0.245440  -0.153812   0.243917   0.245470   0.153727   0.243907
11  0.643D 00       -0.404232   0.000004   0.069724  -0.066699   0.000001  -0.376795   0.095810   0.094673   0.272966
                     0.095809  -0.094671   0.272966   0.404241  -0.000001  -0.069721   0.066690   0.000000   0.376809
                    -0.095804  -0.094661  -0.272973  -0.095804   0.094664  -0.272969
12  0.633D 00        0.000003   0.393546  -0.000002   0.000001   0.025352   0.000000   0.017491  -0.009419   0.414534
                    -0.017495  -0.009410  -0.414532  -0.000002  -0.393554  -0.000001   0.000001  -0.025344  -0.000005
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                  -0.017495   0.009414  -0.414542   0.017492   0.009423   0.414552
 13  0.585D 00     0.100770  -0.000001   0.264298  -0.238549  -0.000000   0.423586   0.210744   0.083001   0.201334
                   0.210743  -0.083001   0.201336  -0.100781  -0.000001  -0.264294   0.238535  -0.000000  -0.423586
                  -0.210726  -0.082979  -0.201335  -0.210727   0.082950  -0.201334
 14  0.534D 00     0.084039   0.000079  -0.044330   0.167710  -0.000122  -0.077349  -0.233727  -0.406376   0.092018
                  -0.233914   0.406567   0.091883   0.084955   0.000091  -0.044348   0.167727  -0.000124  -0.077365
                  -0.233734  -0.406366   0.092000  -0.233926   0.406590   0.091851
 15  0.517D 00     0.044515   0.000001   0.123763   0.053752  -0.000000   0.036305  -0.168740  -0.388223   0.243867
                  -0.168741   0.388213   0.243854  -0.044514  -0.000001  -0.123765  -0.063769  -0.000001  -0.036292
                   0.168748   0.388220  -0.243858   0.168748  -0.388230  -0.243868
 16  0.374D 00     0.000032   0.220097   0.000006  -0.000061  -0.140066   0.000099   0.080409  -0.138937   0.436046
                  -0.080385  -0.139076  -0.436169   0.000032   0.220083   0.000008  -0.000060  -0.140069   0.000098
                   0.080403  -0.138947   0.436039  -0.080388  -0.139064  -0.436151
 17  0.357D 00    -0.266144   0.000044   0.016137   0.216927  -0.000007  -0.494047   0.123119   0.043700   0.227717
                   0.123120  -0.043771   0.227566  -0.266138   0.000042   0.016136   0.216918  -0.000009  -0.494029
                   0.123120   0.043703   0.227712   0.123117  -0.043781   0.227551
 18  0.453D-01    -0.000425  -0.175547   0.000021  -0.000309  -0.320169  -0.000002   0.372692   0.210504  -0.008809
                  -0.372928   0.210257   0.008776  -0.000422  -0.175557   0.000020  -0.000313  -0.320185  -0.000003
                   0.372715   0.210515  -0.008803  -0.372945   0.210261   0.008771
 19  0.761D-02    -0.000018  -0.265161  -0.000013   0.000011  -0.383258  -0.000002   0.353061   0.038643   0.123548
                  -0.353078   0.038643  -0.123563  -0.000003   0.265127  -0.000013   0.000005   0.383232  -0.000010
                  -0.353049  -0.038651  -0.123559   0.353052  -0.038650   0.123552
 20  0.373D-02     0.375745  -0.000010   0.000026   0.414019  -0.000008  -0.202249   0.251359   0.000179   0.100845
                   0.251348  -0.000190   0.100835  -0.375521   0.000011  -0.000023  -0.413863   0.000008   0.202260
                  -0.251262  -0.000181  -0.100844  -0.251253   0.000195  -0.100834
 21  0.320D-02    -0.000001  -0.301166   0.000025  -0.000001  -0.030832   0.000012  -0.134266  -0.407988   0.140310
                   0.134269  -0.407995  -0.140296   0.000012   0.301182   0.000025   0.000014   0.030841   0.000005
                   0.134273   0.408001  -0.140292  -0.134253   0.407994   0.140313
 22  0.157D-04     0.373080  -0.349185  -0.005382   0.270711  -0.102209  -0.002209   0.165632  -0.224430  -0.002265
                   0.163792  -0.224428  -0.002251   0.373200  -0.349190  -0.005382   0.270840  -0.102214  -0.002275
                   0.165712  -0.224433  -0.002229   0.163864  -0.224427  -0.002220
 23 -0.345D-06     0.003643  -0.003117   0.573550   0.002642  -0.000920   0.238743   0.001627  -0.001993   0.238738
                   0.001588  -0.001991   0.238743   0.003647  -0.003129   0.573554   0.002648  -0.000905   0.238743
                   0.001603  -0.002027   0.238748   0.001618  -0.002027   0.238741
 24 -0.460D-03    -0.348715  -0.373413   0.000265  -0.252899  -0.108962   0.000037  -0.153520  -0.240431   0.000094
                  -0.154650  -0.240316   0.000088  -0.348820  -0.373416   0.000262  -0.253024  -0.108983   0.000102
                  -0.153569  -0.240417   0.000069  -0.154753  -0.240291   0.000060

ONLY FIRST 18 VARIED


TEST PROBLEM 3B. MINIMIZE ENERGY AND CALCULATE FREQUENCIES OF MOLECULES          01-06-81
ETHANE. NO SYMMETRY RESTRICTIONS. PARALLEL CARTESIAN SYSTEMS.

CYCLE  2

      WC        WV        WR        WX        WT
    0.0    -11.875    46.519     8.130    42.775

TEST PROBLEM 3B. MINIMIZE ENERGY AND CALCULATE FREQUENCIES OF MOLECULES          01-06-81
ETHANE. NO SYMMETRY RESTRICTIONS. PARALLEL CARTESIAN SYSTEMS.

      WOBS       WCALC BEFORE CYCLE  2
    0.0        42.7753

DERIVATIVES BEFORE CYCLE  2
  J  NAMP(J)  DYC(J)
 24  TX        0.0001
 25  TY       -0.0000
 26  TZ        0.0221
 27  TX        0.0053
 28  TY       -0.0000
 29  TZ        0.0083
 30  TX       -0.0029
 31  TY        0.0050
 32  TZ        0.0087
 33  TX       -0.0029
 34  TY       -0.0050
 35  TZ        0.0087
 36  TX       -0.0001
 37  TY       -0.0000
 38  TZ       -0.0221
 39  TX       -0.0054
 40  TY       -0.0000
 41  TZ       -0.0083
 42  TX        0.0029
 43  TY       -0.0050
 44  TZ       -0.0087
 45  TX        0.0029
 46  TY        0.0050
 47  TZ       -0.0087

FREQ(  1)        CARTESIAN NORMAL COORDINATE
  2963.76        ATOM        DX          DY          DZ
              1  C        0.000087   -0.000209   -0.037266
              2  H        0.370661   -0.000009    0.147516
              3  H       -0.186584    0.323219    0.148718
              4  H       -0.185061   -0.320659    0.147511
              5  C        0.000085   -0.000220   -0.037271
              6  H        0.370726   -0.000012    0.147541
              7  H       -0.186643    0.323318    0.148761
              8  H       -0.185043   -0.320630    0.147496

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
      I          1        2        3        4        5        6        7        8        9       10
                11       12
NAMS(I)       E        C3       C3       C2       C2       C2        I       S6       S6        M
              M        M
CHAR(I)    1.0000   1.0000   1.0000  -1.0000  -1.0000  -1.0000  -1.0000  -1.0000  -1.0000   1.0000
           1.0000   1.0000

-----------------------------------------------------------

FREQ(  2)        CARTESIAN NORMAL COORDINATE
  2954.33        ATOM        DX          DY          DZ
              1  C       -0.000215   -0.000018    0.032112
              2  H       -0.371707   -0.000002   -0.146758
              3  H        0.187096   -0.324107   -0.147894
              4  H        0.187223    0.324322   -0.147997
              5  C        0.000207   -0.000014   -0.032107
              6  H        0.371723   -0.000002    0.146765
              7  H       -0.187170    0.324231    0.147953
              8  H       -0.187071   -0.324060    0.147871

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
      I          1        2        3        4        5        6        7        8        9       10
                11       12
NAMS(I)       E        C3       C3       C2       C2       C2        I       S6       S6        M
              M        M
CHAR(I)    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
           1.0000   1.0000

-----------------------------------------------------------

FREQ(  3)        CARTESIAN NORMAL COORDINATE
  2946.24        ATOM        DX          DY          DZ
              1  C        0.030498   -0.055590    0.000128
              2  H       -0.244335   -0.001561   -0.100861
              3  H       -0.251833    0.436183    0.208166
              4  H        0.132940    0.227286   -0.108813
              5  C        0.030508   -0.055592    0.000140
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          6  H      -0.244564  -0.001559  -0.100951
          7  H      -0.251790   0.436106   0.208130
          8  H       0.132999   0.227388  -0.108859

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
               11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000   -0.5000   -0.5000    0.5370    0.4620   -0.9991   -1.0000    0.5000    0.5000   -0.5370
          -0.4620    0.9991

-----------------------------------------------------------------

FREQ(  4)        CARTESIAN NORMAL COORDINATE
  2946.17        ATOM        DX        DY        DZ
          1  C      -0.055599  -0.030520   0.000023
          2  H       0.442862  -0.000851   0.182840
          3  H       0.003962  -0.010412  -0.004544
          4  H       0.215156   0.374643  -0.178564
          5  C      -0.055585  -0.030503   0.000035
          6  H       0.442620  -0.000854   0.182746
          7  H       0.004059  -0.010581  -0.004621
          8  H       0.215139   0.374611  -0.178549

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
               11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000   -0.5000   -0.5000   -0.5371   -0.4620    0.9991   -1.0000    0.5000    0.5000    0.5371
           0.4620   -0.9991

-----------------------------------------------------------------

FREQ(  5)        CARTESIAN NORMAL COORDINATE
  2938.74        ATOM        DX        DY        DZ
          1  C      -0.000381  -0.063650  -0.000005
          2  H       0.003006  -0.000561   0.001206
          3  H      -0.219659   0.380293   0.171417
          4  H       0.221328   0.382845  -0.172564
          5  C       0.000396   0.063656  -0.000002
          6  H      -0.003156   0.000561  -0.001232
          7  H       0.219819  -0.380221  -0.171383
          8  H      -0.221412  -0.382991   0.172631

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
               11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000   -0.5000   -0.5000   -0.9999    0.5105    0.4894    1.0000   -0.5000   -0.5000   -0.9999
           0.5105    0.4894

-----------------------------------------------------------------

FREQ(  6)        CARTESIAN NORMAL COORDINATE
  2938.66        ATOM        DX        DY        DZ
          1  C      -0.063653   0.000397  -0.000098
          2  H       0.510292   0.000006   0.198933
          3  H       0.127524  -0.221866  -0.099654
          4  H       0.124776   0.217112  -0.097709
          5  C       0.063660  -0.000381   0.000098
          6  H      -0.510334  -0.000001  -0.198951
          7  H      -0.127490   0.221806   0.099825
          8  H      -0.124850  -0.217239   0.097769

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
               11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000   -0.5000   -0.5000    0.9999   -0.5105   -0.4894    1.0000   -0.5000   -0.5000    0.9999
          -0.5105   -0.4894

-----------------------------------------------------------------

FREQ(  7)        CARTESIAN NORMAL COORDINATE
  1477.03        ATOM        DX        DY        DZ
          1  C      -0.000038   0.000000  -0.107329
          2  H      -0.158086  -0.000009   0.307615
          3  H       0.079257  -0.136856   0.307503
          4  H       0.079259   0.136851   0.307507
          5  C       0.000034  -0.000000   0.107339
          6  H       0.158095  -0.000001  -0.307637
          7  H      -0.079256   0.136883  -0.307548
          8  H      -0.079255  -0.136885  -0.307550

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
               11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
           1.0000    1.0000

-----------------------------------------------------------------

FREQ(  8)        CARTESIAN NORMAL COORDINATE
  1466.01        ATOM        DX        DY        DZ
          1  C       0.000012   0.000066   0.083632
          2  H       0.165401  -0.000582  -0.331904
          3  H      -0.083065   0.143401  -0.332198
          4  H      -0.082374  -0.143480  -0.331726
          5  C       0.000009   0.000067   0.083620
          6  H       0.165376  -0.000604  -0.331658
          7  H      -0.083051   0.143395  -0.332175
          8  H      -0.082336  -0.143483  -0.331695

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
               11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000    1.0000    1.0000   -1.0000   -1.0000   -1.0000   -1.0000   -1.0000   -1.0000    1.0000
           1.0000    1.0000

-----------------------------------------------------------------

FREQ(  9)        CARTESIAN NORMAL COORDINATE
  1433.51        ATOM        DX        DY        DZ
          1  C      -0.041659   0.020629  -0.000050
          2  H      -0.118536  -0.222518   0.190348
          3  H       0.185218   0.233861  -0.176354
          4  H       0.429029  -0.257203  -0.013273
          5  C      -0.041650   0.020636  -0.000066
          6  H      -0.116527  -0.222609   0.190336
          7  H       0.185108   0.233794  -0.176347
          8  H       0.429019  -0.257157  -0.013215

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
               11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000   -0.5000   -0.5000   -0.6051    0.9920   -0.3869   -1.0000    0.5000    0.5000    0.6051
          -0.9920    0.3869
```

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FREQ( 10)        CARTESIAN NORMAL COORDINATE
  1433.36        ATOM        DX          DY          DZ
              1  C        0.020665    0.041676   -0.000084
              2  H        0.058583   -0.044905   -0.093987
              3  H       -0.398052   -0.145423   -0.117105
              4  H        0.093509    0.098673    0.212087
              5  C        0.020642    0.041639   -0.000083
              6  H        0.058522   -0.044841   -0.093806
              7  H       -0.397642   -0.145243   -0.117032
              8  H        0.093469    0.098569    0.211915

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
                11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000   -0.5000   -0.5000    0.6052   -0.9920    0.3869   -1.0000    0.5000    0.5000   -0.6052
           0.9920   -0.3869

-----------------------------------------------------------

FREQ( 11)        CARTESIAN NORMAL COORDINATE
  1426.65        ATOM        DX          DY          DZ
              1  C       -0.001143    0.044904    0.000004
              2  H       -0.002961   -0.515882    0.004727
              3  H       -0.264741   -0.034600   -0.163274
              4  H        0.282944   -0.048555    0.158509
              5  C        0.001120   -0.044933   -0.000000
              6  H        0.002906    0.516200   -0.004631
              7  H        0.265088    0.034769    0.163328
              8  H       -0.282946    0.048423   -0.158699

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
                11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000   -0.5000   -0.5000   -0.9987    0.4557    0.5430    1.0000   -0.5000   -0.5000   -0.9987
           0.4557    0.5430

-----------------------------------------------------------

FREQ( 12)        CARTESIAN NORMAL COORDINATE
  1426.54        ATOM        DX          DY          DZ
              1  C       -0.044902   -0.001122    0.000045
              2  H       -0.116437    0.012906    0.185817
              3  H        0.364603    0.274954   -0.089107
              4  H        0.350908   -0.272826   -0.097139
              5  C        0.044920    0.001142   -0.000040
              6  H        0.116500   -0.013104   -0.185922
              7  H       -0.363850   -0.275062    0.089055
              8  H       -0.350942    0.272964    0.097246

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
                11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000   -0.5000   -0.5000    0.9987   -0.4558   -0.5430    1.0000   -0.5000   -0.5000    0.9987
          -0.4558   -0.5430

-----------------------------------------------------------

FREQ( 13)        CARTESIAN NORMAL COORDINATE
  1070.45        ATOM        DX          DY          DZ
              1  C        0.003800   -0.111838   -0.000002
              2  H       -0.002373    0.105577    0.015754
              3  H        0.012016    0.078302   -0.409378
              4  H       -0.018592    0.079355    0.393627
              5  C       -0.003800    0.111841    0.000001
              6  H        0.002373   -0.105595   -0.015753
              7  H       -0.012026   -0.078315    0.409398
              8  H        0.018594   -0.079359   -0.393646

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
                11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000   -0.5000   -0.5000   -0.9977    0.4401    0.5576    1.0000   -0.5000   -0.5000   -0.9977
           0.4401    0.5576

-----------------------------------------------------------

FREQ( 14)        CARTESIAN NORMAL COORDINATE
  1070.45        ATOM        DX          DY          DZ
              1  C       -0.111838   -0.003800    0.000038
              2  H        0.069823    0.003590   -0.463630
              3  H        0.097234    0.018114    0.218141
              4  H        0.096194   -0.012756    0.245425
              5  C        0.111842    0.003801   -0.000038
              6  H       -0.069827   -0.003590    0.463645
              7  H       -0.097241   -0.018116   -0.218147
              8  H       -0.096202    0.012762   -0.245431

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
                11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000   -0.5000   -0.5000    0.9977   -0.4401   -0.5576    1.0000   -0.5000   -0.5000    0.9977
          -0.4401   -0.5576

-----------------------------------------------------------

FREQ( 15)        CARTESIAN NORMAL COORDINATE
   981.37        ATOM        DX          DY          DZ
              1  C       -0.000052   -0.000000   -0.170592
              2  H        0.029149    0.000001   -0.221307
              3  H       -0.014655    0.025296   -0.221274
              4  H       -0.014656   -0.025294   -0.221269
              5  C        0.000051   -0.000000    0.170591
              6  H       -0.029146    0.000002    0.221298
              7  H        0.014659   -0.025292    0.221271
              8  H        0.014658    0.025294    0.221278

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1         2         3         4         5         6         7         8         9        10
                11        12
NAMS(I)       E         C3        C3        C2        C2        C2         I        S6        S6         M
              M         M
CHAR(I)    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
           1.0000    1.0000

-----------------------------------------------------------

FREQ( 16)        CARTESIAN NORMAL COORDINATE
   903.15        ATOM        DX          DY          DZ
              1  C       -0.027141    0.038287    0.000008
              2  H        0.099940   -0.175500   -0.284700
              3  H        0.095690   -0.125638    0.489891
              4  H        0.136602   -0.154635   -0.205290
              5  C       -0.027140    0.038282    0.000008
              6  H        0.090936   -0.175501   -0.284689
              7  H        0.095681   -0.125639    0.489872
              8  H        0.135598   -0.154631   -0.205278
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CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1        2        3        4        5        6        7        8        9       10
               11       12
NAMS(I)        E       C3       C3       C2       C2       C2        I       S6       S6        M
               M        M
CHAR(I)    1.0000  -0.5000  -0.5000   0.3306   0.6520  -0.9826  -1.0000   0.5000   0.5000  -0.3306
          -0.6520   0.9826
-----------------------------------------------------------------------------------------------------

FREQ( 17)        CARTESIAN NORMAL COORDINATE
   908.08        ATOM        DX        DY        DZ
             1   C      -0.038321  -0.027200   0.000011
             2   H       0.128149   0.124499  -0.401378
             3   H       0.178217   0.119794  -0.045684
             4   H       0.149332   0.078839   0.447155
             5   C      -0.038321  -0.027197   0.000009
             6   H       0.128146   0.124500  -0.401369
             7   H       0.178215   0.119794  -0.045683
             8   H       0.149329   0.078829   0.447124

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1        2        3        4        5        6        7        8        9       10
               11       12
NAMS(I)        E       C3       C3       C2       C2       C2        I       S6       S6        M
               M        M
CHAR(I)    1.0000  -0.5000  -0.5000  -0.3307  -0.6519   0.9826  -1.0000   0.5000   0.5000   0.3307
           0.6519  -0.9826
-----------------------------------------------------------------------------------------------------

FREQ( 18)        CARTESIAN NORMAL COORDINATE
   309.92        ATOM        DX        DY        DZ
             1   C       0.000397  -0.000239  -0.000002
             2   H       0.000360   0.406417   0.000041
             3   H      -0.351813  -0.202561   0.000046
             4   H       0.352393  -0.203419  -0.000055
             5   C       0.000396  -0.000240  -0.000002
             6   H       0.000381   0.406436   0.000044
             7   H      -0.351837  -0.203597   0.000049
             8   H       0.352410  -0.203429  -0.000053

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1        2        3        4        5        6        7        8        9       10
               11       12
NAMS(I)        E       C3       C3       C2       C2       C2        I       S6       S6        M
               M        M
CHAR(I)    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000  -1.0000  -1.0000  -1.0000  -1.0000
          -1.0000  -1.0000
-----------------------------------------------------------------------------------------------------

FREQ( 19)        CARTESIAN NORMAL COORDINATE
    34.89        ATOM        DX        DY        DZ
             1   C       0.001197   0.027738  -0.000080
             2   H       0.001824   0.441793  -0.001710
             3   H      -0.344383  -0.157774  -0.031443
             4   H       0.348028  -0.157774   0.032908
             5   C      -0.001233  -0.027871  -0.000080
             6   H      -0.001862  -0.441903   0.001548
             7   H       0.344331   0.157634   0.031282
             8   H      -0.348045   0.157629  -0.033069

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1        2        3        4        5        6        7        8        9       10
               11       12
NAMS(I)        E       C3       C3       C2       C2       C2        I       S6       S6        M
               M        M
CHAR(I)    1.0000   0.9748   0.9748  -0.9999  -0.9736  -0.9761   1.0000   0.9748   0.9748  -0.9999
          -0.9736  -0.9761
-----------------------------------------------------------------------------------------------------

FREQ( 20)        CARTESIAN NORMAL COORDINATE
    19.07        ATOM        DX        DY        DZ
             1   C      -0.009426   0.149115   0.000036
             2   H      -0.014245   0.152047   0.012526
             3   H       0.049839   0.263252  -0.179246
             4   H      -0.078327   0.263261   0.166839
             5   C       0.009200  -0.148924   0.000031
             6   H       0.014015  -0.151861  -0.012455
             7   H      -0.050068  -0.263062   0.179315
             8   H       0.078091  -0.263054  -0.166769

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1        2        3        4        5        6        7        8        9       10
               11       12
NAMS(I)        E       C3       C3       C2       C2       C2        I       S6       S6        M
               M        M
CHAR(I)    1.0000  -0.4024  -0.4024  -0.9927   0.2979   0.4995   1.0000  -0.4024  -0.4024  -0.9927
           0.2979   0.4995
-----------------------------------------------------------------------------------------------------

FREQ( 21)        CARTESIAN NORMAL COORDINATE
    18.44        ATOM        DX        DY        DZ
             1   C      -0.152172  -0.008646   0.000095
             2   H      -0.230566  -0.005506   0.203322
             3   H      -0.237252  -0.017114  -0.091095
             4   H      -0.223819  -0.017184  -0.111846
             5   C       0.150954   0.009222   0.000018
             6   H       0.229351   0.006091  -0.203220
             7   H       0.236028   0.017686   0.091209
             8   H       0.222611   0.017752   0.111958

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1        2        3        4        5        6        7        8        9       10
               11       12
NAMS(I)        E       C3       C3       C2       C2       C2        I       S6       S6        M
               M        M
CHAR(I)    1.0000  -0.4989  -0.4989   0.9916  -0.3952  -0.5986   1.0000  -0.4989  -0.4989   0.9916
          -0.3952  -0.5986
-----------------------------------------------------------------------------------------------------

FREQ( 22)        CARTESIAN NORMAL COORDINATE
     5.20        ATOM        DX        DY        DZ
             1   C       0.132161  -0.125050  -0.000989
             2   H       0.131881  -0.126137  -0.000261
             3   H       0.132780  -0.124473  -0.001457
             4   H       0.130975  -0.124471  -0.001252
             5   C       0.133242  -0.125219  -0.000990
             6   H       0.133520  -0.126184  -0.001713
             7   H       0.134234  -0.124837  -0.000535
             8   H       0.132793  -0.124833  -0.000724

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1        2        3        4        5        6        7        8        9       10
               11       12
NAMS(I)        E       C3       C3       C2       C2       C2        I       S6       S6        M
               M        M
CHAR(I)    1.0000  -0.4999  -0.4999  -0.0585   0.8937  -0.8352  -1.0000   0.4999   0.4999   0.0585
          -0.8937   0.8352
-----------------------------------------------------------------------------------------------------
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FREQ( 23)        CARTESIAN NORMAL COORDINATE
    0.44          ATOM        DX          DY          DZ
              1  C        0.000838   -0.000615    0.182400
              2  H        0.000862   -0.000442    0.182337
              3  H        0.000707   -0.000711    0.182444
              4  H        0.001018   -0.000711    0.182415
              5  C        0.000747   -0.000590    0.182401
              6  H        0.000723   -0.000778    0.182463
              7  H        0.000891   -0.000487    0.182356
              8  H        0.000555   -0.000488    0.182384

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1        2        3        4        5        6        7        8        9       10
               11       12
NAMS(I)       E        C3       C3       C2       C2       C2       I        S6       S6       M
              M        M
CHAR(I)     1.0000   1.0000   1.0000  -1.0000  -0.9999  -1.0000  -1.0000  -1.0000  -1.0000   1.0000
            0.9999   1.0000

-----------------------------------------------------------

FREQ( 24)        CARTESIAN NORMAL COORDINATE
   -27.54         ATOM        DX          DY          DZ
              1  C        0.124945    0.132694   -0.000109
              2  H        0.124876    0.132732    0.000059
              3  H        0.125090    0.132846   -0.000252
              4  H        0.124933    0.132762   -0.000077
              5  C        0.125291    0.132682   -0.000108
              6  H        0.125404    0.132437   -0.000412
              7  H        0.125860    0.132970   -0.000007
              8  H        0.125221    0.132880    0.000140

CHARACTER OF VIBRATION WITH RESPECT TO SYMMETRY OPERATION I
     I          1        2        3        4        5        6        7        8        9       10
               11       12
NAMS(I)       E        C3       C3       C2       C2       C2       I        S6       S6       M
              M        M
CHAR(I)     1.0000  -0.5000  -0.5000   0.0585  -0.8938   0.8353  -1.0000   0.5000   0.5000  -0.0585
            0.8938  -0.8353

-----------------------------------------------------------

  J  NAME    IKA    IRB          X          Y          Z
  1  C         1      1    0.00020    0.00000    0.76105
  2  H         2      2    1.02054    0.00000    1.15462
  3  H         2      3    0.00030    1.02024    1.15501
  4  H         2      4   -1.01994   -1.02024    1.15501
  5  C         1      5   -0.00020    0.00000   -0.76105
  6  H         2      6   -1.02054    0.00000   -1.15462
  7  H         2      7   -0.00030   -1.02024   -1.15501
  8  H         2      8    1.01994    1.02024   -1.15501


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TEST PROBLEM 3B. MINIMIZE ENERGY AND CALCULATE FREQUENCIES OF MOLECULES          01-06-81
ETHANE. NO SYMMETRY RESTRICTIONS. PARALLEL CARTESIAN SYSTEMS.

  MODE     NC    NPC   ILSQ   IWGT   IPLM   IPRT   NSTG   IBPC          ARE          SLIM          CMPR          XORD          EPSC
     4      1     17      0      0      0      3      4      1    0.100D-01    0.100D-05    0.0           0.200D-02    0.100D 02

    ARC       ARH       BRC       BRH       PLC       PLH       TBR       DCC
    KCC       DCH       KCH       ACCC      KCCC      ACCH      KCCH      AHCH
    KHCH
 1.71100   1.23400   0.14070   0.14590  22.64000   4.94000   0.28167   1.36586
 4.26800   1.05714   6.35100101.92153   0.01169109.50000   0.01673109.96982
 0.01799

   NA    NKA     NS  ICENT  HXNEG  HYNEG  HZNEG    NRB    NPX    NRP   ICMB   IVDW   IREP   IMOL    NCT   IRSC   IZAM   IGEM   IRBA  ISETA
    8      2     12      1    1.0    1.0    0.0      8      0     10      0      1      1      1      2      6      0      0      1      0

   NO     NV    NOV     LS    IWT
   24     24     24      0      0

                      PARAMETERS AFTER EACH CYCLE
  J  NAMP    DKT       INITIAL        1
 24  TX     1.000    0.0          0.000196
 25  TY     1.000    0.0          0.000000
 26  TZ     1.000    0.0         -0.005947
 27  TX     1.000    0.0         -0.001084
 28  TY     1.000    0.0          0.000000
 29  TZ     1.000    0.0         -0.006483
 30  TX     1.000    0.0          0.000987
 31  TY     1.000    0.0         -0.001196
 32  TZ     1.000    0.0         -0.006091
 33  TX     1.000    0.0          0.000987
 34  TY     1.000    0.0          0.001196
 35  TZ     1.000    0.0         -0.006091
 36  TX     1.000    0.0         -0.000196
 37  TY     1.000    0.0          0.000000
 38  TZ     1.000    0.0          0.005947
 39  TX     1.000    0.0          0.001084
 40  TY     1.000    0.0          0.000000
 41  TZ     1.000    0.0          0.006483
 42  TX     1.000    0.0         -0.000987
 43  TY     1.000    0.0          0.001196
 44  TZ     1.000    0.0          0.006091
 45  TX     1.000    0.0         -0.000987
 46  TY     1.000    0.0         -0.001196
 47  TZ     1.000    0.0          0.005091

            NVU                        18

            RDWS 0.8406D 01

            W        42.8260     42.7753

FREQ(I)

   2963.76    2954.33    2946.24    2946.17    2938.74    2938.66    1477.03    1466.01

   1433.51    1433.36    1426.65    1426.54    1070.45    1070.45     981.37     908.15

    908.08     309.92      34.89      19.07      18.44       5.20       0.44     -27.54

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