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PROGRAM MDCSPC4: MOLECULAR DYNAMICS COMPUTER SIMULATION OF MOLECULAR IONIC CRYSTALS

by

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PROGRAM MDCSPC4: MOLECULAR DYNAMICS COMPUTER SIMULATION OF MOLECULAR IONIC CRYSTALS

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Abstract

The program MDCSPC4, performs molecular dynamics computer simulations of phase changes in molecular ionic crystals. The program employs the equations of motion derived by Parrinello and Rahman, in which the simulation cell is permitted to change volume and shape in response to an applied isotropic pressure. The nature of the ionic species handled by the program include monatomic ions (e.g. K^+, Cl^- etc.), molecular ions (SO_4^{2-}, NO_3^- etc.) and neutral molecules with anisotropic charge distributions (e.g. CF_2Cl_2 etc.) The molecular species are treated as rigid and non-polarisable.

1 PROGRAM SUMMARY

Title of program: MDCSPC4

Program obtainable from:

The CCP5 Program Library, SERC Daresbury Laboratory, Daresbury, Warrington WA4 4AD, England.

Computer for which the program is designed and others on which it is operable:

Convex C220. Suitable for other mainframes with vector processing capability.

Operating system:

Unix.

Programming language:

FORTRAN 77 (plus NAMELIST extensions).

High speed storage required:

Variable. 580175 bytes for test case provided.

Number of bits per word:

64.

Number of lines in combined program and test data:

4049 + 130.

Keywords:

Molecular Dynamics, molecular ionic crystals, phase transitions, constant pressure.

Nature of the physical problem:

Calculation of the structural properties of crystalline ionic systems: the temperature and pressure dependence of the lattice parameters; the positions and orientations of molecular ions in the crystal basis; the relationships between thermodynamic variables (e.g. configuration and kinetic energies, enthalpy, pressure, volume and temperature); and the occurrence of phase transitions.

Method of solution:

The program is based on the Parrinello-Rahman Molecular Dynamics (PRMD)constant pressure method [1] for crystalline solids.

Restrictions on complexity of problem:

The ionic species handled by the program must either be point ions, rigid sub-molecules or rigid molecules. The charge distribution on each species must be represented as a fixed (distributed) set of point charges. Polarisation, molecular flexibility and three-body (or higher order) forces are not included.

Typical running time:

Variable. On the Convex C220, a 2000 timestep simulation requires ~2400 seconds for the test case provided.

Other applications:

The program can be switched to a constant volume mode, suitable for simulating ionic melts. Simulation of melts under constant pressure conditions is *not recommended.*

2 LONG WRITE UP

2.1 Introduction

Polymorphism in crystalline materials is a well known phenomenon. Under certain conditions of temperature and pressure a given material may undergo a *phase transition* and assume a new structural form. Thermodynamically this happens because the system achieves a state of lower free energy. A theoretical prediction of the phase transition can be made if the relative free energies of the two states are calculable beforehand, but this is only possible if the structure of the transformed material is already known. Unfortunately, the experimental elucidation of new structures, particularly under conditions of high temperature or pressure, is extremely difficult. What is required is the ability to predict the new structural form *a priori*. The Parrinello-Rahman Molecular Dynamics (PRMD) method [1], has this capability and has been successfully applied in many studies to date.

(In what follows it is assumed that the reader has some familiarity with the basics of molecular dynamics [2].) The PRMD method is similar to the earlier constant pressure method of Andersen [3], in that the simulated system is allowed to change volume in response to an applied isotropic pressure. However it has the additional ability to change the *shape* of the simulation cell to accommodate any anisotropic stresses that may develop. In crystallographic terms, this means the vectors defining the crystal lattice are completely variable, as are the relative positions of the ions within the unit cell (the so-called crystal basis). These degrees of freedom permit the occurrence of phase transitions in the simulations.

The method works by treating the parameters defining the lattice vectors as dynamical variables coupled to the motions of the ions in the system. Formally this is done by writing a Lagrangian [1] or Hamiltonian [4] including these variables and the appropriate coupling with the *stress tensor*. The stress tensor is defined by the kinetic energy of the ions and the molecular virial. The imbalance between the applied *isotropic pressure* and the stress tensor generates the motion of the cell parameters, leading eventually to the establishment of a dynamic equilibrium for the given temperature and pressure. In other words the structure of the crystal evolves towards the thermodynamically stable phase for the given state point. It therefore represents an *a priori* approach to the study of phase transitions in crystalline solids by virtue of the fact that it is not intrinsically dependent upon the chosen starting structure. In principle the method is capable of generating the correct crystal structure for any desired state point. All that is required is a suitable representation of the interionic potential energy.

2.2 The Program MDCSPC4

The program MDCSPC4 is based on the PRMD method for ionic crystals, where the ionic species exist either as point ions (e.g. K^+, Cl^- etc.) or "rigid" sub-molecular species (e.g. SO_4^{2-}, NH_4^+ etc.), and is also able to handle crystals of neutral "rigid" molecules with polar bonds (e.g. $CFCl_3$, H_2O etc.) Its implementation for molecular (sub-)species with long ranged Coulombic interactions, employs the Ewald summation method [5], and follows the prescription of Nosé and Klein [6], to which the reader is directed for a detailed description of the theory.

Within the program an ionic species is treated as either a single fixed charge (located on an atomic nucleus) in the case of the point ions, or a fixed set of point charges (not

necessarily located on the nuclei) at fixed locations in the molecular framework in the case of neutral molecules or molecular ions. Polarisation is not treated, nor is molecular flexiblity. The molecular species are regarded as dynamically rigid bodies. The only non-Coulombic forces permitted are Buckingham *exp-6* [7] pair potentials between atomic sites on different molecules. The system must be electrically neutral. No hard restrictions on the system size or on the (crystallographic) shape of the simulation cell exist. Though efficiency considerations apply to large systems or highly noncubic simulations cells. The equations of motion, for the simulation cell and the translational motions of the ions, are solved using the fifth order Gear predictor-corrector [8]. The rotational motion is handled with the Evans quaternion algorithm [9] with a fifth order Gear integrator.

3 The Program Structure

The subprograms in the program MDCSPC4 are listed in Table 1. There are essentially five types of subprogram:

1. Subprograms MAIN and CYCLE control the execution of the program by calling the principal subroutines. MAIN is the root subprogram of MDCSPC4 and CYCLE controls the molecular dynamics simulation.
2. SYSDEF, START and BLOCKDATA are concerned with data initialisation.
3. SETVEC, EWALD, FORCES and MOTION, perform the molecular dynamics simulation and are called by CYCLE.
4. SYSAVG, ENFOLD, CRYSTL, ORIENT, TRAJIC and RESULT are concerned with analysing the properties of the simulated system.
5. DCELL, INVERT, JACOBI, MATMUL, RANDUM, SDOT, SSUM and TIMCHK are simple utility routines or functions.

Few of the subprograms are called with an argument list. In most cases the data are transferred via COMMON blocks. The calling heirarchy of the subprograms is presented in Table 2. Program MDCSPC4 makes extensive use of FORTRAN COMMON blocks. These are listed in Table 3. A more detailed description of the elements of each block appears as FORTRAN comment lines in the main segment of the program.

3.1 Subprogram descriptions

3.1.1 Control subprograms

The execution of the program is controlled by the MAIN subprogram. This calls the major subroutines SYSDEF, START, CYCLE and RESULT and also makes the first (initialising) call to the timing routine TIMCHK. On completion of a successful run of MDCSPC4, the MAIN routine terminates the program. The primary I/O files DATA05 (input) and DATA06 (output), are opened by MAIN. (A list of the files accessed by MDCSPC4 is given in Table 4.)

Subroutine CYCLE controls the molecular dynamics simulation. This is done primarily by calling the main simulation routines: SETVEC, FORCES, EWALD and MOTION. CYCLE also monitors the usage of CPU time and compares the time consumed

against a user specified limit and, if necessary, brings about a controlled termination of the job. CYCLE also updates the timestep number (NSTEP) with each MD step and terminates the job if the number of steps reaches the required limit (NRUN). At user selected intervals CYCLE prints data to file DATA06, which indicates the status of the simulation. These data include: energy, temperature, pressure, cell parameters, time and timestep number etc. During the MD cycle, subroutine CYCLE calls the analysis routines SYSAVG and ORIENT, to accumulate data on the system properties, and the subroutine TRAJIC, to write out configuration data.

MAIN and CYCLE are called once only during a run of MDCSPC4.

3.1.2 Initialisation subprograms

Subroutine SYSDEF reads the input data supplied by the user in the file DAT05 and performs some rudimentary data checking prior to the start of the simulation. Apart from a job title, all data appearing in DATA05 are specified in NAMELIST format. A full description of these data is given in section 4. SYSDEF defines the internal units for the program and converts the user supplied data accordingly. Some basic properties of the input species are calculated, such as the principal moments of inertia (which determines the number of rotational degrees of freedom), molecular mass, and so on. SYSDEF also calculates the long ranged corrections for the short-ranged forces (based on the specified potential cutoff radius) and the fixed intramolecular corrections for the Ewald summation. Finally, SYSDEF prints a summary of the user supplied data in the file DATA06.

The BLOCKDATA subprogram contains some initial values for variables in the COMMON blocks, and also the default values for some parameters appearing in the namelists read by SYSDEF. It is not possible to give all variables sensible defaults (e.g. potential parameters) and hence these are left undefined. The contents of each namelist are specified in Tables 6 to 9.

Subroutine START generates the initial configuration of the simulated system and has three different modes of use, depending on the input parameter KEYRES (see section 4.3). These different modes allow simulations to commence from different starting conditions

The initialisation subprograms are called once only during a run of MDCSPC4.

3.1.3 Molecular dynamics subprograms

These subroutines are called exclusively by the control subprogram CYCLE. They are called many times in the course of a simulation. Most are called once only per timestep, except subroutine MOTION, which is called twice.

Subroutine SETVEC is a simple subprogram which initialises certain arrays at the start of every timestep. Its other principal function is to reorientate the atomic site vectors of the molecular ions in an absolute frame of reference after the ions have been dynamically rotated in the previous timestep. SETVEC also renormalises the quaternions every timestep as demanded by the Evans-Murad algorithm [9].

Subroutine MOTION performs the integration of the equations of motion for both the molecular ions (translational and rotational motion) and the simulation cell. The algorithm used for these tasks is the appropriate 5th-order Gear predictor-corrector [8]. Subroutine MOTION is called twice during each MD cycle. On the first call it uses

a Taylor expansion to predict the positions and orientations of the ions (and the new simulation cell parameters). The subroutine then returns control to CYCLE. Later, after the molecular forces and torques (and the stress tensor) have been calculated, MOTION is called again to determine the corrected positions and orientations (and cell parameters). Lastly, MOTION accumulates data for an approximate calculation of the mean square displacement of the ionic species.

Subroutine EWALD calculates the reciprocal space contributions to the potential energy, virial, stress tensor and ionic forces. The calculation of these quantities follows the method of Nosé and Klein [6] and the implementation is derived from the CPC program MDIONS [15].

Subroutine FORCES calculates the real space contribution to the potential energy, virial, stress tensor and ionic forces and also the contributions to these quantities arising from the short-ranged Buckingham potentials. The calculation of these quantities also closely follows the method of Nosé and Klein [6]. FORCES also (conditionally) accumulates data for the site-site radial distribution functions, as specified by the user with the logical control variable LRDF.

3.1.4 Analysis subprograms

A group of subprograms are called during the MD cycle by the subprogram CYCLE. These include SYSAVG, ORIENT and TRAJIC.

Subroutine SYSAVG calculates the statistics of the fundamental thermodynamic quantities of the system under study. The quantities of interest are: potential (configuration) energy, total energy, virial, enthalpy, pressure, volume, kinetic energy and temperature (rotational and translational) and the cell parameters (cell vector lengths and angle cosines). SYSAVG also accumulates the quantities to enable the calculation of *fluctuations* of the basic thermodynamic variables and *rolling averages* over a user-defined number of preceeding MD steps. During the nominated equilibration period, SYSAVG will zero these variables, and/or rescale the system temperature, as instructed by the user. SYSAVG also includes a check on the size (perpendicular width) of the simulation cell in relation to the user specified cutoff radius. The program will terminate if the cutoff exceeds the cell half-width (see section 4.3).

Subroutine ORIENT calculates *orientational distribution functions* (ODFs) for the site vectors of the ionic species. The site vectors being the vectors drawn from the centre of mass of a species, to each of the atomic sites within the species. In a perfect crystal, these vectors have preferred directions, which give rise to peaks in the orientational distribution function, which is defined in terms of *real* spherical harmonics by the series [11, 12]:

$$Z(\theta,\phi) = \sum_{\ell}^{\infty} \sum_{m=-\ell}^{m=+\ell} C_{\ell m} Y_{\ell m}(\theta,\phi) \qquad (1)$$

Where the $C_{\ell m}$ are calculated as ensemble averages of the corresponding spherical harmonics for each site vector. (i.e. $C_{\ell m} =< Y_{\ell m} >$). In ORIENT the limit $\ell \leq 12$ is used. The spherical harmonics are generated by an algorithm due to Smith [13].

Subroutine TRAJIC opens and writes to the file DATA09, the configuration data at user selected intervals. In the supplied version of the program, these data consist of positions, orientations and corresponding velocities of the ions. TRAJIC is called by CYCLE.

Subroutine RESULT is the primary analysis routine of program MDCSPC4, and is usually called by MAIN. (It can also be called by SYSAVG if an error condition is encountered. See above.) It provides the final summary of the results of the simulation at the time of termination. The final thermodynamic averages and fluctuations are written to DATA06, along with the normalised site-site RDFS, mean ion positions and final positions, orientations and velocities of the ions. RESULT writes the final configuration data and all internal accumulators to the *restart file* DATA08 and optionally writes a summary of the structural data to the file DATA10. RESULT also optionally calls the analysis routines CRYSTL and ENFOLD.

MDCSPC4 contains a number of structural analysis routines to help the user unravel the structure of an undetermined phase. Though experience has shown that these are helpful in many cases, the user is warned that these are not foolproof.

Subroutine CRYSTL peforms a 3D spatial fourier transform of the *mean positions* of the ionic species, with a view to projecting out any periodicity in the structure. (This should not be confused with a structure factor calculation, which is an ensemble average of the Fourier transform of the charge density.) CRYSTL is meant to provide a quick and inexpensive indication of the presence of Bragg planes in the overall structure.

Subroutine ENFOLD attempts to "fold" the contents of the simulation cell back onto a user defined "unit cell", using the average ion positions calculated by RESULT. If all the enfolded ions are within the RMS fluctuation of each other the enfolding is deemed successful and a reasonably reliable crystal structure is obtained. However, if the system has become disorganised, the enfolding will fail and an error message is printed along with the unresolved enfolded structure.

3.1.5 Utility subprograms

MDCSPC4 has a number of utility routines, some of which are likely to exist on other computing systems, but which have been included for transportability. The user may wish to replace them with more familiar local facilities. These routines (which are internally documented) are as follows.

Subroutine DCELL calculates the dimensional properties of the simulation cell (i.e. the lengths of the cell vectors, the cosines of the angles between the cell vectors, the perpendicular widths of the cell and the cell volume.) Subroutine INVERT calculates the inverse of a 3×3 matrix. Subroutine JACOBI diagonalises a *real symmetric* matrix, giving the eigenvalues and eigenvectors. Subroutine MATMUL multiplies two 3×3 matrices. Function RANDUM is an approximate random number generator, which produces pseudo random numbers in the interval $(0, 1)$. (An exact random sequence is not essential in MDCSPC4.) Function SDOT calculates the scalar product of two vectors. Function SSUM calculates the scalar sum of the elements of a vector. Subroutine TIMCHK is a simple timing routine that makes use of the *local intrinsic* timing routine. (In the case of the Convex C220, the local routine is called ETIME.) On other machines this must be replaced by a local intrinsic function to provide the CPU time in seconds. Note that MDCSPC4 only ever calls the timing intrinsic via TIMCHK.

4 Running the Program

4.1 PARAMETER Specification

Prior to using MDCSPC4 it may be necessary to adjust some of the internal array sizes throughout the program. These are defined by PARAMETER statements. The relevant parameters are listed in Table 5, with the current default values. They must be located and adjusted wherever they appear in the program.

The defaults appearing in Table 5 are based on the supplied test case, a potassium nitrate simulation, and have the following significance. The compound has two species: K^+ and NO_3^-, hence NST=2. There are 5 atomic sites in the KNO_3 molecule, hence MSITES=5. The unit cell has 4 K^+ and 4 NO_3^- sites, hence MBAS=8. MSP is the total number of ionic species to be simulated, which for the test case provided is 144 species or 72 potassium nitrate molecules (this is equivalent to 18 unit cells).

KMAX is is the parameter in subroutine EWALD that effectively defines the range of the Ewald sum in reciprocal space. Section 4.5 describes how this parameter should be fixed.

MAXRDF determines the size of the RDF arrays (see section 4.7.1).

4.2 The Input File DATA05

The execution of the program is controlled by the input file DAT05. The user supplied data consist of five types:

1. The Job title.
2. System data, specifying temperature, pressure etc.(/NLSYST/).
3. Simulation control data (/NLCNTL/).
4. Species parameters, defining the structure of the ions etc. (/NLSPE/).
5. Potential energy parameters for the Buckingham potentials (/NLPOTL/).

Items 2 to 5 are supplied in NAMELIST format, the names of which appear in brackets. This sequence of the data indicated must be adhered to. The job title appears once only in DATA05, as does the namelists /NLSYST/ and /NLCNTL/. The namelist /NLSPEC/ appears once for each distinct species type in the simulation and /NLPOTL/ appears once for every distinct pair potential required.

4.2.1 The Job Title

The job title is the first record in file DATA05. It must be less than 80 characters (including spaces). It is reprinted as a header record in the output file DATA06, the restart file DATA08 and the structure file DATA10.

4.2.2 The NAMELIST /NLSYST/

The namelist /NLSYST/ specifies the primary system variables as described in Table 6. It must be the second data item in file DATA05. The units are generally MKS, except the variable DAMP, which is treated as a dimensionless scaling parameter. The array CVEC(9) contains the vectors defining the simulation cell. The first three elements represent the vector a, the second three b etc.

4.2.3 The NAMELIST /NLCNTL/

The namelist /NLCNTL/ defines the variables which control the execution of the program. They are specified in Table 7. They are generally logical or integer variables without units, except for the time variables TIMJOB and TCLOSE, which are real numbers in units of seconds. The namelist /NLCNTL/ must be the third data item in file DATA05.

4.2.4 The NAMELIST /NLSPEC/

The namelist /NLSPEC/ defines the structures of the ionic and molecular species and their location within the crystal unit cell. (The latter should not be confused with the simulation cell, which is built from multiples of the crystal unit cell.) There are NST occurences of the /NLSPEC/ namelist in DATA05 i.e. one such namelist for every unique species type in the simulation. Collectively the set of namelists /NLSPEC/ comprise the fourth data item in the file DATA05.

To specify each species, the following information is required (MKS units are used where appropriate):

1. the number of atoms (or sites) in the species;
2. the mass associated with each site (this can be zero if the site is a distributed charge) and the associated electronic charge (which can be zero);
3. the positions of the atomic sites within the species;
4. the number of times the species appears in the unit cell (i.e. number of locations)
5. the positions and orientations of the species in the unit cell.

It should be noted that the specified positions of the species in the unit cell are defined by their centres of mass in fractional coordinates of the unit cell (i.e. in the range 0~1). The orientations are defined in terms of the Euler angles (in degrees) written in the X convention [10]. Atomic ions must be assigned zero values for the Euler angles. The positions of sites within a species must be defined with reference to an internal coordinate system in which the moment of inertia tensor is diagonal i.e. the principal moments of inertia must define the molecular axes. (Note that it is not necessary to specify the principal moments of inertia; these are calculated internally.) Failure to use the principal axes in defining the site locations, will result in a redefinition of the molecular orientation and hence an incorrect specification of the initial molecular orientation. Users are advised to examine the printed coordinates in the output file DATA06 to see if such a redefinition has occurred.

The contents of the namelist /NLSPEC/ are described in Table 8. None of the variables have default values, but limits on their number do exist, as indicated in the table. (Note: MBAS is defined by a PARAMETER statement in subroutine SYSDEF.)

4.2.5 The NAMELIST /NLPOTL/

The namelist /NLSPEC/ defines the short ranged pair potentials that act between atomic sites. Any number of occurrences of the namelist /NLPOTL/ may appear, up to

a maximum of MSITES(MSITES+1)/2 (see Table 5). Collectively these form the fifth and final item of data in file DATA05.

The form of the pair potential is the Buckingham exp-6 type [7]:

$$V(r_{ij}) = A_{\ell m} exp(-r_{ij}/\rho_{\ell m}) + C_{\ell m}/r_{ij}^6 \qquad (2)$$

where $A_{\ell m}$, $\rho_{\ell m}$ and $C_{\ell m}$ are the appropriate empirical parameters defining the potential between sites of types ℓ and m; $V(r_{ij})$ being the potential as a function of the inter-site separation r_{ij}. (Note the + sign before the parameter $C_{\ell m}$ in the above equation.) The contents of the namelist /NLPOTL/ are listed in Table 9. The parameters are defined in units of *Joules* (J) and *nanometres* (nm).

To define a pair potential correctly with the namelist /NLPOTL/, use is made of the *site index*, which is a unique number automatically assigned to each site specified by the namelist /NLSPEC/, preserving the order in which each site occurs. If more than one type of species is present in the system (i.e. more than one namelist /NLSPEC/ is present in the input file DATA05) the site index continues to increase with each new site encountered. It is important to note that the program MDCSPC4 does not recognise the symmetry equivalence of sites within a molecular species. Each individual site must be treated as if unique within the species concerned. The site index appears in the output file DATA06.

In order to reduce the number of occurrences of the /NLPOTL/ namelist in DATA05, it is possible to characterise several pair potentials with a single /NLPOTL/ namelist. The number of potentials that may be specified for each namelist occurrence is limited by the parameter MSITES (Table 5). The method is to specify the index of the first site (parameter IXP - Table 9) followed by the several possible second sites (parameter array JXP(n) - Table 9). Use of the condition IXP<JXP will prevent unnecessary double specification of the potentials. (Note that if double specification occurs, the last entry will be adopted.) The entry of the pair potentials is terminated by an empty /NLPOTL/ namelist. Any pair potentials not specified by this stage will be assumed null (i.e. $A_{\ell m} = C_{\ell m} = \rho_{\ell m}^{-1} = 0$). It is assumed that all specified potentials act only between sites on *different* molecular species. No intramolecular terms are calculated.

4.3 General Comments on the Use of the Program

The normal use of the program MDCSPC4 assumes that a simulation will begin with an *Equilibration Period* of the order of one or two thousand timesteps, during which the temperature and pressure of the simulation achieve the required targets, within statistical fluctuations. There follows a *Production Period*, typically of several thousand timesteps, during which data are accumulated to calculate the desired properties, after which the program *Summarises* the results and *Terminates* the simulation. In terms of the input variables in Table 7, the equilibration period lasts NSEQL timesteps and the production period for the subsequent NRUN-NSEQL timesteps.

The starting conditions for a simulation are controlled by the parameter KEYRES (Table 7) chosen by the user:

1. KEYRES=0, generates the initial system from the lattice data provided by the user. These data include the fractional coordinates of the ionic species in the unit cell and the orientations of the molecular ions. The initial lattice is

created by repetition of the unit cell in all three principal directions, as specified by the user (section 4.9). Random translational and angular velocities are assigned to the ions, the bulk motions extracted and then scaling to the desired temperature is performed. Allowance is automatically made in the rotational motion for species possessing fewer that three rotational degrees of freedom. Step counters and accumulators are initialised to zero, as are the higher derivatives of the velocity and angular momentum arrays.

2. KEYRES=1, assumes the simulation is a continuation of a previous run. In which case all configurational data are read from the *restart file:* DATA07. Step counters and accumulators assume their previous values.
3. KEYRES=2, reads all the configuration data from the restart file DATA07, but ignores the step counters and accumulators of any previous run. The temperature of the initial system will be adjusted to that desired by the user, as an aid to equilibration.

As indicated above, the program has the capability of restarting a simulation once it has terminated. It requires that the file DATA08, which is automatically written at termination, be renamed DATA07 and the control variable KEYRES (Table 7) in the input file DATA05 be reset to a nonzero value. (Other changes may be necessary in the input file according to requirements.)

The variable LTEMP (Table 7) determines the use of temperature scaling during the equilibration period. It must be set .TRUE. if scaling is required. NSBTS (Table 7) determines the timestep interval between the rescaling operations. It is possible to define an equilibration period without temperature scaling, by setting LTEMP to .FALSE. Both LTEMP and NSBTS are valid during the equilibration period only; outside this period they are ignored.

The equilibration period can be reimposed during a simulation by restarting the simulation from a previous run, selecting the start conditions from the file DATA07 with control option KEYRES=2 (Table 7). Such a re-equilibration is recommended if the system has undergone a phase transition, or if there is a drift in the thermodynamic quantities during the production period. The user is advised to re-equilibrate the system before accumulating fresh data. With KEYRES=2, the user may select a new temperature or pressure for the system at restart.

The program may sometimes terminate before the desired number of timesteps has been completed because the run comes within TCLOSE seconds of the allocated job time TIMJOB (see Table 7). In which case the program may be restarted from the restart file with KEYRES=1. The simulation will continue as if uninterrupted. A simulation can also be continued beyond the originally specified production period by restarting the program with KEYRES=1 and the control variable NRUN increased to the desired value. The user is advised that it is dangerous to change any other variables in the main input file DATA05 in this case.

During constant pressure simulations, the program may sometimes terminate automatically if the half-width of the simulation cell shrinks to less than the specified radius of cutoff. In this circumstance the user may choose to restart the simulation with a reduced cutoff (but beware of reduced accuracy!) or consider a larger simulation.

Finally, it should be remarked that, while program MDCSPC4 is capable of recreating phase transitions in inorganic crystals, in practice such transitions may be few and

far between. It is frequently the case that phase transitions are "relocated" in phase space (particularly if the potential functions are approximate), or that they are inhibited for mechanistic reasons [12]. Furthermore, when a phase transition occurs, it will sometimes mean that the program control parameters, the Ewald convergence parameter and even the system size need to be reconsidered before characterising the new structure. It is incorrect to attempt to characterise the new structure during a simulation designed for the preceeding structure, not least because the accumulated averages will pertain to both structures.

4.4 Constant Volume and Constant Pressure

Program MDCSPC4 contains three alternative MD algorithms, which are controlled by the variable KPRESS (Table 7):

1. KPRESS = 0, standard NVT (constant volume) simulation.
2. KPRESS = 1, Parrinello-Rahman NPT (constant pressure) [1] simulation.
3. KPRESS = 2, Brown-Clarke NPT (constant pressure) [14] simulation.

The parameter KPRESS is set by the user in the file DATA05 (Table 7). The Brown-Clarke algorithm is an alternative to the Parrinello-Rahman algorithm, though in MDCSPC4 it is included purely to assist with equilibration to a specified pressure.

Note that it is necessary to set a fictitious mass for the MD cell (CMASS - Table 6). This is usually set equal to the mass of the molecular species being simulated, though higher values sometimes improve the stability of the simulation.

Equilibration of a system in a constant pressure simulation is sometimes problematical, particularly if the empirical potentials have not been optimised for the starting structure. The following strategies may help: (i) Equilibration of the system at constant volume sometimes helps to resolve internal stresses (option KPRESS=0, see Table 7); (ii) Equilibration using the Brown-Clarke constant pressure algorithm (option KPRESS=2) is usually more stable than Parrinello-Rahman (option KPRESS=1) under these circumstances and can be used to relax the system to equilibrium. A large value of the damping parameter DAMP ($10^3 \sim 10^6$) may be used to control the rate of attainment of the desired pressure.

4.5 Controlling the Program Accuracy

The accuracy of the program is determined by a few key parameters and control variables.

The accuracy of the short-ranged potential and forces is determined entirely by the chosen radius of the cutoff (RCUT, Table 6). If this variable is not specified in the input file DATA05, a default value is used, which equals half the width of the simulation cell if the constant volume option applies and 0.8 times the initial half width if constant pressure is chosen. It should be noted that the use of a cutoff implies a long-range correction to the short-ranged terms. In MDCSPC4 this correction is based on the assumption of uniform density outside the spherical cutoff, and should be regarded as a first order correction only. The correction fluctuates with the system volume when the constant pressure algorithm is used. The initial values of these corrections are printed in datset DATA06.

The accuracy of the long-ranged Coulombic terms, as treated by the Ewald method, depends on choosing the correct cutoff range in the real and reciprocal space domains and a suitable convergence parameter α [2, 5]. In MDCSPC4 the cutoff in real space is set equal to that of the short-ranged terms (i.e. RCUT). The cutoff range in reciprocal space is effectively governed by the parameter KMAX (Table 5), since this sets the limit on the largest k-vector used in the reciprocal space summation.

It is easily shown [6] that the terms $exp(i\mathbf{k}\cdot\mathbf{r}_j)$ in the Ewald sum readily reduce to the form $exp(i2\pi(\ell s_j^x + m s_j^y + n s_j^z))$, where $\mathbf{k}$ is a reciprocal lattice vector, $\mathbf{r}_j$ and s_j the ion positions in the simulation cell in real and fractional coordinates and ℓ, m and n are integers. The parameter KMAX defines the largest values of ℓ, m and n the program uses. Typical values of KMAX range between 6 and 8, assuming a reasonably cubic simulation cell. (The default value is KMAX=8.) It should be noted that the running time of the program will increase rapidly as KMAX increases.

Assuming that the KMAX range is sufficient, a suitable value of α must be found. (Note that α is units of m^{-1}.) In practice this may be easily obtained for a given system by performing a series of one-step MD runs, gradually increasing α from zero until the potential energy achieves a plateau value. (As a rule-of-thumb, the product αr_{cut}, where r_{cut} is the applied potential cutoff, is $\approx 3 \sim 4$.) The obtained value of α, and the calculated potential energy, should be verified by increasing KMAX and repeating the determination. If a plateau value does not occur in the first instance KMAX is too small, and should be increased. Note that the larger KMAX, the broader will be the range of acceptable α values. Also, since large KMAX values greatly increase the computing time per timestep, the smallest KMAX compatible with the required accuracy is desirable.

4.6 Thermodynamic Quantities

Program MDCSPC4 prints a number of thermodynamic and structural quantities at user selected timestep intervals while the simulation proceeds. The frequency of printing is controlled by variable NSBPO (Table 7). The data printed include: configuration energy; virial; translational and rotational kinetic energy and associated temperatures; total energy; enthalpy; pressure; volume and the lengths of the simulation cell vectors and angle cosines. The rolling averages of the quantities over the previous NSTK timesteps are also printed (see Table 7). At the termination of a run MDCSPC4 prints the final averages of these quantities and their associated fluctuations. It should be noted that the extensive properties are quoted for *Avogadro's number of species* and not necessarily for one mole of the material (unless a single, neutral species is simulated.) Further (trivial) conversion to molar quantities is therefore usually necessary. The averages are calculated from data samples taken every timestep after the end of the equilibration period (i.e. after timestep NSEQL), as are the fluctuations.

4.7 Structural Analysis

The primary structural analysis facility within MDCSPC4 is the set of partial radial distribution functions. However some additional low level facilities have been included, which help with the data interpretation. These include orientational distribution functions, average particle positions, folding analysis and Bragg plane projection. The results of all these analyses are printed in the output file DATA06.

4.7.1 Radial Distribution Functions

This option is activated by setting LRDF to .TRUE. in /NLCNTL/ (Table 7). The data accumulation begins at the user specified timestep NSTRDF and is sampled every subsequent INCRDF timesteps.

In principle MDCSPC4 calculates one partial radial distribution function (RDF) for each pair of site indices. The program does not average the RDFs over sites equivalent by symmetry until the RDFs are finally printed. The facility exists within MDCSPC4 for the user to define the averaging process, in terms of the partial RDFs that are to be averaged together. This is done by equivalencing the RDFs via the array IDTRDF in the namelist /NLCNTL/. In this array the partial RDFs to be equivalenced are indicated by backwards referral to the first equivalent RDF. In the case of no equivalent RDFs being specified the contents of the array are as indicated in Table 10. If for example, RDFs 3,5 and 6 were equivalent, entries for IDTRDF(3), IDTRDF(5) and IDTRDF(6) would specify the number 3. (In which case IDTRDF(7) would continue the sequence with the number 7, unless it too refers to a previous RDF etc.) Normalisation of the RDFs automatically makes allowance for the averaging process.

It should also be noted that the partial RDFs are stored in the restart file DATA07 in the pre-averaged state. This means that a subsequent run of the program will permit a new specification of the averaging process, without loss of previously accumulated data. The new structure file DATA10 will however contain the new averages.

An example of the use of this facility is given in the provided input file.

4.7.2 Orientational Distribution Functions

This option is activated by the same variables that select the RDF option (i.e. LRDF, NSTRDF and INCRDF).

The orientational distibution functions (ODFs) indicate the preferred directions of the site vectors in terms of the components of the spherical harmonic expansion (equation (1)). The coefficients $C_{\ell m}$ obtained are printed in DATA06 when the job terminates. In DATA06, the $C_{\ell m}$s are printed as a 13×13 matrix, and there is one such matrix for each site vector in the molecular unit. (There is no $C_{\ell m}$ matrix printed for point ions and ions at the centre of mass of the molecular unit.) It is possible to average the ODF matrix elements arithmetically, for symmetry-equivalent site vectors, though MDCSPC4 does not do this.

The ODF matrices are written so the the $\ell = 0$ terms appear along the diagonal. Below and above the diagonal the terms corresponding to the normalised combinations $(Y_{\ell m} + Y_{\ell -m})/2^{1/2}$ and $-i(Y_{\ell m} - Y_{\ell -m})/2^{1/2}$ respectively appear (here using the complex spherical harmonic notation). Terms closest to the diagonal have the lowest m values. The pattern is exemplified by Table 11.

The conversion of these parameters into contour plots of $Z(\theta, \phi)$ via equation (1) simple and very revealing [12].

4.7.3 Average Species Positions

The program calculates the average positions of each species in the simulation cell and the associated fluctuations. To be of maximum use these data must be accumulated for a stable crystal structure. Structures which are disordered, or have mobile ions do not

provide meaningful data. The average is performed in terms of the fractional coordinates of the ions within the simulation cell.

These data are also used in the folding analysis and Bragg plane projection decribed below.

4.7.4 Folding Analysis

The folding analysis uses the average species positions described above. In this technique the user specifies the number of unit cells in each direction in the simulation cell with the user defined variables KLX, KLY and KLZ (Table 7) and the program will attempt to superimpose these "unit" cells on top of each other to determine if they have the same structure. The tolerance of the fit is set by the fluctuations of the ions concerned. If this tolerance is not satisfied, then all non-superimposable ions are listed, with an error message. A satisfactory folding indicates a correct unit cell, though not necessarily the primitive cell.

Unless the structure has undergone a phase transition, KLX, KLY and KLZ should correspond to NLX, NLY and NLZ (Table 7) respectively.

4.7.5 Bragg Plane Projection

The Bragg plane projection is based simply on a Fourier transform of the average species positions i.e.

$$S(\mathbf{k}) = N_s^{-1} \left| \sum_{j=1}^{N_s} exp(i\mathbf{r}_j \cdot \mathbf{k}) \right|^2 \qquad (3)$$

where N_s is the number of species of a given type, $\mathbf{r}_j$ is the location of the species in the MD cell and $\mathbf{k}$ is a reciprocal lattice vector. $S(\mathbf{k})$ is a *pseudo*-structure factor, which indicates the presence of Bragg planes in the average structure when its magnitude is of the same order as N_s. Values of $S(\mathbf{k})$ less than 1.0 are not printed in the output.

4.7.6 The Trajectory File DATA09

The trajectories of the species may be written into a file (DATA09) if requested by the user. The control variable for this facility is LTRAJ (Table 7), which must be set to .TRUE.. The writing of the data starts at the timestep NSTRAJ and at timestep intervals NITRAJ (Table 7). In the supplied program, the data written to DATA09 include the species positions and quaternions. Modifications of the subroutine TRAJIC to write other data, are trivial.

4.7.7 The Structural File DATA10

The user may instruct MDCSPC4 to write a structural file (DATA10) at job completion, which contains the RDFs, ODFs and average particle positions. (Modifications, if desired, should be made to subroutine RESULT.) This option is activated by setting the control variable LSTRFL (Table 7) to .TRUE..

4.8 Units

The program MDCSPC4 adopts MKS units for input and output, wherever practical. The main departure from this rule occurs in the definition of the potential parameters, which requires the use of nanometers (see section 4.2.5).

Internally, the program uses suitably scaled units for dealing with molecular quantities. These units appear in the output file DATA06. The restart file DATA08 is generally written in these units as are the sample input and output positions and velocities appearing in file DATA06.

4.9 Additional Program Controls

Further control options are presented in Table 7. The following points should be noted.

1. The input variable NPC and the variables NLX, NLY and NLZ are mutually exclusive. If NPC is nonzero, (NLX,NLY,NLZ) are each set to $(NPC)^{1/3}$, from which it follows that NPC must be of the form M^3, where M is integer. Only if NPC is zero, will the values of (NLX,NLY,NLZ) specified in the input file be used, in which case NPC will default internally to NLX×NLY×NLZ.
2. At the end of the equilibration period, it is usual to set the accumulators of thermodynamic properties to zero. The variable LZEQL can be used to prevent this. If LZEQL is .FALSE. the accumulators are not zeroed. This allows the accumulation of data while temperature scaling is occuring.
3. The program contains a simple (single-origin) mean square displacement (MSD) algorithm. It is activated by setting LMSD to .TRUE., and starts at timestep NSTMSD. The computed MSD is printed in file DATA06.
4. NSTK specifies the number of timesteps over which the rolling averages are calculated. The maximum is 100 steps.
5. The option to randomise the orientations of the species (i.e. using random Euler angles) is controlled by the variable LORAND. If set .TRUE., random initial orientations are created. In this case the EULER parameters (Table 8) should be set to zero in /NLSPEC/.

5 Example Run of Program MDCSPC4

5.1 Compilation and Execution

Program MDCSPC4 was developed in a Unix environment. Readers are therefore advised to consult local Unix documentation for specific details on standard procedures.

On the Daresbury Laboratory Convex C220, compilation of the entire source code followed by execution of the program is achieved by the unix commands:

```
fc -o mdcspc4 -O2 mdcspc4.f
mdcspc4
```

Which may be inserted into a *shell script* and submitted into the background.

It is assumed that the program source is contained in the file mdcspc4.f and the input data is in the file DATA05. The reader is referred to Section 4.3 and Table 4 for further details regarding input and output files.

5.2 The Test Case

The test case supplied is an example simulation of potassium nitrate. The basic input file (DATA05) is shown in Table 12. Two example runs are performed. The first is an NVT simulation of potassium nitrate at 200 K (Table 13). The second is a similar simulation at NPT, with the required pressure set to 0.0 Pa (Table 14). The latter run requires KPRESS=1. Note also that option KEYRES=2 should be used in the second case, which means that the NPT run takes the final configuration of the NVT run as input. A brief summary of the contents of a typical output file (DATA06) follows.

1. A presentation of all supplied input data characterising the system to be simulated and the job specification.
2. A sample of species positions, orientations, translational velocities and quaternions at the start of the run, either generated from an initial lattice or taken from a previous run.
3. A running commentary of the progress of the job, presenting the computed thermodynamic properties, cell structure and their rolling averages, and the elapsed computing time at user specified intervals. The mean square displacements and an announcement of the end of the equilibration period and job termination may also appear.
4. A summary of the mean values of the thermodynamic variables and cell parameters and their fluctuations for the entire simulation production period.
5. A sample of species positions, orientations, translational velocities and quaternions at the end of the run.
6. Computed structural properties: partial radial distribution functions; orientational order parameters; average species positions and RMS deviations; folding analysis and bragg plane projection results.

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Table 1: Program MDCSPC4: Subprograms

ROUTINE	TYPE	FUNCTION
BLOCKDATA	Initialisation	Default values and parameter initialisation
CRYSTL	Analysis	Fourier transforms average particle position
CYCLE	Control	Controls molecular dynamics cycle
DCELL	Utility	Calculates dimensional properties of MD cell
ENFOLD	Analysis	Performs folding analysis of MD cell (see text)
EWALD	Dynamics	Calculates reciprocal space force and energy terms
FORCES	Dynamics	Calculates real space and short ranged terms
INVERT	Utility	Inverts 3×3 matrices
JACOBI	Utility	Diagonalises the moment of inertia tensor
MAIN	Control	Main program, calls major subroutines
MATMUL	Utility	Multiplies two 3×3 matrices
MOTION	Dynamics	Integrates equations of motion
ORIENT	Analysis	Calculates bond orientation distribution function
RANDUM	Utility	Rough and ready pseudo randum number generator
RESULT	Analysis	Produces final simulation summary
SDOT	Utility	Calculates scalar product of two vectors
SETVEC	Dynamics	Sets up vector arrays for forces calculations
SSUM	Utility	Calculates scalar sum of array elements
START	Initialisation	Generates inital crystal structure and velocities
SYSAVG	Analysis	Accumulates system averages
SYSDEF	Initialisation	Processes input data and defines simulation
TIMCHK	Utility	Program timing routine
TRAJIC	Analysis	Writes a trajectory file

Table 2: Program MDCSPC4: Subprogram Heirarchy

	CALLING ROUTINE								
CALLED ROUTINE	MAIN	SYSDEF	START	CYCLE	EWALD	FORCES	MOTION	SYSAVG	RESULT
BLOCKDATA	X								X
CRYSTL									
CYCLE	X								
DCELL		X			X		X	X	
ENFOLD									X
EWALD				X					
FORCES				X					
INVERT		X					X		
JACOBI		X							
MATMUL							X		
MOTION				X					
ORIENT				X					
RANDUM			X						
RESULT	X						X		
SDOT						X			
SETVEC				X					
SSUM						X			
START	X								
SYSAVG				X					
SYSDEF	X								
TIMCHK	X			X					X
TRAJIC				X					

Table 3: Program MDCSPC4: COMMON Blocks

Block	Function of Data
/CMANGL/	Species angular momenta and derivatives
/CMCALC/	Calculated thermodynamic properties
/CMCDYN/	MD cell dynamical quantities
/CMCELL/	Unit cell properties
/CMCHNL/	FORTRAN channel numbers
/CMCNST/	Fundamental physical constants
/CMCRDS/	Species coordinates and derivatives
/CMCTRL/	Program execution control parameters
/CMENGY/	Energy and virial accumulators
/CMFACT/	Conversion factors and correction terms
/CMFRCS/	Force and torque arrays
/CMMSD0/	Mean square displacement variables and arrays
/CMPARD/	Potential energy parameters
/CMPARM/	Potential energy parameters (MKS)
/CMPHYS/	Specified system properties
/CMQTNS/	Species quaternions and derivatives
/CMRDF0/	Radial distribution variables and arrays
/CMSAVG/	Structural average accumulators
/CMSITE/	Specified site numbers
/CMSPEC/	Species mass parameters
/CMTIME/	Simulation timing parameters
/CMTITL/	Job titles
/CMWORK/	Temporary workspace

Table 4: Program MDCSPC4 Files

File	Function
DATA05	Main input file
DATA06	Main output file
DATA07	Restart file (input)
DATA08	Restart file (output)
DATA09	Trajectory file (output)
DATA10	Structure file (output)

Table 5: Program MDCSPC4 Parameters

Parameter	Function	Default
NST	Number of species types	2
MSP	Total number of ions in MD cell	144
KMAX	Range of k-vectors (section 4.5)	8
MSITES	Maximum No. of sites	5
MBAS	Maximum No. of basis species	8
MAXRDF	Length of RDF array	128

Table 6: Program MDCSPC4: NAMELIST /NLSYST/ Specification

Parameter	Definition	Default
TEMP	System temperature (K)	None
PZERO	System pressure (Pa)	None
ALPHA	Ewald Convergence Parameter (m^{-1})	0.0
CVEC(9)	MD cell vectors (a,b,c) in columns (m).	9×0.0
CMASS	Mass of MD cell (~ mass of molecule) (Kg).	10^{-26}
DAMP	Damping factor for Brown-Clarke algorithm	10^{6}
RCUT	Cutoff for Buckingham/Erfc potentials (m).	1/2 Cell Width
DT	Timestep (s).	10^{-14}

Table 7: Program MDCSPC4: NAMELIST /NLCNTL/ Specification

Parameter	Definition	Default
NPC	Number of primitive cells in MD cell.	0
NRUN	Number of timesteps in entire simulation.	10
KEYRES	Restart Control option = 0 for start from perfect crystal = 1 to continue a simulation unchanged = 2 to start simulation from old configuration	0
NBAS	Number of ionic species in PRIMITIVE cell.	None
LTEMP	Temperature scaling ON if .TRUE. (until NSEQL).	.FALSE.
NSBTS	Temperature scaling interval (timesteps).	10
NSEQL	Number of timesteps in equilibration period.	0
LRDF	RDF option ON if .TRUE..	.FALSE.
INCRDF	RDF accumulation interval (timesteps).	5
NSTRDF	Start timestep of RDF accumulation.	0
LMSD	MSD option ON if .TRUE..	.FALSE.
NSTMSD	Start timestep of MSD accumulation.	0
NSTK	Number of timesteps in rolling averages.	100
LORAND	Initial orientations randomised if .TRUE..	.FALSE.
LZEQL	Zeros averages during equilibration if .TRUE..	.TRUE.
KPRESS	Constant pressure option control = 0 for constant volume simulation = 1 for Parrinello-Rahman algorithm = 2 for Brown-Clarke algorithm	0
NSBPO	Print out running summary every NSBPO timesteps.	5
LSTRFL	Write out structural data file if .TRUE..	.FALSE.
NLX	Number of primive cells in MD cell (X direction).	None
NLY	Number of primive cells in MD cell (Y direction).	None
NLZ	Number of primive cells in MD cell (Z direction).	None
KLX	Folding analysis factor (X direction).	None
KLY	Folding analysis factor (Y direction).	None
KLZ	Folding analysis factor (Z direction).	None
LTRAJ	Write trajectory file if .TRUE.	.FALSE.
NSTRAJ	Timestep for start of trajectory file	0
NITRAJ	Timestep interval between trajectory samples	10
TIMJOB	Allocated job time (S).	10.0
TCLOSE	Job close-down time (S).	5.0
IDTRDF(n)	RDF equivalence array	1,2,3,..etc.

Table 8: Program MDCSPC4: NAMELIST /NLSPEC/ Specification

Parameter	Definition	Limit
NSIT	Number of interaction sites (atoms) on species.	MSITES
NPOS	Number of locations of species in primitive cell.	MBAS
MASS(NSIT)	Masses of atoms on species (Kg).	MSITES
BPOS(3*NPOS)	Coordinates of species in primitive cell (x,y,z,...)	3*MBAS
SITE(3*NSIT)	Relative positions of atoms in species (x,y,z,...) (m).	3*MBAS
CHARGE(NSIT)	Charges on atoms in species (C).	MSITES
EULER(3*NPOS)	Euler angles (ϕ, θ, ψ) of species in each location in primitive cell (X convention).	3*MBAS

Table 9: Program MDCSPC4: NAMELIST /NLPOTL/ Specification

Parameter	Definition	Default
IXP	Site index of first atom.	None
JXP(n)	Site indices of second atoms.	None
AIJ	Buckingham pre-exponential factor (J).	None
RIJ	Buckingham rho parameters (nm).	None
CIJ	Buckingham C parameter (J-nm^6)	None

Table 10: Program MDCSPC4: Radial Distribution Function Indices

JXP=	1	2	3	4	5
IXP=1	1				
2	2	3			
3	4	5	6		
4	7	8	9	10	
5	11	12	13	14	15

Table 11: Program MDCSPC4: Orientational Distribution Function Indices

	1	2	3	4	
1	Y_{00}	$-i(Y_{11} - Y_{1-1})$	$-i(Y_{22} - Y_{2-2})$	$-i(Y_{33} - Y_{3-3})$	etc.
2	$(Y_{11} + Y_{1-1})$	Y_{10}	$-i(Y_{21} - Y_{2-1})$	$-i(Y_{32} - Y_{3-2})$	etc.
3	$(Y_{22} + Y_{2-2})$	$(Y_{21} + Y_{2-1})$	Y_{20}	$-i(Y_{31} - Y_{3-1})$	etc.
4	$(Y_{33} + Y_{3-3})$	$(Y_{32} + Y_{3-2})$	$(Y_{31} + Y_{3-1})$	Y_{30}	etc.
	etc.	etc.	etc.	etc.	etc.

Note: all entries must be divided by $\sqrt{2}$ for exactness

Table 12: Program MDCSPC4: Example Input Dataset DATA05

```
POTASSIUM NITRATE SIMULATION Pmcn PHASE (NPT)
 &NLSYST
 TEMP=200.0,PZERO=0.0E0,ALPHA=4.5E9,
 CVEC=1.653E-9,0.0,0.0,0.0,1.906E-9,0.0,0.0,0.0,1.917E-9,
 CMASS=1.67881E-25,DAMP=0.0,RCUT=0.7E-9,DT=2.0E-15,
 &END
 &NLCNTL
 NPC=0,NRUN=2000,KEYRES=0,NBAS=8,LTEMP=.TRUE.,NSBTS=5,NSEQL=1000,
 LRDF=.TRUE.,INCRDF=5,NSTRDF=1000,LMSD=.TRUE.,NSTMSD=1000,NSTK=100,
 LORAND=.FALSE.,LZEQL=.TRUE.,KPRESS=0,NSBPO=100,LSTRFL=.FALSE.,
 NLX=3,NLY=2,NLZ=3,KLX=3,KLY=2,KLZ=3,LTRAJ=.FALSE.,NSTRAJ=500,
 NITRAJ=10,TIMJOB=4200.0,TCLOSE=20.0,
 IDTRDF=1,2,3,4,5,6,4,5,6,6,4,5,6,6,6,
 &END
 &NLSPEC
 NSIT=1,NPOS=4,MASS=6.4926E-26,CHARGE=1.6021E-19,
 SITE=0.0,0.0,0.0,
 BPOS=0.25,0.416,0.75,0.25,0.048,0.25,0.75,0.583,0.25,0.75,0.917,0.75,
 EULER=12*0.0
 &END
 &NLSPEC
 NSIT=4,NPOS=4,MASS=2.3257E-26,3*2.6566E-26,
 CHARGE=2.0928E-19,3*-1.2316E-19,
 SITE=0.0,0.0,0.0,0.12446E-9,0.0,0.0, -0.06223E-9,-0.107786E-9,0.0,
 -0.06223E-9,0.107786E-9,0.0,
 BPOS=0.25,0.75,0.00,0.25,0.75,0.50,0.75,0.25,0.00,0.75,0.25,0.50,
 EULER=12*0.0
 &END
 &NLPOTL IXP=1,JXP=1,AIJ=1.991415E-16,RIJ=.033670,CIJ=-2.4300E-24 &END
 &NLPOTL IXP=2,JXP=2,AIJ=2.9224E-16,RIJ=.026455,CIJ=-1.7999E-24 &END
 &NLPOTL IXP=3,JXP=3,4,5,AIJ=5.3964E-16,RIJ=.023923,CIJ=-1.8016E-24 &END
 &NLPOTL IXP=4,JXP=4,5,AIJ=5.3964E-16,RIJ=.023923,CIJ=-1.8016E-24 &END
 &NLPOTL IXP=5,JXP=5,AIJ=5.3964E-16,RIJ=.023923,CIJ=-1.8016E-24 &END
 &NLPOTL IXP=1,JXP=2,AIJ=2.41241E-16,RIJ=.029630,CIJ=-2.09135E-24 &END
 &NLPOTL IXP=1,JXP=3,4,5,AIJ=3.27818E-16,RIJ=.027927,CIJ=-2.09234E-24 &END
 &NLPOTL IXP=2,JXP=3,4,5,AIJ=3.9712E-16,RIJ=.025126,CIJ=-1.8007E-24 &END
 &NLPOTL &END
```

Table 13

```
**********  CCP5 PROGRAM LIBRARY  (SERC)
            DARESBURY LABORATORY
M D C S P C MOLECULAR DYNAMICS OF PHASE
            CHANGES.   BY W. SMITH
**********  VERSION 4.3 , MAY 1991

POTASSIUM NITRATE SIMULATION PHASE A (NVT)

PHYSICAL SPECIFICATION
                        INITIAL MOLAR VOLUME        =     2.5258E-05 M**3
                        SPECIFIED TEMPERATURE       =     2.0000E+02 K
                        SPECIFIED PRESSURE          =     0.0000E+00 PA
                        CELL MASS PARAMETER         =     0.0000E+00 KG
                        EWALD CONVERGENCE PARAMETER =     4.5000E+09 M**-1
                        INITIAL CELL VECTOR NO. 1   =  1.6530000 0.0000000 0.0000000 NM
                        INITIAL CELL VECTOR NO. 2   =  0.0000000 1.9060000 0.0000000 NM
                        INITIAL CELL VECTOR NO. 3   =  0.0000000 0.0000000 1.9170000 NM


INTERNAL PROGRAM UNITS
                        UNIT OF LENGTH              =     1.0000E-09 M
                        UNIT OF MASS                =     1.0000E-26 KG
                        UNIT OF TIME                =     2.0000E-15 S
                        UNIT OF ENERGY              =     2.5000E-15 J
                        UNIT OF PRESSURE            =     2.5000E+12 PA
                        UNIT OF CHARGE              =     1.6022E-19 C


VALUE OF CUTOFF RADIUS =  0.7000000 NM


JOB CONTROL PARAMETERS

                        CONSTANT PRESSURE OPTION    =        0

                        RANDOM ORIENTATION OPTION   =        F

                        NUMBER OF TIMESTEPS IN RUN  =     2000
                        RESTART CONTROL PARAMETER   =        0

                        NUMBER OF SPECIES TYPES     =        2
                        NUMBER OF PRIMITIVE CELLS   =       18
                        NUMBER OF PRIMITIVE CELLS X =        3
                        NUMBER OF PRIMITIVE CELLS Y =        2
                        NUMBER OF PRIMITIVE CELLS Z =        3
                        SPECIES IN PRIMITIVE CELL   =        8

                        TEMPERATURE SCALING OPTION  =        T
                        TEMPERATURE SCALING INTERVAL=        5
                        LAST TEMP. SCALING STEP     =     1000
```

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                          RDF OPTION                    =        T
                          RDF ARRAY LENGTH              =      128
                          RDF TIMESTEP INTERVAL         =        5
                          RDF START TIMESTEP            =     1000

                          MSD OPTION                    =        T
                          MSD START TIMESTEP            =     1000

                          STRUCTURAL DATA FILE OPTION =          F

                          TRAJECTORY FILE OPTION        =        F
                          TRAJECTORY FILE START STEP    =        0
                          TRAJECTORY SAMPLING INTERVAL=          0

                          ZERO AVERAGES OPTION          =        T
                          NO. STEPS IN ROLLING AVERAGE=      100

PARAMETERS FOR SPECIES NUMBER   1

                          NO. PLES. IN PRIMITIVE CELL =          4
                          NO. PARTICLES IN MD CELL      =       72
                          TOTAL PARTICLE MASS           =     6.4926E-26 KG
                          MOMENT OF INERTIA IXX         =     0.0000E+00 KG M**2
                          MOMENT OF INERTIA IYY         =     0.0000E+00 KG M**2
                          MOMENT OF INERTIA IZZ         =     0.0000E+00 KG M**2
PARTICLE POSITIONS AND ORIENTATIONS IN PRIMITIVE CELL
                            0.250000  0.416000  0.750000  0.000000  0.000000  0.000000
                            0.250000  0.048000  0.250000  0.000000  0.000000  0.000000
                            0.750000  0.583000  0.250000  0.000000  0.000000  0.000000
                            0.750000  0.917000  0.750000  0.000000  0.000000  0.000000
SITE PARAMETERS AND BONDLENGTHS
SITE INDEX     BOND X (NM)     BOND Y (NM)     BOND Z (NM)    AT.MASS (KG)    AT.CHGE  (C)
    1            0.000000        0.000000        0.000000    6.49260E-26    1.60210E-19

PARAMETERS FOR SPECIES NUMBER   2

                          NO. PLES. IN PRIMITIVE CELL =          4
                          NO. PARTICLES IN MD CELL      =       72
                          TOTAL PARTICLE MASS           =     1.0295E-25 KG
                          MOMENT OF INERTIA IXX         =     6.1728E-46 KG M**2
                          MOMENT OF INERTIA IYY         =     6.1727E-46 KG M**2
                          MOMENT OF INERTIA IZZ         =     1.2346E-45 KG M**2
PARTICLE POSITIONS AND ORIENTATIONS IN PRIMITIVE CELL
                            0.250000  0.750000  0.000000  0.000000  0.000000  0.000000
                            0.250000  0.750000  0.500000  0.000000  0.000000  0.000000
                            0.750000  0.250000  0.000000  0.000000  0.000000  0.000000
                            0.750000  0.250000  0.500000  0.000000  0.000000  0.000000
SITE PARAMETERS AND BONDLENGTHS
SITE INDEX     BOND X (NM)     BOND Y (NM)     BOND Z (NM)    AT.MASS (KG)    AT.CHGE  (C)
```

2	0.000000	0.000000	0.000000	2.32570E-26	2.09280E-19
3	0.124460	0.000000	0.000000	2.65660E-26	-1.23160E-19
4	-0.062230	-0.107786	0.000000	2.65660E-26	-1.23160E-19
5	-0.062230	0.107786	0.000000	2.65660E-26	-1.23160E-19

RDF EQUIVALENCES

```
IXP:
   1  1
   2  2  3
   3  4  5  6
   4  4  5  6  6
   5  4  5  6  6  6
JXP-  1  2  3  4  5
```

BUCKINGHAM POTENTIAL PARAMETERS

FORM OF POTENTIAL: V(R)=Q*Q/R+AAA*EXP(-R/RHO)+CCC/R**6

SITE	SITE	AAA(I,J) (J)	RHO(I,J) (NM)	CCC(I,J) (J-NM6)
1	1	1.991415E-16	3.367000E-02	-2.430000E-24
2	1	2.412410E-16	2.963000E-02	-2.091350E-24
2	2	2.922400E-16	2.645500E-02	-1.799900E-24
3	1	3.278180E-16	2.792700E-02	-2.092340E-24
3	2	3.971200E-16	2.512600E-02	-1.800700E-24
3	3	5.396400E-16	2.392300E-02	-1.801600E-24
4	1	3.278180E-16	2.792700E-02	-2.092340E-24
4	2	3.971200E-16	2.512600E-02	-1.800700E-24
4	3	5.396400E-16	2.392300E-02	-1.801600E-24
4	4	5.396400E-16	2.392300E-02	-1.801600E-24
5	1	3.278180E-16	2.792700E-02	-2.092340E-24
5	2	3.971200E-16	2.512600E-02	-1.800700E-24
5	3	5.396400E-16	2.392300E-02	-1.801600E-24
5	4	5.396400E-16	2.392300E-02	-1.801600E-24
5	5	5.396400E-16	2.392300E-02	-1.801600E-24

LONG RANGE CORRECTIONS

```
POTENTIAL CORRECTION          =    -1.0516E+03 J/M
VIRIAL    CORRECTION          =     6.3083E+03 J/M
EWALD SELF CORRECTION (PE)    =    -3.0285E+05 J/M
EWALD SELF CORRECTION (VIR)   =     2.5747E+05 J/M
```

STARTING CONFIGURATION CONSTRUCTED FROM LATTICE

SAMPLE OF INITIAL PARTICLE POSITIONS

ABSOLUTE POSITIONS MD CELL POSITIONS

1	-0.68875000E+00	-0.55655200E+00	-0.47925000E+00	-0.83333333E+00	-0.58400000E+00	-0.50000000E+00
9	0.41325000E+00	-0.55655200E+00	0.15975000E+00	0.50000000E+00	-0.58400000E+00	0.16666667E+00
17	-0.13775000E+00	0.39644800E+00	0.79875000E+00	-0.16666667E+00	0.41600000E+00	0.83333333E+00
25	-0.68875000E+00	-0.90725600E+00	-0.15975000E+00	-0.83333333E+00	-0.95200000E+00	-0.16666667E+00
33	0.41325000E+00	-0.90725600E+00	0.47925000E+00	0.50000000E+00	-0.95200000E+00	0.50000000E+00
41	0.13775000E+00	0.55559900E+00	-0.79875000E+00	0.16666667E+00	0.58300000E+00	-0.83333333E+00
49	-0.41325000E+00	-0.39740100E+00	0.47925000E+00	-0.50000000E+00	-0.41700000E+00	0.50000000E+00
57	0.68875000E+00	-0.79099000E-01	-0.47925000E+00	0.83333333E+00	-0.83000000E-01	-0.50000000E+00
65	0.13775000E+00	0.87390100E+00	0.15975000E+00	0.16666667E+00	0.91700000E+00	0.16666667E+00
73	-0.68875000E+00	-0.23825000E+00	-0.95850000E+00	-0.83333333E+00	-0.25000000E+00	-0.10000000E+01
81	0.41325000E+00	-0.23825000E+00	-0.31950000E+00	0.50000000E+00	-0.25000000E+00	-0.33333333E+00
89	-0.13775000E+00	0.71475000E+00	0.31950000E+00	-0.16666667E+00	0.75000000E+00	0.33333333E+00
97	-0.68875000E+00	-0.23825000E+00	-0.10641488E-15	-0.83333333E+00	-0.25000000E+00	-0.11102230E-15
105	0.41325000E+00	-0.23825000E+00	0.63900000E+00	0.50000000E+00	-0.25000000E+00	0.66666667E+00
113	0.13775000E+00	0.23825000E+00	-0.95850000E+00	0.16666667E+00	0.25000000E+00	-0.10000000E+01
121	-0.41325000E+00	-0.71475000E+00	0.31950000E+00	-0.50000000E+00	-0.75000000E+00	0.33333333E+00
129	0.68875000E+00	-0.71475000E+00	-0.63900000E+00	0.83333333E+00	-0.75000000E+00	-0.66666667E+00
137	0.13775000E+00	0.23825000E+00	-0.10641488E-15	0.16666667E+00	0.25000000E+00	-0.11102230E-15

SAMPLE OF INITIAL PARTICLE VELOCITIES

	ABSOLUTE VELOCITIES			MD CELL VELOCITIES		
1	0.28980115E-03	-0.52766437E-03	0.55841303E-03	0.35063660E-03	-0.55368769E-03	0.58259054E-03
9	0.41051800E-03	-0.17541371E-03	0.10025246E-03	0.49669450E-03	-0.18406475E-03	0.10459307E-03
17	0.13719889E-04	0.22057542E-03	-0.70255411E-03	0.16599986E-04	0.23145374E-03	-0.73297247E-03
25	0.26790199E-03	0.21290868E-03	0.23961564E-03	0.32414034E-03	0.22340889E-03	0.24999024E-03
33	0.62369842E-03	0.67122735E-03	-0.24604518E-03	0.75462604E-03	0.70433090E-03	-0.25669816E-03
41	0.56366675E-03	0.28063724E-03	0.57924008E-04	0.68199244E-03	0.29447769E-03	0.60431934E-04
49	0.38109383E-03	0.48983040E-03	0.11649736E-03	0.46109356E-03	0.51398783E-03	0.12154133E-03
57	-0.30681535E-03	-0.19475358E-03	-0.51529976E-03	-0.37122245E-03	-0.20435843E-03	-0.53761060E-03
65	0.16182560E-03	-0.52605001E-03	-0.49824830E-03	0.19579625E-03	-0.55199371E-03	-0.51982086E-03
73	-0.49670348E-03	-0.35305395E-04	0.28450770E-03	-0.60097214E-03	-0.37046585E-04	0.29682597E-03
81	-0.11958290E-03	0.74650531E-04	-0.10300217E-03	-0.14468590E-03	0.78332142E-04	-0.10746184E-03
89	0.24133584E-03	0.69278858E-04	0.48999143E-03	0.29199738E-03	0.72695549E-04	0.51120650E-03
97	0.14106854E-03	-0.73534732E-04	0.20955012E-03	0.17068183E-03	-0.77161313E-04	0.21862297E-03
105	0.10645247E-03	0.13446038E-03	-0.49499645E-03	0.12879911E-03	0.14109169E-03	-0.51642822E-03
113	0.12759563E-04	-0.15615528E-03	0.25528568E-03	0.15438067E-04	-0.16385653E-03	0.26633873E-03
121	0.72239213E-04	0.39559561E-03	0.28693481E-03	0.87403766E-04	0.41510557E-03	0.29935817E-03
129	-0.20883973E-03	-0.48828615E-03	0.48821262E-03	-0.25267965E-03	-0.51236742E-03	0.50935068E-03
137	-0.46121734E-03	-0.83560181E-04	-0.58450944E-04	-0.55803671E-03	-0.87681197E-04	-0.60981684E-04

SAMPLE OF INITIAL PARTICLE ORIENTATIONS

	QUATERNIONS				QUATERNION DERIVATIVES			
1	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
9	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
17	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
25	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00

33	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
41	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
49	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
57	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
65	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
73	0.100000E+01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.643372E-03	-0.264999E-02	-0.192451E-03
81	0.100000E+01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.800763E-03	-0.158470E-02	-0.457837E-03
89	0.100000E+01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	-0.165481E-02	0.213325E-02	0.764993E-03
97	0.100000E+01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.429592E-03	0.192594E-02	-0.389277E-03
105	0.100000E+01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	-0.128688E-02	-0.208989E-02	-0.306206E-04
113	0.100000E+01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.348511E-02	-0.206457E-02	-0.487203E-03
121	0.100000E+01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.266028E-03	-0.131198E-02	-0.156886E-02
129	0.100000E+01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	-0.277888E-02	0.185705E-04	-0.444759E-03
137	0.100000E+01	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.391076E-02	-0.664334E-03	-0.135151E-03

TIME ELAPSED SINCE JOB START = 0.19578999 SECONDS

STEP TIME (S)	PE (J/M) VIR (J/M)	TKE (J/M) RKE (J/M)	TE (J/M) EPV (J/M)	T. TEMP (K) R. TEMP (K)	PRS (PA) VOL (M**3)	VL1 (M) DC1	VL2 (M) DC2	VL3 (M) DC3
1	-3.390188E+05	2.487123E+03	-3.352834E+05	1.994203E+02	-1.765063E+08	1.653000E-09	1.906000E-09	1.917000E-09
1.39	1.834905E+04	1.248256E+03	-3.397417E+05	2.001730E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.390188E+05	2.487123E+03	-3.352834E+05	1.994203E+02	-1.765063E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.834905E+04	1.248256E+03	-3.397417E+05	2.001730E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
100	-3.369671E+05	2.637106E+03	-3.330047E+05	2.114460E+02	-1.849570E+08	1.653000E-09	1.906000E-09	1.917000E-09
115.32	1.928937E+04	1.325337E+03	-3.376764E+05	2.125339E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.373717E+05	2.460723E+03	-3.336983E+05	1.973035E+02	-1.139226E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.355395E+04	1.212616E+03	-3.365758E+05	1.944578E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
200	-3.377395E+05	2.516434E+03	-3.339584E+05	2.017704E+02	-2.330044E+08	1.653000E-09	1.906000E-09	1.917000E-09
231.53	2.268882E+04	1.264596E+03	-3.398438E+05	2.027933E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.375169E+05	2.531675E+03	-3.337445E+05	2.029925E+02	-2.295366E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	2.245654E+04	1.240653E+03	-3.395423E+05	1.989538E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
300	-3.371577E+05	2.479519E+03	-3.334242E+05	1.988106E+02	-1.705133E+08	1.653000E-09	1.906000E-09	1.917000E-09
348.42	1.787972E+04	1.253943E+03	-3.377311E+05	2.010851E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.373155E+05	2.484932E+03	-3.335909E+05	1.992446E+02	-1.905024E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.940523E+04	1.239750E+03	-3.384026E+05	1.988091E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
400	-3.371323E+05	2.510545E+03	-3.334455E+05	2.012982E+02	-2.039807E+08	1.653000E-09	1.906000E-09	1.917000E-09
465.65	2.047777E+04	1.176303E+03	-3.385977E+05	1.886346E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.373721E+05	2.498859E+03	-3.336286E+05	2.003612E+02	-2.079056E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	2.075181E+04	1.244638E+03	-3.388799E+05	1.995928E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
500	-3.366789E+05	2.479422E+03	-3.329609E+05	1.988028E+02	-2.364501E+08	1.653000E-09	1.906000E-09	1.917000E-09
582.59	2.287590E+04	1.238515E+03	-3.389333E+05	1.986110E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.370463E+05	2.483780E+03	-3.333142E+05	1.991522E+02	-2.453856E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	2.356171E+04	1.248271E+03	-3.395123E+05	2.001755E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00

600	-3.371597E+05	2.483228E+03	-3.334036E+05	1.991080E+02	-1.556187E+08	1.653000E-09	1.906000E-09	1.917000E-09
700.04	1.675850E+04	1.272869E+03	-3.373342E+05	2.041200E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.370329E+05	2.508487E+03	-3.332748E+05	2.011333E+02	-1.819511E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.880436E+04	1.249634E+03	-3.378706E+05	2.003940E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
700	-3.371200E+05	2.535227E+03	-3.333354E+05	2.032773E+02	-1.395733E+08	1.653000E-09	1.906000E-09	1.917000E-09
817.85	1.564665E+04	1.249412E+03	-3.368608E+05	2.003584E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.370503E+05	2.501511E+03	-3.333134E+05	2.005739E+02	-1.070368E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.311376E+04	1.235428E+03	-3.360169E+05	1.981160E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
800	-3.376475E+05	2.607360E+03	-3.337500E+05	2.090610E+02	-1.718580E+08	1.653000E-09	1.906000E-09	1.917000E-09
935.09	1.823730E+04	1.290162E+03	-3.380909E+05	2.068932E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.372830E+05	2.508686E+03	-3.335214E+05	2.011492E+02	-1.561507E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.684972E+04	1.252843E+03	-3.374655E+05	2.009087E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
900	-3.372065E+05	2.555174E+03	-3.333771E+05	2.048767E+02	-4.111026E+07	1.653000E-09	1.906000E-09	1.917000E-09
1052.89	8.225488E+03	1.274201E+03	-3.344155E+05	2.043337E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.372855E+05	2.487191E+03	-3.335583E+05	1.994257E+02	-1.313504E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.492749E+04	1.240061E+03	-3.368760E+05	1.988588E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00

1 STEP TIME (S)	PE (J/M) VIR (J/M)	TKE (J/M) RKE (J/M)	TE (J/M) EPV (J/M)	T.TEMP (K) R.TEMP (K)	PRS (PA) VOL (M**3)	VL1 (M) DC1	VL2 (M) DC2	VL3 (M) DC3
1000	-3.375250E+05	2.554913E+03	-3.337447E+05	2.048557E+02	-1.688464E+08	1.653000E-09	1.906000E-09	1.917000E-09
1171.01	1.790420E+04	1.225379E+03	-3.380095E+05	1.965045E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.375914E+05	2.496489E+03	-3.338392E+05	2.001712E+02	-1.480386E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.621064E+04	1.255760E+03	-3.375784E+05	2.013764E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00

SWITCHING OFF TEMPERATURE SCALING AT STEP 1000

1100	-3.376836E+05	2.712655E+03	-3.337293E+05	2.175037E+02	-2.110477E+08	1.653000E-09	1.906000E-09	1.917000E-09
1292.05	2.141750E+04	1.241650E+03	-3.390600E+05	1.991138E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.373772E+05	2.600260E+03	-3.336691E+05	2.084917E+02	-2.078335E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	2.094915E+04	1.107803E+03	-3.389187E+05	1.776498E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
MSD (M**2)	1.065013E-21	1.073190E-21						
1200	-3.375439E+05	2.764065E+03	-3.335634E+05	2.216258E+02	-1.925243E+08	1.653000E-09	1.906000E-09	1.917000E-09
1413.00	2.011670E+04	1.216434E+03	-3.384262E+05	1.950700E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.375402E+05	2.615350E+03	-3.336021E+05	2.097017E+02	-1.802592E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.888988E+04	1.322702E+03	-3.381552E+05	2.121115E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
MSD (M**2)	1.160313E-21	1.159178E-21						
1300	-3.374634E+05	2.321818E+03	-3.335383E+05	1.861660E+02	-1.534969E+08	1.653000E-09	1.906000E-09	1.917000E-09
1533.65	1.627490E+04	1.603321E+03	-3.374154E+05	2.571120E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.374318E+05	2.628632E+03	-3.335640E+05	2.107666E+02	-1.631417E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.761936E+04	1.239112E+03	-3.376847E+05	1.987067E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00

MSD(M**2)	1.268265E-21	1.209292E-21						
1400	-3.376035E+05	2.385840E+03	-3.337040E+05	1.912993E+02	-1.597180E+08	1.653000E-09	1.906000E-09	1.917000E-09
1653.99	1.687435E+04	1.513701E+03	-3.377382E+05	2.427404E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.375194E+05	2.476717E+03	-3.336292E+05	1.985859E+02	-1.678682E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.767369E+04	1.413530E+03	-3.378693E+05	2.266767E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
MSD(M**2)	1.167457E-21	1.299099E-21						
1500	-3.375003E+05	2.536469E+03	-3.334564E+05	2.033769E+02	-1.893914E+08	1.653000E-09	1.906000E-09	1.917000E-09
1774.81	1.942412E+04	1.507400E+03	-3.382401E+05	2.417300E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.373828E+05	2.545979E+03	-3.334844E+05	2.041394E+02	-1.648437E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.758302E+04	1.352354E+03	-3.376481E+05	2.168664E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
MSD(M**2)	1.133233E-21	1.316537E-21						
1600	-3.372089E+05	2.516328E+03	-3.333636E+05	2.017620E+02	-1.207807E+08	1.653000E-09	1.906000E-09	1.917000E-09
1896.09	1.418484E+04	1.328928E+03	-3.364143E+05	2.131099E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.373766E+05	2.581347E+03	-3.334259E+05	2.069753E+02	-1.514118E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.663596E+04	1.369316E+03	-3.372504E+05	2.195865E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
MSD(M**2)	1.171933E-21	1.092204E-21						
1700	-3.371392E+05	2.286528E+03	-3.334248E+05	1.833363E+02	-1.406149E+08	1.653000E-09	1.906000E-09	1.917000E-09
2017.84	1.522818E+04	1.427873E+03	-3.369765E+05	2.289768E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.373742E+05	2.692583E+03	-3.333056E+05	2.158943E+02	-1.550737E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.713591E+04	1.376092E+03	-3.372225E+05	2.206732E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
MSD(M**2)	1.257431E-21	1.546984E-21						
1800	-3.372622E+05	2.449543E+03	-3.332330E+05	1.964071E+02	-1.537466E+08	1.653000E-09	1.906000E-09	1.917000E-09
2138.23	1.654927E+04	1.579659E+03	-3.371164E+05	2.533176E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.372631E+05	2.555212E+03	-3.333019E+05	2.048797E+02	-1.799390E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.874534E+04	1.406024E+03	-3.378468E+05	2.254731E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
MSD(M**2)	1.128066E-21	1.417963E-21						
1900	-3.372881E+05	2.854179E+03	-3.330745E+05	2.288512E+02	-1.126285E+08	1.653000E-09	1.906000E-09	1.917000E-09
2258.44	1.424281E+04	1.359387E+03	-3.359193E+05	2.179944E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.373013E+05	2.687491E+03	-3.331531E+05	2.154860E+02	-1.295156E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.518906E+04	1.460773E+03	-3.364244E+05	2.342528E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
MSD(M**2)	1.161852E-21	1.433570E-21						

1 STEP TIME(S)	PE(J/M) VIR(J/M)	TKE(J/M) RKE(J/M)	TE(J/M) EPV(J/M)	T.TEMP(K) R.TEMP(K)	PRS(PA) VOL(M**3)	VL1(M) DC1	VL2(M) DC2	VL3(M) DC3
2000	-3.366811E+05	2.632286E+03	-3.328427E+05	2.110596E+02	-1.228673E+08	1.653000E-09	1.906000E-09	1.917000E-09
2378.26	1.457487E+04	1.206138E+03	-3.359461E+05	1.934190E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
ROLLING	-3.372011E+05	2.771685E+03	-3.329970E+05	2.222368E+02	-1.000747E+08	1.653000E-09	1.906000E-09	1.917000E-09
AVERAGES	1.312655E+04	1.432422E+03	-3.355247E+05	2.297063E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
MSD(M**2)	1.385201E-21	1.217798E-21						

RUN TERMINATING. ELAPSED CPU TIME = 2378.2690, JOB TIME = 4200.0000, CLOSE TIME = 20.0000

RUN TERMINATED AFTER 2000 STEPS. FINAL AVERAGES CALCULATED OVER 1000 STEPS.

SUMMARY OF SYSTEM AVERAGES AND CELL STRUCTURE.

STEP TIME(S)	PE(J/M) VIR(J/M)	TKE(J/M) RKE(J/M)	TE(J/M) EPV(J/M)	T.TEMP(K) R.TEMP(K)	PRS(PA) VOL(M**3)	VL1(M) DC(1,2)	VL2(M) DC(1,3)	VL3(M) DC(2,3)
2000	-3.373768E+05	2.615526E+03	-3.334132E+05	2.097157E+02	-1.599961E+08	1.653000E-09	1.906000E-09	1.917000E-09
2378.28	1.735479E+04	1.348013E+03	-3.374545E+05	2.161703E+02	2.525841E-05	0.000000E+00	0.000000E+00	0.000000E+00
R.M.S.	1.865802E+02	1.549795E+02	2.194254E+02	1.242643E+01	3.692017E+07	3.790440E-16	4.894749E-16	5.551115E-17
FLUCT.	2.805172E+03	1.457755E+02	1.084283E+03	2.337687E+01	4.003327E-12	0.000000E+00	0.000000E+00	0.000000E+00

SAMPLE OF FINAL PARTICLE POSITIONS

	ABSOLUTE POSITIONS			MD CELL POSITIONS		
1	-0.67601151E+00	-0.53421269E+00	-0.46334764E+00	-0.81792076E+00	-0.56055896E+00	-0.48340912E+00
9	0.42035490E+00	-0.56691922E+00	0.15106461E+00	0.50859637E+00	-0.59487851E+00	0.15760523E+00
17	-0.13557932E+00	0.40222956E+00	0.79049686E+00	-0.16404032E+00	0.42206669E+00	0.82472286E+00
25	-0.69584414E+00	-0.86105895E+00	-0.13629686E+00	-0.84191668E+00	-0.90352461E+00	-0.14219808E+00
33	0.41267365E+00	-0.89053644E+00	0.48892214E+00	0.49930266E+00	-0.93445587E+00	0.51009091E+00
41	0.13892713E+00	0.56833102E+00	-0.77776640E+00	0.16809090E+00	0.59635994E+00	-0.81144121E+00
49	-0.39321195E+00	-0.37490768E+00	0.47191138E+00	-0.47575554E+00	-0.39339736E+00	0.49234364E+00
57	0.68345911E+00	-0.10401934E+00	-0.46495074E+00	0.82693177E+00	-0.10914936E+00	-0.48508163E+00
65	0.12492491E+00	0.86455346E+00	0.16728913E+00	0.15114932E+00	0.90719146E+00	0.17453221E+00
73	-0.72499113E+00	-0.24591554E+00	-0.94952138E+00	-0.87718225E+00	-0.25804359E+00	-0.99063264E+00
81	0.38115397E+00	-0.22889291E+00	-0.33371560E+00	0.46116633E+00	-0.24018144E+00	-0.34816442E+00
89	-0.13544314E+00	0.69899599E+00	0.31048751E+00	-0.16387554E+00	0.73346904E+00	0.32393063E+00
97	-0.68251474E+00	-0.22475351E+00	-0.10052705E-01	-0.82578916E+00	-0.23583789E+00	-0.10487955E-01
105	0.44097274E+00	-0.24397642E+00	0.62855581E+00	0.53354234E+00	-0.25600884E+00	0.65577028E+00
113	0.14816677E+00	0.24308312E+00	-0.93035629E+00	0.17927014E+00	0.25507148E+00	-0.97063776E+00
121	-0.39729918E+00	-0.72300003E+00	0.32079642E+00	-0.48070076E+00	-0.75865691E+00	0.33468588E+00
129	0.70306567E+00	-0.70814416E+00	-0.61786014E+00	0.85065417E+00	-0.74306838E+00	-0.64461152E+00
137	0.13649316E+00	0.24680113E+00	0.18630419E-01	0.16514599E+00	0.25897286E+00	0.19437057E-01

SAMPLE OF FINAL PARTICLE VELOCITIES

	ABSOLUTE VELOCITIES			MD CELL VELOCITIES		
1	-0.62183728E-04	0.73403524E-03	0.35706597E-03	-0.75237420E-04	0.77023635E-03	0.37252579E-03
9	-0.48335362E-03	0.33787651E-03	-0.28260907E-03	-0.58481987E-03	0.35453989E-03	-0.29484515E-03
17	-0.20993188E-03	0.70793460E-03	-0.22631932E-03	-0.25400106E-03	0.74284848E-03	-0.23611823E-03
25	-0.43366253E-03	0.64795373E-04	0.22857530E-03	-0.52469756E-03	0.67990948E-04	0.23847188E-03
33	-0.95927361E-03	-0.22915186E-03	-0.26418859E-03	-0.11606456E-02	-0.24045316E-03	-0.27562712E-03

41	-0.74812795E-03	0.43513033E-03	-0.24558088E-03	-0.90517598E-03	0.45659006E-03	-0.25621375E-03
49	0.37528279E-03	-0.55336151E-03	0.38663016E-03	0.45406266E-03	-0.58065216E-03	0.40337001E-03
57	-0.24619341E-04	-0.72458536E-03	-0.11051993E-03	-0.29787467E-04	-0.76032042E-03	-0.11530510E-03
65	0.81081832E-03	-0.50226725E-03	0.40252015E-03	0.98102641E-03	-0.52703803E-03	0.41994799E-03
73	-0.11092104E-03	-0.10594885E-03	-0.52865494E-03	-0.13420574E-03	-0.11117403E-03	-0.55154402E-03
81	-0.37175301E-03	0.11112941E-03	0.47228240E-03	-0.44979191E-03	0.11661008E-03	0.49273073E-03
89	-0.19684471E-03	0.48531787E-04	-0.86197625E-04	-0.23816662E-03	0.50925275E-04	-0.89929708E-04
97	0.17055670E-03	-0.27377188E-03	-0.29278396E-03	0.20636019E-03	-0.28727374E-03	-0.30546057E-03
105	0.17541811E-03	0.20513611E-03	0.31184800E-03	0.21224212E-03	0.21525300E-03	0.32535003E-03
113	-0.40460420E-03	0.41942474E-03	-0.48805589E-03	-0.48953926E-03	0.44010991E-03	-0.50918716E-03
121	0.19467857E-03	0.17215686E-03	-0.71989512E-04	0.23554576E-03	0.18064728E-03	-0.75106428E-04
129	-0.39083117E-04	0.37912645E-03	-0.17796901E-03	-0.47287497E-04	0.39782419E-03	-0.18567451E-03
137	-0.21679058E-03	-0.98438364E-04	0.36668696E-03	-0.26229955E-03	-0.10329314E-03	0.38256334E-03

SAMPLE OF FINAL PARTICLE ORIENTATIONS

	QUATERNIONS				QUATERNION DERIVATIVES			
1	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
9	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
17	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
25	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
33	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
41	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
49	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
57	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
65	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
73	0.800686E+00	-0.379673E-01	0.799509E-01	0.592510E+00	-0.581471E-03	0.921919E-03	-0.213348E-02	0.113274E-02
81	0.732768E+00	-0.104541E+00	-0.956694E-01	0.665560E+00	0.742159E-03	-0.248526E-02	-0.332471E-03	-0.125526E-02
89	0.995303E+00	-0.205963E-01	0.777859E-01	-0.538182E-01	0.231901E-03	0.985753E-03	-0.318433E-02	-0.690971E-03
97	0.995252E+00	-0.625282E-01	0.627776E-01	0.402935E-01	-0.138933E-03	-0.410124E-03	0.121010E-02	0.909876E-03
105	0.992437E+00	-0.107590E-01	0.300314E-01	0.118544E+00	0.691606E-04	-0.210020E-02	-0.218813E-02	-0.214994E-03
113	0.982997E+00	-0.122079E+00	-0.140030E-01	0.136446E+00	-0.101783E-03	-0.545408E-03	0.705768E-04	0.252541E-03
121	0.975617E+00	-0.857558E-01	0.731784E-01	0.188312E+00	-0.995017E-04	0.872425E-03	0.137554E-02	0.378266E-03
129	0.995056E+00	0.774601E-02	-0.422506E-01	0.895519E-01	0.643835E-04	0.186045E-02	0.753086E-03	-0.520941E-03
137	0.983782E+00	-0.288856E-01	0.125424E+00	-0.124927E+00	-0.231066E-03	0.412015E-03	0.894253E-03	-0.101707E-02

RADIAL DISTRIBUTION FUNCTIONS AVERAGED OVER 200 CONFIGURATIONS RESOLUTION = 5.468750E-12 M

RADIUS (NM)	RDF(1)	RDF(2)	RDF(3)	RDF(4)	RDF(5)	RDF(6)
0.002734	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.013672	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.024609	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.035547	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.046484	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.057422	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.068359	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.079297	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.090234	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.101172	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

0.112109	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.123047	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.133984	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.144922	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.155859	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.166797	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.177734	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.188672	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.199609	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.210547	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.221484	0.000000	0.000000	0.000000	0.001728	0.000000	0.000000
0.232422	0.000000	0.000000	0.000000	0.130758	0.000000	0.000000
0.243359	0.000000	0.000000	0.000000	1.403086	0.000000	0.000000
0.254297	0.000000	0.000000	0.000000	4.183538	0.001311	0.001748
0.265234	0.000000	0.000000	0.000000	4.919996	0.016869	0.013655
0.276172	0.000000	0.000000	0.015559	3.389625	0.045195	0.078536
0.287109	0.000000	0.000000	0.238564	1.759067	0.191263	0.273298
0.298047	0.000000	0.004771	1.919869	0.915405	0.531813	0.648650
0.308984	0.000000	0.235281	4.306082	0.584799	1.064535	1.017084
0.319922	0.000000	1.224883	3.889149	0.518167	1.755473	1.276139
0.330859	0.000000	4.069898	1.522340	0.663346	2.103607	1.352847
0.341797	0.000000	7.467570	0.354078	0.878666	2.079001	1.371973
0.352734	0.000000	8.430744	0.066765	1.128641	1.549213	1.520297
0.363672	0.000000	5.338143	0.001282	1.196580	0.890011	1.583761
0.374609	0.000000	2.196260	0.004832	1.246521	0.439534	1.546859
0.385547	0.006843	0.656355	0.000000	1.051916	0.221066	1.419282
0.396484	0.052844	0.162844	0.000000	0.827703	0.245525	1.215402
0.407422	0.461634	0.025022	0.000000	0.651769	0.482571	0.969682
0.418359	1.514909	0.009686	0.000000	0.529185	0.803463	0.752181
0.429297	3.156126	0.000000	0.000000	0.817931	0.857946	0.582696
0.440234	4.561795	0.000000	0.000000	1.353668	0.687404	0.495397
0.451172	4.254186	0.000000	0.000000	1.755365	0.526221	0.445203
0.462109	2.643654	0.000000	0.000000	1.325267	0.532171	0.543021
0.473047	1.327321	0.000000	0.003030	0.748386	0.713031	0.649266
0.483984	0.408918	0.000000	0.010132	0.499507	0.878510	0.762992
0.494922	0.171644	0.002768	0.038758	0.556459	1.013831	0.831920
0.505859	0.338542	0.012256	0.231215	0.784962	1.219235	0.920812
0.516797	0.877241	0.052685	0.856929	1.031489	1.282960	1.007720
0.527734	1.898001	0.240446	1.831650	1.204461	1.281161	1.096109
0.538672	2.832469	0.709578	3.020015	1.339210	1.219243	1.247969
0.549609	2.793256	1.542549	3.085658	1.366415	1.079718	1.306363
0.560547	2.039480	2.358351	1.998474	1.341668	1.172971	1.277163
0.571484	0.955126	2.624780	0.931767	1.245990	1.279644	1.239357
0.582422	0.359840	1.972620	0.457796	1.126081	1.469345	1.215514
0.593359	0.139160	1.150597	0.753582	0.974200	1.498096	1.202949
0.604297	0.273907	0.639503	1.752077	0.819168	1.513375	1.211484
0.615234	0.430870	0.536796	3.446510	0.777163	1.470869	1.249313
0.626172	0.659379	0.930264	4.983606	0.784408	1.404585	1.245493
0.637109	0.670764	1.570824	4.932163	0.851611	1.338257	1.276791
0.648047	0.543760	1.951803	3.161235	0.842956	1.293398	1.203287

0.658984	0.313095	1.680252	1.633795	0.790481	1.268648	1.146845
0.669922	0.284068	1.075642	0.540560	0.688008	1.276857	1.077930
0.680859	0.674736	0.552955	0.160913	0.628352	1.189230	0.978520
0.691797	1.433957	0.211126	0.029048	0.684270	1.125179	0.932867

ORIENTATIONAL ORDER PARAMETERS Y(L,M) AVERAGED OVER 200 CONFIGURATIONS. SITE NUMBER 3

	0	1	2	3	4	5	6	7	8	9	10	11	12
0	0.2821	-0.0182	0.0000	0.0160	0.0000	-0.0133	0.0000	0.0112	0.0000	-0.0096	0.0000	0.0084	0.0000
1	0.0000	-0.0015	-0.0008	0.0000	0.0018	0.0000	-0.0022	0.0000	0.0024	0.0000	-0.0025	0.0000	0.0025
2	-0.1224	0.0000	-0.2950	0.0146	0.0000	-0.0104	0.0000	0.0076	0.0000	-0.0057	0.0000	0.0043	0.0000
3	0.0000	-0.0005	0.0000	0.0026	0.0015	0.0000	-0.0026	0.0000	0.0028	0.0000	-0.0028	0.0000	0.0028
4	0.0939	0.0000	0.0913	0.0000	0.2543	-0.0110	0.0000	0.0072	0.0000	-0.0049	0.0000	0.0034	0.0000
5	0.0000	0.0004	0.0000	0.0010	0.0000	-0.0024	-0.0021	0.0000	0.0030	0.0000	-0.0030	0.0000	0.0028
6	-0.0778	0.0000	-0.0604	0.0000	-0.0704	0.0000	-0.2004	0.0074	0.0000	-0.0049	0.0000	0.0033	0.0000
7	0.0000	-0.0003	0.0000	-0.0006	0.0000	-0.0013	0.0000	0.0017	0.0028	0.0000	-0.0032	0.0000	0.0028
8	0.0656	0.0000	0.0448	0.0000	0.0424	0.0000	0.0512	0.0000	0.1456	-0.0046	0.0000	0.0034	0.0000
9	0.0000	0.0002	0.0000	0.0004	0.0000	0.0006	0.0000	0.0013	0.0000	-0.0014	-0.0033	0.0000	0.0029
10	-0.0560	0.0000	-0.0344	0.0000	-0.0289	0.0000	-0.0288	0.0000	-0.0353	0.0000	-0.0980	0.0029	0.0000
11	0.0000	-0.0001	0.0000	-0.0002	0.0000	-0.0002	0.0000	-0.0003	0.0000	-0.0009	0.0000	0.0017	0.0034
12	0.0484	0.0000	0.0269	0.0000	0.0205	0.0000	0.0185	0.0000	0.0191	0.0000	0.0236	0.0000	0.0615

ORIENTATIONAL ORDER PARAMETERS Y(L,M) AVERAGED OVER 200 CONFIGURATIONS. SITE NUMBER 4

	0	1	2	3	4	5	6	7	8	9	10	11	12
0	0.2821	-0.3115	0.0000	0.2749	0.0000	-0.2329	0.0000	0.1968	0.0000	-0.1674	0.0000	0.1438	0.0000
1	0.0000	0.0042	-0.0093	0.0000	0.0096	0.0000	-0.0089	0.0000	0.0081	0.0000	-0.0073	0.0000	0.0067
2	-0.3404	0.0000	-0.2927	0.2546	0.0000	-0.1776	0.0000	0.1272	0.0000	-0.0922	0.0000	0.0672	0.0000
3	0.0000	-0.0088	0.0000	-0.0085	0.0142	0.0000	-0.0109	0.0000	0.0081	0.0000	-0.0061	0.0000	0.0046
4	0.2913	0.0000	0.2457	0.0000	0.2473	-0.1971	0.0000	0.1177	0.0000	-0.0723	0.0000	0.0445	0.0000
5	0.0000	0.0087	0.0000	0.0114	0.0000	0.0105	-0.0151	0.0000	0.0088	0.0000	-0.0048	0.0000	0.0022
6	-0.2471	0.0000	-0.1753	0.0000	-0.1788	0.0000	-0.1876	0.1361	0.0000	-0.0700	0.0000	0.0365	0.0000
7	0.0000	-0.0081	0.0000	-0.0089	0.0000	-0.0105	0.0000	-0.0099	0.0122	0.0000	-0.0045	0.0000	0.0004
8	0.2105	0.0000	0.1281	0.0000	0.1106	0.0000	0.1180	0.0000	0.1279	-0.0823	0.0000	0.0360	0.0000
9	0.0000	0.0073	0.0000	0.0067	0.0000	0.0061	0.0000	0.0066	0.0000	0.0067	-0.0065	0.0000	-0.0006
10	-0.1809	0.0000	-0.0948	0.0000	-0.0701	0.0000	-0.0636	0.0000	-0.0692	0.0000	-0.0781	0.0425	0.0000
11	0.0000	-0.0066	0.0000	-0.0050	0.0000	-0.0031	0.0000	-0.0016	0.0000	-0.0012	0.0000	-0.0021	0.0002
12	0.1570	0.0000	0.0707	0.0000	0.0449	0.0000	0.0349	0.0000	0.0324	0.0000	0.0356	0.0000	0.0427

ORIENTATIONAL ORDER PARAMETERS Y(L,M) AVERAGED OVER 200 CONFIGURATIONS. SITE NUMBER 5

	0	1	2	3	4	5	6	7	8	9	10	11	12
0	0.2821	0.3296	0.0000	-0.2916	0.0000	0.2478	0.0000	-0.2104	0.0000	0.1800	0.0000	-0.1555	0.0000
1	0.0000	-0.0027	-0.0068	0.0000	0.0080	0.0000	-0.0087	0.0000	0.0091	0.0000	-0.0093	0.0000	0.0094
2	-0.3371	0.0000	-0.2944	-0.2750	0.0000	0.1969	0.0000	-0.1457	0.0000	0.1101	0.0000	-0.0846	0.0000
3	0.0000	0.0064	0.0000	0.0058	0.0107	0.0000	-0.0102	0.0000	0.0097	0.0000	-0.0092	0.0000	0.0087
4	0.2864	0.0000	0.2482	0.0000	0.2520	0.2213	0.0000	-0.1397	0.0000	0.0920	0.0000	-0.0621	0.0000

5	0.0000	-0.0069	0.0000	-0.0095	0.0000	-0.0084	-0.0122	0.0000	0.0100	0.0000	-0.0086	0.0000	0.0074
6	-0.2418	0.0000	-0.1788	0.0000	-0.1868	0.0000	-0.1955	-0.1627	0.0000	0.0917	0.0000	-0.0537	0.0000
7	0.0000	0.0070	0.0000	0.0090	0.0000	0.0108	0.0000	0.0099	0.0112	0.0000	-0.0081	0.0000	0.0062
8	0.2056	0.0000	0.1328	0.0000	0.1190	0.0000	0.1295	0.0000	0.1377	0.1081	0.0000	-0.0541	0.0000
9	0.0000	-0.0071	0.0000	-0.0087	0.0000	-0.0094	0.0000	-0.0104	0.0000	-0.0098	-0.0083	0.0000	0.0052
10	-0.1765	0.0000	-0.1005	0.0000	-0.0787	0.0000	-0.0737	0.0000	-0.0814	0.0000	-0.0879	-0.0643	0.0000
11	0.0000	0.0072	0.0000	0.0085	0.0000	0.0085	0.0000	0.0082	0.0000	0.0082	0.0000	0.0080	0.0046
12	0.1533	0.0000	0.0772	0.0000	0.0532	0.0000	0.0435	0.0000	0.0414	0.0000	0.0460	0.0000	0.0510

AVERAGE PARTICLE POSITIONS AND RMS DEVIATIONS

1	-0.83072270E+00	-0.58549028E+00	-0.49918835E+00	0.14654553E-01	0.13938081E-01	0.11264709E-01
9	0.50350883E+00	-0.58542690E+00	0.16484407E+00	0.12749961E-01	0.14699471E-01	0.15197839E-01
17	-0.17607636E+00	0.40448745E+00	0.83796883E+00	0.15804625E-01	0.10502581E-01	0.12633467E-01
25	-0.83167615E+00	-0.92087435E+00	-0.16679645E+00	0.14524983E-01	0.99118186E-02	0.17642946E-01
33	0.50265918E+00	-0.92247786E+00	0.50509315E+00	0.20419819E-01	0.12624982E-01	0.98683415E-02
41	0.17432025E+00	0.58112880E+00	-0.83163249E+00	0.15342008E-01	0.14832516E-01	0.15268499E-01
49	-0.49697332E+00	-0.42189348E+00	0.49724117E+00	0.19564484E-01	0.14931575E-01	0.14271171E-01
57	0.82885650E+00	-0.86301224E-01	-0.50226569E+00	0.10199484E-01	0.12759383E-01	0.12837957E-01
65	0.16407432E+00	0.91423606E+00	0.16867522E+00	0.15699347E-01	0.13238042E-01	0.15259484E-01
73	-0.84908207E+00	-0.26007468E+00	0.99919427E+00	0.16322878E-01	0.10262690E-01	0.19281669E-01
81	0.49711811E+00	-0.25454773E+00	-0.33786768E+00	0.14879652E-01	0.12445767E-01	0.13612054E-01
89	-0.16343559E+00	0.74452624E+00	0.33474019E+00	0.15131654E-01	0.14786962E-01	0.13247824E-01
97	-0.83248210E+00	-0.25347503E+00	-0.53553063E-02	0.94218368E-02	0.10457516E-01	0.13998140E-01
105	0.50127137E+00	-0.25361840E+00	0.66551565E+00	0.20171659E-01	0.12610297E-01	0.12116398E-01
113	0.15852517E+00	0.24127077E+00	0.99915223E+00	0.14122849E-01	0.15269122E-01	0.18437475E-01
121	-0.49302436E+00	-0.75340717E+00	0.33465533E+00	0.17158853E-01	0.10669177E-01	0.14196591E-01
129	0.83603708E+00	-0.75145415E+00	-0.65884022E+00	0.14755707E-01	0.13044334E-01	0.11783132E-01
137	0.16215469E+00	0.24781591E+00	-0.43151161E-02	0.16037344E-01	0.14563687E-01	0.18062752E-01

ANALYSIS OF CRYSTAL STRUCTURE

BASED ON 3 2 3 ENFOLDING

NUMBER OF BASIS SITES IN UNIT CELL = 8

SITE	NAVG	SX-COORD	SY-COORD	SZ-COORD	X-RMS ERR	Y-RMS ERR	Z-RMS ERR
1	18	0.249533	0.412718	0.749984	0.025823	0.013733	0.021252
2	18	0.249003	0.079831	0.249962	0.024950	0.012613	0.021113
3	18	0.751289	0.580155	0.249704	0.023077	0.013509	0.023525
4	18	0.751932	0.913495	0.749867	0.022849	0.012316	0.021103
5	18	0.251609	0.746282	0.000096	0.024463	0.013075	0.020838
6	18	0.250824	0.746973	0.500080	0.022070	0.012231	0.020640
7	18	0.749256	0.245839	0.000228	0.026211	0.013586	0.020674
8	18	0.747203	0.246908	0.499900	0.026493	0.013509	0.020424

BRAGG PLANE PROJECTION

L	M	N	STR.FAC	L	M	N	STR.FAC
0	0	6	71.7080	0	0	6	71.6672
0	4	-6	17.7710	0	4	-6	71.4804
0	4	-3	53.9599	0	4	-3	0.0026
0	4	0	17.8892	0	4	0	71.8840
0	4	3	53.9497	0	4	3	0.0017
0	4	6	17.8613	0	4	6	71.6235
0	8	-6	18.0174	0	8	-6	71.0653
0	8	-3	53.4263	0	8	-3	0.0095
0	8	0	18.0698	0	8	0	71.5373
0	8	3	53.5165	0	8	3	0.0078
0	8	6	17.9774	0	8	6	71.3496
3	-6	-6	71.4082	3	-6	-6	71.3761
3	-6	0	71.5889	3	-6	0	71.5591
3	-6	6	71.1890	3	-6	6	71.0820
3	-2	-6	18.0038	3	-2	-6	71.4920
3	-2	-3	53.6461	3	-2	-3	0.0032
3	-2	0	18.0946	3	-2	0	71.7467
3	-2	3	53.5537	3	-2	3	0.0043
3	-2	6	18.0389	3	-2	6	71.3387
3	2	-6	17.8292	3	2	-6	71.3778
3	2	-3	53.7933	3	2	-3	0.0002
3	2	0	17.8546	3	2	0	71.7036
3	2	3	53.8009	3	2	3	0.0004
3	2	6	17.7359	3	2	6	71.3671
3	6	-6	71.1769	3	6	-6	71.0347
3	6	0	71.4626	3	6	0	71.4301
3	6	6	71.1684	3	6	6	71.1665
6	-8	-6	18.0393	6	-8	-6	70.6305
6	-8	-3	52.7193	6	-8	-3	0.0266
6	-8	0	18.1012	6	-8	0	70.7357
6	-8	3	52.5466	6	-8	3	0.0294
6	-8	6	18.0180	6	-8	6	70.1907
6	-4	-6	17.4417	6	-4	-6	70.8172
6	-4	-3	53.5451	6	-4	-3	0.0140
6	-4	0	17.4397	6	-4	0	70.9921
6	-4	3	53.4697	6	-4	3	0.0160
6	-4	6	17.2962	6	-4	6	70.5130
6	0	-6	70.8405	6	0	-6	70.7764
6	0	0	71.0153	6	0	0	71.0214
6	0	6	70.6140	6	0	6	70.6115
6	4	-6	17.7605	6	4	-6	70.5086
6	4	-3	52.9744	6	4	-3	0.0015
6	4	0	17.8534	6	4	0	70.8231
6	4	3	52.8763	6	4	3	0.0017
6	4	6	17.8003	6	4	6	70.4847
6	8	-6	17.5246	6	8	-6	70.0165
6	8	-3	52.8504	6	8	-3	0.0022
6	8	0	17.5422	6	8	0	70.3988

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 6 8 3    52.8601 6 8 3     0.0011
 6 8 6    17.4199 6 8 6    70.1333

TIME ELAPSED SINCE JOB START =    2378.63574219 SECONDS
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Table 14

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************  CCP5 PROGRAM LIBRARY  (SERC)
              DARESBURY LABORATORY
M D C S P C   MOLECULAR DYNAMICS OF PHASE
              CHANGES.   BY W. SMITH
************  VERSION 4.3 , MAY 1991

POTASSIUM NITRATE SIMULATION PHASE A (NPT)

PHYSICAL SPECIFICATION
                        INITIAL MOLAR VOLUME        =     2.5258E-05 M**3
                        SPECIFIED TEMPERATURE       =     2.0000E+02 K
                        SPECIFIED PRESSURE          =     0.0000E+00 PA
                        CELL MASS PARAMETER         =     1.6788E-25 KG
                        EWALD CONVERGENCE PARAMETER =     4.5000E+09 M**-1
                        INITIAL CELL VECTOR NO. 1   =  1.6530000 0.0000000 0.0000000 NM
                        INITIAL CELL VECTOR NO. 2   =  0.0000000 1.9060000 0.0000000 NM
                        INITIAL CELL VECTOR NO. 3   =  0.0000000 0.0000000 1.9170000 NM


INTERNAL PROGRAM UNITS
                        UNIT OF LENGTH              =     1.0000E-09 M
                        UNIT OF MASS                =     1.0000E-26 KG
                        UNIT OF TIME                =     2.0000E-15 S
                        UNIT OF ENERGY              =     2.5000E-15 J
                        UNIT OF PRESSURE            =     2.5000E+12 PA
                        UNIT OF CHARGE              =     1.6022E-19 C


VALUE OF CUTOFF RADIUS =  0.7000000 NM


JOB CONTROL PARAMETERS

                        CONSTANT PRESSURE OPTION    =        1

                        RANDOM ORIENTATION OPTION   =        F

                        NUMBER OF TIMESTEPS IN RUN  =     2000
                        RESTART CONTROL PARAMETER   =        2

                        NUMBER OF SPECIES TYPES     =        2
                        NUMBER OF PRIMITIVE CELLS   =       18
                        NUMBER OF PRIMITIVE CELLS X =        3
                        NUMBER OF PRIMITIVE CELLS Y =        2
                        NUMBER OF PRIMITIVE CELLS Z =        3
                        SPECIES IN PRIMITIVE CELL   =        8

                        TEMPERATURE SCALING OPTION  =        T
                        TEMPERATURE SCALING INTERVAL=        5
                        LAST TEMP. SCALING STEP     =     1000
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                        RDF OPTION                    =        T
                        RDF ARRAY LENGTH              =      128
                        RDF TIMESTEP INTERVAL         =        5
                        RDF START TIMESTEP            =     1000

                        MSD OPTION                    =        T
                        MSD START TIMESTEP            =     1000

                        STRUCTURAL DATA FILE OPTION   =        F

                        TRAJECTORY FILE OPTION        =        F
                        TRAJECTORY FILE START STEP    =        0
                        TRAJECTORY SAMPLING INTERVAL  =        0

                        ZERO AVERAGES OPTION          =        T
                        NO. STEPS IN ROLLING AVERAGE  =      100


PARAMETERS FOR SPECIES NUMBER   1

                        NO. PLES. IN PRIMITIVE CELL   =        4
                        NO. PARTICLES IN MD CELL      =       72
                        TOTAL PARTICLE MASS           =     6.4926E-26 KG
                        MOMENT OF INERTIA IXX         =     0.0000E+00 KG M**2
                        MOMENT OF INERTIA IYY         =     0.0000E+00 KG M**2
                        MOMENT OF INERTIA IZZ         =     0.0000E+00 KG M**2
PARTICLE POSITIONS AND ORIENTATIONS IN PRIMITIVE CELL
                          0.250000  0.416000  0.750000  0.000000  0.000000  0.000000
                          0.250000  0.048000  0.250000  0.000000  0.000000  0.000000
                          0.750000  0.583000  0.250000  0.000000  0.000000  0.000000
                          0.750000  0.917000  0.750000  0.000000  0.000000  0.000000
SITE PARAMETERS AND BONDLENGTHS
SITE INDEX     BOND X (NM)     BOND Y (NM)     BOND Z (NM)    AT.MASS (KG)    AT.CHGE  (C)
    1            0.000000        0.000000        0.000000     6.49260E-26     1.60210E-19

PARAMETERS FOR SPECIES NUMBER   2

                        NO. PLES. IN PRIMITIVE CELL   =        4
                        NO. PARTICLES IN MD CELL      =       72
                        TOTAL PARTICLE MASS           =     1.0295E-25 KG
                        MOMENT OF INERTIA IXX         =     6.1728E-46 KG M**2
                        MOMENT OF INERTIA IYY         =     6.1727E-46 KG M**2
                        MOMENT OF INERTIA IZZ         =     1.2346E-45 KG M**2
PARTICLE POSITIONS AND ORIENTATIONS IN PRIMITIVE CELL
                          0.250000  0.750000  0.000000  0.000000  0.000000  0.000000
                          0.250000  0.750000  0.500000  0.000000  0.000000  0.000000
                          0.750000  0.250000  0.000000  0.000000  0.000000  0.000000
                          0.750000  0.250000  0.500000  0.000000  0.000000  0.000000
SITE PARAMETERS AND BONDLENGTHS
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SITE INDEX	BOND X (NM)	BOND Y (NM)	BOND Z (NM)	AT.MASS (KG)	AT.CHGE (C)
2	0.000000	0.000000	0.000000	2.32570E-26	2.09280E-19
3	0.124460	0.000000	0.000000	2.65660E-26	-1.23160E-19
4	-0.062230	-0.107786	0.000000	2.65660E-26	-1.23160E-19
5	-0.062230	0.107786	0.000000	2.65660E-26	-1.23160E-19

RDF EQUIVALENCES

IXP:					
1	1				
2	2	3			
3	4	5	6		
4	4	5	6	6	
5	4	5	6	6	6
JXP-	1	2	3	4	5

BUCKINGHAM POTENTIAL PARAMETERS

FORM OF POTENTIAL: V(R)=Q*Q/R+AAA*EXP(-R/RHO)+CCC/R**6

SITE	SITE	AAA(I,J) (J)	RHO(I,J) (NM)	CCC(I,J) (J-NM6)
1	1	1.991415E-16	3.367000E-02	-2.430000E-24
2	1	2.412410E-16	2.963000E-02	-2.091350E-24
2	2	2.922400E-16	2.645500E-02	-1.799900E-24
3	1	3.278180E-16	2.792700E-02	-2.092340E-24
3	2	3.971200E-16	2.512600E-02	-1.800700E-24
3	3	5.396400E-16	2.392300E-02	-1.801600E-24
4	1	3.278180E-16	2.792700E-02	-2.092340E-24
4	2	3.971200E-16	2.512600E-02	-1.800700E-24
4	3	5.396400E-16	2.392300E-02	-1.801600E-24
4	4	5.396400E-16	2.392300E-02	-1.801600E-24
5	1	3.278180E-16	2.792700E-02	-2.092340E-24
5	2	3.971200E-16	2.512600E-02	-1.800700E-24
5	3	5.396400E-16	2.392300E-02	-1.801600E-24
5	4	5.396400E-16	2.392300E-02	-1.801600E-24
5	5	5.396400E-16	2.392300E-02	-1.801600E-24

LONG RANGE CORRECTIONS

POTENTIAL CORRECTION	=	-1.0516E+03 J/M
VIRIAL CORRECTION	=	6.3083E+03 J/M
EWALD SELF CORRECTION (PE)	=	-3.0285E+05 J/M
EWALD SELF CORRECTION (VIR)	=	2.5747E+05 J/M

STARTING CONFIGURATION OBTAINED FROM RESTART FILE

PREVIOUS JOB ENTITLED <POTASSIUM NITRATE SIMULATION PHASE A (NVT) >

SAMPLE OF INITIAL PARTICLE POSITIONS

	ABSOLUTE POSITIONS			MD CELL POSITIONS		
1	-0.67601151E+00	-0.53421269E+00	-0.46334764E+00	-0.81792076E+00	-0.56055896E+00	-0.48340912E+00
9	0.42035490E+00	-0.56691922E+00	0.15106461E+00	0.50859637E+00	-0.59487851E+00	0.15760523E+00
17	-0.13557932E+00	0.40222956E+00	0.79049686E+00	-0.16404032E+00	0.42206669E+00	0.82472286E+00
25	-0.69584414E+00	-0.86105895E+00	-0.13629686E+00	-0.84191668E+00	-0.90352461E+00	-0.14219808E+00
33	0.41267365E+00	-0.89053644E+00	0.48892214E+00	0.49930266E+00	-0.93445587E+00	0.51009091E+00
41	0.13892713E+00	0.56833102E+00	-0.77776640E+00	0.16809090E+00	0.59635994E+00	-0.81144121E+00
49	-0.39321195E+00	-0.37490768E+00	0.47191138E+00	-0.47575554E+00	-0.39339736E+00	0.49234364E+00
57	0.68345911E+00	-0.10401934E+00	-0.46495074E+00	0.82693177E+00	-0.10914936E+00	-0.48508163E+00
65	0.12492491E+00	0.86455346E+00	0.16728913E+00	0.15114932E+00	0.90719146E+00	0.17453221E+00
73	-0.72499113E+00	-0.24591554E+00	-0.94952138E+00	-0.87718225E+00	-0.25804359E+00	-0.99063264E+00
81	0.38115397E+00	-0.22889291E+00	-0.33371560E+00	0.46116633E+00	-0.24018144E+00	-0.34816442E+00
89	-0.13544314E+00	0.69899599E+00	0.31048751E+00	-0.16387554E+00	0.73346904E+00	0.32393063E+00
97	-0.68251474E+00	-0.22475351E+00	-0.10052705E-01	-0.82578916E+00	-0.23583789E+00	-0.10487955E-01
105	0.44097274E+00	-0.24397642E+00	0.62855581E+00	0.53354234E+00	-0.25600884E+00	0.65577028E+00
113	0.14816677E+00	0.24308312E+00	-0.93035629E+00	0.17927014E+00	0.25507148E+00	-0.97063776E+00
121	-0.39729918E+00	-0.72300003E+00	0.32079642E+00	-0.48070076E+00	-0.75865691E+00	0.33468588E+00
129	0.70306567E+00	-0.70814416E+00	-0.61786014E+00	0.85065417E+00	-0.74306838E+00	-0.64461152E+00
137	0.13649316E+00	0.24680113E+00	0.18630419E-01	0.16514599E+00	0.25897286E+00	0.19437057E-01

SAMPLE OF INITIAL PARTICLE VELOCITIES

	ABSOLUTE VELOCITIES			MD CELL VELOCITIES		
1	-0.60532587E-04	0.71454469E-03	0.34758493E-03	-0.73239670E-04	0.74978456E-03	0.36263425E-03
9	-0.47051932E-03	0.32890501E-03	-0.27510506E-03	-0.56929137E-03	0.34512593E-03	-0.28701624E-03
17	-0.20435764E-03	0.68913709E-03	-0.22030995E-03	-0.24725667E-03	0.72312391E-03	-0.22984867E-03
25	-0.42214766E-03	0.63074887E-04	0.22250603E-03	-0.51076547E-03	0.66185610E-04	0.23213983E-03
33	-0.93380239E-03	-0.22306728E-03	-0.25717370E-03	-0.11298275E-02	-0.23406850E-03	-0.26830850E-03
41	-0.72826319E-03	0.42357648E-03	-0.23906007E-03	-0.88114119E-03	0.44446640E-03	-0.24941061E-03
49	0.36531805E-03	-0.53866831E-03	0.37636412E-03	0.44200611E-03	-0.56523433E-03	0.39265948E-03
57	-0.23965633E-04	-0.70534572E-03	-0.10758534E-03	-0.28996531E-04	-0.74013192E-03	-0.11224344E-03
65	0.78928898E-03	-0.48893074E-03	0.39183219E-03	0.95497759E-03	-0.51304380E-03	0.40879727E-03
73	-0.10797580E-03	-0.10313563E-03	-0.51461777E-03	-0.13064223E-03	-0.10822206E-03	-0.53689908E-03
81	-0.36188200E-03	0.10817863E-03	0.45974207E-03	-0.43784876E-03	0.11351378E-03	0.47964744E-03
89	-0.19161797E-03	0.47243142E-04	-0.83908853E-04	-0.23184267E-03	0.49573076E-04	-0.87541839E-04
97	0.16602797E-03	-0.26650252E-03	-0.28500978E-03	0.20088079E-03	-0.27964587E-03	-0.29734979E-03
105	0.17076030E-03	0.19968921E-03	0.30356762E-03	0.20660653E-03	0.20953747E-03	0.31671114E-03
113	-0.39386090E-03	0.40828792E-03	-0.47509673E-03	-0.47654071E-03	0.42842384E-03	-0.49566691E-03
121	0.18950935E-03	0.16758564E-03	-0.70078002E-04	0.22929140E-03	0.17585062E-03	-0.73112156E-04
129	-0.38045358E-04	0.36905965E-03	-0.17324347E-03	-0.46031891E-04	0.38726091E-03	-0.18074436E-03
137	-0.21103422E-03	-0.95824568E-04	0.35695046E-03	-0.25533481E-03	-0.10055044E-03	0.37240528E-03

SAMPLE OF INITIAL PARTICLE ORIENTATIONS

	QUATERNIONS				QUATERNION DERIVATIVES			
1	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00

9	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
17	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
25	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
33	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
41	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
49	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
57	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
65	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
73	0.800686E+00	-0.379673E-01	0.799509E-01	0.592510E+00	-0.591281E-03	0.937472E-03	-0.216947E-02	0.115185E-02
81	0.732768E+00	-0.104541E+00	-0.956694E-01	0.665560E+00	0.754679E-03	-0.252718E-02	-0.338080E-03	-0.127643E-02
89	0.995303E+00	-0.205963E-01	0.777859E-01	-0.538182E-01	0.235813E-03	0.100238E-02	-0.323805E-02	-0.702628E-03
97	0.995252E+00	-0.625282E-01	0.627776E-01	0.402935E-01	-0.141277E-03	-0.417043E-03	0.123052E-02	0.925226E-03
105	0.992437E+00	-0.107590E-01	0.300314E-01	0.118544E+00	0.703273E-04	-0.213563E-02	-0.222504E-02	-0.218621E-03
113	0.982997E+00	-0.122079E+00	-0.140030E-01	0.136446E+00	-0.103500E-03	-0.554610E-03	0.717675E-04	0.256801E-03
121	0.975617E+00	-0.857558E-01	0.731784E-01	0.188312E+00	-0.101180E-03	0.887143E-03	0.139874E-02	0.384648E-03
129	0.995056E+00	0.774601E-02	-0.422506E-01	0.895519E-01	0.654697E-04	0.189184E-02	0.765790E-03	-0.529729E-03
137	0.983782E+00	-0.288856E-01	0.125424E+00	-0.124927E+00	-0.234964E-03	0.418966E-03	0.909339E-03	-0.103423E-02

TIME ELAPSED SINCE JOB START = 0.20029400 SECONDS

STEP TIME (S)	PE (J/M) VIR (J/M)	TKE (J/M) RKE (J/M)	TE (J/M) EPV (J/M)	T. TEMP (K) R. TEMP (K)	PRS (PA) VOL (M**3)	VL1 (M) DC1	VL2 (M) DC2	VL3 (M) DC3
1	-3.366701E+05	2.485935E+03	-3.329399E+05	1.993250E+02	-1.283289E+08	1.652998E-09	1.905998E-09	1.916999E-09
1.40	1.469600E+04	1.244215E+03	-3.361813E+05	1.995251E+02	2.525834E-05	-6.395852E-07	-8.054649E-09	-6.001741E-07
ROLLING	-3.366701E+05	2.485935E+03	-3.329399E+05	1.993250E+02	-1.283289E+08	1.652998E-09	1.905998E-09	1.916999E-09
AVERAGES	1.469600E+04	1.244215E+03	-3.361813E+05	1.995251E+02	2.525834E-05	-6.395852E-07	-8.054649E-09	-6.001741E-07
100	-3.383812E+05	2.554467E+03	-3.345549E+05	2.048200E+02	-3.117715E+06	1.641191E-09	1.902731E-09	1.910962E-09
106.15	5.342296E+03	1.271813E+03	-3.346327E+05	2.039507E+02	2.495003E-05	2.603366E-03	1.902796E-02	1.088695E-02
ROLLING	-3.376413E+05	2.519854E+03	-3.338544E+05	2.020446E+02	3.968553E+06	1.642898E-09	1.899834E-09	1.912690E-09
AVERAGES	4.779526E+03	1.267043E+03	-3.337676E+05	2.031859E+02	2.496452E-05	5.000939E-06	9.201309E-03	2.927411E-03
200	-3.376536E+05	2.606055E+03	-3.337699E+05	2.089563E+02	-7.934449E+06	1.645761E-09	1.899362E-09	1.910919E-09
210.25	5.806502E+03	1.277566E+03	-3.339681E+05	2.048733E+02	2.497097E-05	-2.289023E-03	2.379426E-02	1.437561E-02
ROLLING	-3.378336E+05	2.490570E+03	-3.341105E+05	1.996967E+02	1.339962E+07	1.649112E-09	1.898579E-09	1.907542E-09
AVERAGES	3.983806E+03	1.232449E+03	-3.337781E+05	1.976383E+02	2.497199E-05	-3.262326E-03	1.257635E-02	1.357665E-02
300	-3.377407E+05	2.468326E+03	-3.340246E+05	1.979131E+02	3.352375E+07	1.646293E-09	1.902881E-09	1.900424E-09
315.17	2.433295E+03	1.247737E+03	-3.331901E+05	2.000898E+02	2.489138E-05	-1.305981E-02	1.784452E-02	2.933087E-03
ROLLING	-3.377888E+05	2.514724E+03	-3.340366E+05	2.016333E+02	-1.049022E+07	1.641146E-09	1.900719E-09	1.911916E-09
AVERAGES	5.836358E+03	1.237473E+03	-3.343056E+05	1.984439E+02	2.493637E-05	-3.652025E-03	1.716778E-02	5.609690E-03
400	-3.378851E+05	2.506110E+03	-3.340544E+05	2.009427E+02	1.777124E+08	1.634690E-09	1.893401E-09	1.911913E-09
419.05	-8.181111E+03	1.324605E+03	-3.296566E+05	2.124166E+02	2.474660E-05	7.367758E-03	-1.948158E-03	-5.300977E-03
ROLLING	-3.375692E+05	2.496508E+03	-3.338218E+05	2.001728E+02	4.149796E+07	1.648685E-09	1.903258E-09	1.900594E-09
AVERAGES	1.977883E+03	1.250889E+03	-3.328167E+05	2.005954E+02	2.493611E-05	-1.667756E-03	1.327361E-02	4.120392E-03
500	-3.379650E+05	2.428320E+03	-3.342270E+05	1.947054E+02	6.211101E+07	1.661802E-09	1.884666E-09	1.897047E-09

523.42	2.270862E+02	1.309687E+03	-3.326838E+05	2.100242E+02	2.484559E-05	2.237983E-04	5.580841E-03	-1.045931E-02
ROLLING	-3.377384E+05	2.484887E+03	-3.339972E+05	1.992410E+02	3.097412E+06	1.647281E-09	1.898726E-09	1.908920E-09
AVERAGES	4.797265E+03	1.256339E+03	-3.339397E+05	2.014692E+02	2.496422E-05	2.244103E-03	1.248335E-02	-1.223637E-02
600	-3.377883E+05	2.417339E+03	-3.341253E+05	1.938249E+02	-1.015637E+08	1.644584E-09	1.906314E-09	1.921039E-09
630.64	1.250849E+04	1.245667E+03	-3.366832E+05	1.997580E+02	2.518555E-05	8.446202E-04	9.553603E-03	-4.009248E-03
ROLLING	-3.378493E+05	2.492616E+03	-3.341094E+05	1.998607E+02	8.471847E+06	1.644974E-09	1.901695E-09	1.908934E-09
AVERAGES	4.367752E+03	1.247264E+03	-3.339036E+05	2.000141E+02	2.497013E-05	-9.910660E-04	2.068894E-03	-1.152191E-02
700	-3.384306E+05	2.464508E+03	-3.346947E+05	1.976070E+02	-1.088984E+08	1.657643E-09	1.896940E-09	1.895642E-09
738.29	1.307281E+04	1.271419E+03	-3.374093E+05	2.038876E+02	2.492780E-05	1.580119E-03	3.527988E-03	2.946648E-03
ROLLING	-3.379621E+05	2.497575E+03	-3.341993E+05	2.002583E+02	-2.078662E+06	1.646629E-09	1.902974E-09	1.904911E-09
AVERAGES	5.177874E+03	1.265199E+03	-3.342603E+05	2.028901E+02	2.496203E-05	2.645741E-03	3.670116E-03	2.704736E-03
800	-3.376437E+05	2.513439E+03	-3.338972E+05	2.015303E+02	1.701261E+08	1.640012E-09	1.893323E-09	1.905904E-09
842.83	-7.602677E+03	1.233045E+03	-3.296873E+05	1.977338E+02	2.474548E-05	4.607483E-03	1.245793E-03	1.660782E-02
ROLLING	-3.377033E+05	2.488887E+03	-3.339836E+05	1.995617E+02	-7.264750E+06	1.647152E-09	1.899152E-09	1.909100E-09
AVERAGES	5.592095E+03	1.230807E+03	-3.341884E+05	1.973750E+02	2.497282E-05	3.825454E-03	2.587706E-05	1.244239E-02
900	-3.380700E+05	2.529536E+03	-3.342780E+05	2.028210E+02	2.707499E+07	1.642854E-09	1.899017E-09	1.914851E-09
946.98	3.030020E+03	1.262491E+03	-3.336016E+05	2.024559E+02	2.498064E-05	-1.929382E-05	9.854543E-03	1.099018E-02
ROLLING	-3.379804E+05	2.494030E+03	-3.342212E+05	1.999740E+02	4.335684E+07	1.647197E-09	1.895853E-09	1.905177E-09
AVERAGES	1.780113E+03	1.265168E+03	-3.331519E+05	2.028852E+02	2.487777E-05	-2.541555E-03	2.705256E-03	1.575410E-02

1 STEP TIME (S)	PE (J/M) VIR (J/M)	TKE (J/M) RKE (J/M)	TE (J/M) EPV (J/M)	T.TEMP (K) R.TEMP (K)	PRS (PA) VOL (M**3)	VL1 (M) DC1	VL2 (M) DC2	VL3 (M) DC3
1000	-3.379254E+05	2.467457E+03	-3.342097E+05	1.978434E+02	-8.212583E+07	1.658875E-09	1.895608E-09	1.899269E-09
1050.14	1.108820E+04	1.248242E+03	-3.362608E+05	2.001708E+02	2.497504E-05	-5.327384E-03	-3.972247E-03	-9.837498E-03
ROLLING	-3.381359E+05	2.491171E+03	-3.343954E+05	1.997448E+02	1.163762E+06	1.646175E-09	1.897922E-09	1.907150E-09
AVERAGES	4.928183E+03	1.249329E+03	-3.343774E+05	2.003451E+02	2.491654E-05	-4.096103E-03	6.734353E-03	6.181769E-03

SWITCHING OFF TEMPERATURE SCALING AT STEP 1000

1100	-3.380600E+05	2.640124E+03	-3.341332E+05	2.116880E+02	-2.190564E+08	1.643338E-09	1.915607E-09	1.919929E-09
1158.93	2.188745E+04	1.286608E+03	-3.396690E+05	2.063232E+02	2.527082E-05	4.723332E-03	-1.825890E-02	-6.919125E-03
ROLLING	-3.379937E+05	2.461087E+03	-3.342629E+05	1.973327E+02	-4.054769E+05	1.642366E-09	1.902304E-09	1.908530E-09
AVERAGES	4.995891E+03	1.269675E+03	-3.342875E+05	2.036079E+02	2.493298E-05	7.724980E-03	-1.044717E-02	-7.279575E-03
MSD (M**2)	1.159790E-21	1.045737E-21						
1200	-3.377791E+05	2.329357E+03	-3.341548E+05	1.867704E+02	-5.007724E+06	1.652658E-09	1.896668E-09	1.907883E-09
1266.12	5.034385E+03	1.294929E+03	-3.342800E+05	2.076577E+02	2.500609E-05	-4.698675E-03	-1.698014E-02	2.396119E-03
ROLLING	-3.380620E+05	2.544614E+03	-3.342126E+05	2.040299E+02	3.681777E+06	1.647138E-09	1.902751E-09	1.904672E-09
AVERAGES	4.867657E+03	1.304731E+03	-3.341388E+05	2.092296E+02	2.495849E-05	-6.843447E-03	-1.684779E-02	-9.061926E-03
MSD (M**2)	1.349977E-21	1.218545E-21						
1300	-3.379621E+05	2.437265E+03	-3.341722E+05	1.954226E+02	8.558589E+06	1.645107E-09	1.908539E-09	1.899029E-09

1371.84	4.234328E+03	1.352623E+03	-3.339588E+05	2.169096E+02	2.493413E-05	-4.422319E-03	-5.728820E-03	-6.592846E-03
ROLLING	-3.379406E+05	2.490950E+03	-3.341398E+05	1.997271E+02	-6.159711E+06	1.638927E-09	1.902536E-09	1.916072E-09
AVERAGES	5.448317E+03	1.309878E+03	-3.342953E+05	2.100550E+02	2.498222E-05	-1.180775E-03	-1.353788E-02	-1.033567E-03
MSD(M**2)	1.121271E-21	9.048962E-22						
1400	-3.376822E+05	2.226334E+03	-3.340148E+05	1.785099E+02	-3.623759E+07	1.643614E-09	1.889752E-09	1.928441E-09
1478.14	7.175737E+03	1.441081E+03	-3.349225E+05	2.310949E+02	2.504829E-05	4.911760E-03	6.411262E-03	-5.611331E-03
ROLLING	-3.380451E+05	2.572700E+03	-3.341239E+05	2.062819E+02	3.194330E+07	1.655030E-09	1.894727E-09	1.897710E-09
AVERAGES	2.769433E+03	1.348468E+03	-3.333319E+05	2.162434E+02	2.488543E-05	1.677678E-03	-1.107192E-03	1.661932E-03
MSD(M**2)	9.271576E-22	1.245908E-21						
1500	-3.380642E+05	2.474757E+03	-3.340024E+05	1.984287E+02	1.337301E+08	1.647064E-09	1.897306E-09	1.884477E-09
1583.83	-4.928331E+03	1.587111E+03	-3.307097E+05	2.545127E+02	2.462135E-05	-1.749218E-02	1.492210E-02	7.530880E-04
ROLLING	-3.379187E+05	2.426788E+03	-3.340651E+05	1.945826E+02	3.047312E+06	1.637791E-09	1.898961E-09	1.914581E-09
AVERAGES	4.647242E+03	1.426768E+03	-3.339964E+05	2.287996E+02	2.489701E-05	6.347375E-04	1.452488E-02	-4.461768E-03
MSD(M**2)	1.155137E-21	1.493389E-21						
1600	-3.374867E+05	2.352390E+03	-3.339491E+05	1.886172E+02	2.463341E+07	1.640707E-09	1.896517E-09	1.911870E-09
1691.64	2.866269E+03	1.185148E+03	-3.333363E+05	1.900529E+02	2.487828E-05	3.727786E-03	-3.282045E-03	6.199403E-03
ROLLING	-3.379110E+05	2.598949E+03	-3.339573E+05	2.083866E+02	2.390603E+07	1.651396E-09	1.894557E-09	1.897072E-09
AVERAGES	3.440105E+03	1.354776E+03	-3.333713E+05	2.172549E+02	2.481952E-05	-2.304200E-03	7.837698E-03	1.399587E-03
MSD(M**2)	1.065709E-21	1.224238E-21						
1700	-3.377128E+05	2.495209E+03	-3.339116E+05	2.000686E+02	-8.832768E+07	1.661074E-09	1.901387E-09	1.898829E-09
1799.68	1.163578E+04	1.305991E+03	-3.361267E+05	2.094316E+02	2.507846E-05	-9.635543E-03	6.606975E-03	-3.836419E-03
ROLLING	-3.378172E+05	2.555978E+03	-3.339654E+05	2.049411E+02	-1.951283E+06	1.649324E-09	1.900105E-09	1.900097E-09
AVERAGES	5.291087E+03	1.295805E+03	-3.340251E+05	2.077981E+02	2.490073E-05	4.938551E-03	-1.322942E-03	5.566520E-03
MSD(M**2)	9.263810E-22	1.048786E-21						
1800	-3.377727E+05	2.472654E+03	-3.339490E+05	1.982601E+02	-1.109646E+08	1.660439E-09	1.904305E-09	1.894919E-09
1907.29	1.328616E+04	1.350994E+03	-3.367293E+05	2.166484E+02	2.505559E-05	5.837758E-03	-3.313794E-03	-1.051507E-02
ROLLING	-3.379290E+05	2.594092E+03	-3.339221E+05	2.079972E+02	-4.182172E+07	1.648973E-09	1.903800E-09	1.909515E-09
AVERAGES	8.398291E+03	1.412868E+03	-3.349921E+05	2.265706E+02	2.506809E-05	-3.903325E-04	2.236807E-03	-1.179669E-03
MSD(M**2)	8.688077E-22	1.022166E-21						
1900	-3.378067E+05	2.623907E+03	-3.338595E+05	2.103877E+02	1.472822E+08	1.641800E-09	1.884913E-09	1.918697E-09
2014.95	-5.723591E+03	1.323291E+03	-3.302024E+05	2.122058E+02	2.483081E-05	-2.143810E-03	-8.111471E-03	7.714577E-05
ROLLING	-3.378069E+05	2.583525E+03	-3.338790E+05	2.071498E+02	2.631963E+07	1.653078E-09	1.899529E-09	1.894249E-09
AVERAGES	3.370194E+03	1.344389E+03	-3.332800E+05	2.155892E+02	2.487397E-05	3.560274E-04	-2.694159E-03	-9.318427E-03
MSD(M**2)	1.184764E-21	1.347905E-21						

STEP TIME(S)	PE(J/M) VIR(J/M)	TKE(J/M) RKE(J/M)	TE(J/M) EPV(J/M)	T.TEMP(K) R.TEMP(K)	PRS(PA) VOL(M**3)	VL1(M) DC1	VL2(M) DC2	VL3(M) DC3
2000	-3.380557E+05	2.798787E+03	-3.337343E+05	2.244098E+02	3.238844E+08	1.639206E-09	1.907959E-09	1.871844E-09
2123.45	-1.818730E+04	1.522679E+03	-3.258060E+05	2.441801E+02	2.447876E-05	6.773389E-03	-1.437979E-02	-8.736514E-03
ROLLING	-3.380310E+05	2.735495E+03	-3.339131E+05	2.193350E+02	4.451744E+07	1.640774E-09	1.904801E-09	1.901727E-09
AVERAGES	2.266592E+03	1.382394E+03	-3.328450E+05	2.216838E+02	2.485348E-05	-1.334673E-04	-9.806603E-03	-1.632219E-04

MSD(M**2) 1.100667E-21 1.303988E-21

RUN TERMINATING. ELAPSED CPU TIME = 2123.4497, JOB TIME = 4200.0000, CLOSE TIME = 20.0000

RUN TERMINATED AFTER 2000 STEPS. FINAL AVERAGES CALCULATED OVER 1000 STEPS.

SUMMARY OF SYSTEM AVERAGES AND CELL STRUCTURE.

STEP TIME(S)	PE(J/M) VIR(J/M)	TKE(J/M) RKE(J/M)	TE(J/M) EPV(J/M)	T.TEMP(K) R.TEMP(K)	PRS(PA) VOL(M**3)	VL1(M) DC(1,2)	VL2(M) DC(1,3)	VL3(M) DC(2,3)
2000	-3.379455E+05	2.556418E+03	-3.340441E+05	2.049764E+02	8.307730E+06	1.646480E-09	1.900407E-09	1.904423E-09
2123.46	4.549481E+03	1.344975E+03	-3.338563E+05	2.156832E+02	2.491719E-05	4.479752E-04	-3.116435E-03	-2.387011E-03
R.M.S.	1.765736E+02	1.371425E+02	1.400943E+02	1.099623E+01	1.220521E+08	9.125257E-12	7.226844E-12	1.370710E-11
FLUCT.	9.121298E+03	9.554259E+01	3.045170E+03	1.532142E+01	1.715310E-07	6.929687E-03	1.002446E-02	6.415218E-03

SAMPLE OF FINAL PARTICLE POSITIONS

	ABSOLUTE POSITIONS			MD CELL POSITIONS		
1	-0.66266951E+00	-0.55119886E+00	-0.45055450E+00	-0.81013031E+00	-0.57742438E+00	-0.48944395E+00
9	0.42239550E+00	-0.53652869E+00	0.15935192E+00	0.51875298E+00	-0.56327274E+00	0.17131290E+00
17	-0.15332297E+00	0.38878592E+00	0.77418282E+00	-0.18233196E+00	0.41168953E+00	0.82778366E+00
25	-0.67638104E+00	-0.88222611E+00	-0.13765785E+00	-0.82307276E+00	-0.92294594E+00	-0.15671831E+00
33	0.40194645E+00	-0.88416873E+00	0.46772012E+00	0.49761628E+00	-0.92620506E+00	0.49906793E+00
41	0.15077029E+00	0.54186540E+00	-0.77761330E+00	0.17563132E+00	0.56389386E+00	-0.82721336E+00
49	-0.39463899E+00	-0.43377559E+00	0.49592210E+00	-0.47589023E+00	-0.45097408E+00	0.52468629E+00
57	0.70603245E+00	-0.93554630E-01	-0.47821457E+00	0.85801864E+00	-0.10289500E+00	-0.50560536E+00
65	0.13602903E+00	0.85926927E+00	0.14563255E+00	0.16387484E+00	0.90092514E+00	0.16067292E+00
73	-0.65816869E+00	-0.22521342E+00	-0.91783112E+00	-0.80965258E+00	-0.23786388E+00	-0.98723506E+00
81	0.38492408E+00	-0.24238969E+00	-0.32087553E+00	0.46803256E+00	-0.25700004E+00	-0.34080938E+00
89	-0.13392920E+00	0.72188567E+00	0.29445511E+00	-0.16380911E+00	0.75859528E+00	0.31684317E+00
97	-0.69667893E+00	-0.21948646E+00	-0.72412178E-02	-0.84932293E+00	-0.22752934E+00	-0.14494570E-01
105	0.44835371E+00	-0.22692747E+00	0.58176902E+00	0.55265030E+00	-0.23687550E+00	0.62432720E+00
113	0.15105381E+00	0.23766377E+00	-0.93209990E+00	0.17589461E+00	0.24429168E+00	-0.99368283E+00
121	-0.43441568E+00	-0.73904711E+00	0.32548666E+00	-0.52463385E+00	-0.77162229E+00	0.34083862E+00
129	0.69825085E+00	-0.69120330E+00	-0.62889166E+00	0.84959333E+00	-0.73006641E+00	-0.66941301E+00
137	0.14468015E+00	0.23375770E+00	0.13903373E-01	0.17576044E+00	0.24457150E+00	0.17120751E-01

SAMPLE OF FINAL PARTICLE VELOCITIES

	ABSOLUTE VELOCITIES			MD CELL VELOCITIES		
1	-0.52627595E-03	-0.93874146E-03	-0.16606255E-03	-0.63992404E-03	-0.98287865E-03	-0.18608985E-03

9	0.29580485E-03	-0.21834920E-03	-0.43554043E-03	0.35827070E-03	-0.23199492E-03	-0.46396318E-03
17	-0.91203015E-03	-0.56791911E-03	0.23853722E-03	-0.11087854E-02	-0.59085618E-03	0.24476567E-03
25	0.13127776E-03	0.50789021E-04	0.51198833E-03	0.16412244E-03	0.55108369E-04	0.54841353E-03
33	-0.30609206E-03	-0.32240781E-03	0.56291947E-03	-0.36772877E-03	-0.33424957E-03	0.59751851E-03
41	-0.56181900E-03	-0.92813237E-05	0.35552354E-04	-0.68522233E-03	-0.74783361E-05	0.33308655E-04
49	-0.50013563E-03	0.16761459E-03	0.79588572E-03	-0.60450017E-03	0.18122703E-03	0.84709931E-03
57	0.29504885E-03	-0.68889408E-03	0.36360725E-03	0.36559124E-03	-0.72158280E-03	0.38782622E-03
65	-0.99114334E-03	0.17161219E-03	-0.15818197E-03	-0.12113476E-02	0.18285428E-03	-0.17642838E-03
73	0.10329226E-03	0.37010029E-04	-0.13225451E-03	0.12483165E-03	0.37805054E-04	-0.14030144E-03
81	-0.97181010E-04	-0.86637146E-04	0.37582286E-04	-0.11794822E-03	-0.90286637E-04	0.38960662E-04
89	-0.31810283E-03	-0.29269763E-03	0.85494538E-03	-0.38014340E-03	-0.30171708E-03	0.90960641E-03
97	-0.59964943E-03	0.12171124E-03	0.14794156E-03	-0.73097846E-03	0.13049693E-03	0.15369160E-03
105	-0.12054847E-03	0.70816471E-03	0.41556350E-05	-0.14977003E-03	0.74282693E-03	0.66845538E-05
113	-0.14083549E-03	-0.25299891E-04	0.68005144E-03	-0.16627033E-03	-0.22870566E-04	0.72540630E-03
121	-0.44871689E-03	-0.49380860E-03	-0.64174000E-03	-0.55082145E-03	-0.51893722E-03	-0.69171049E-03
129	-0.20032070E-03	0.32293705E-03	-0.26010682E-03	-0.24776801E-03	0.33807881E-03	-0.27812018E-03
137	-0.23429948E-04	0.10704429E-03	0.41787670E-03	-0.25629435E-04	0.11422207E-03	0.44682817E-03

SAMPLE OF FINAL PARTICLE ORIENTATIONS

	QUATERNIONS				QUATERNION DERIVATIVES			
1	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
9	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
17	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
25	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
33	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
41	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
49	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
57	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
65	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
73	0.854654E+00	0.816618E-02	0.215399E-01	0.518695E+00	-0.641773E-03	0.953964E-03	-0.302176E-04	0.104377E-02
81	0.878890E+00	-0.265508E-01	0.311975E-01	0.475263E+00	-0.105934E-02	-0.255018E-02	-0.399058E-02	0.207848E-02
89	0.856720E+00	0.237789E-01	-0.620694E-02	0.515196E+00	0.636610E-03	-0.178305E-02	0.113423E-02	-0.962669E-03
97	0.997802E+00	0.381223E-01	0.219859E-01	0.495340E-01	0.224740E-04	-0.816551E-03	0.199677E-02	-0.710570E-03
105	0.981964E+00	0.143078E+00	0.918179E-01	0.827379E-01	0.274111E-05	0.156527E-02	-0.125839E-02	-0.134267E-02
113	0.827039E+00	0.230172E-01	0.311790E-01	-0.560805E+00	0.718793E-03	-0.496761E-03	0.334419E-03	0.105817E-02
121	0.910651E+00	-0.189041E-01	0.100492E+00	0.400323E+00	-0.957799E-03	0.288409E-02	0.430245E-03	0.220698E-02
129	0.991928E+00	0.178851E-01	0.115443E+00	-0.493093E-01	0.250492E-03	0.611657E-03	-0.124681E-02	0.234184E-02
137	0.481554E+00	0.525192E-01	-0.121076E-01	0.874757E+00	-0.122040E-02	-0.237523E-02	0.274511E-02	0.852428E-03

RADIAL DISTRIBUTION FUNCTIONS AVERAGED OVER 200 CONFIGURATIONS RESOLUTION = 5.468750E-12 M

RADIUS (NM)	RDF(1)	RDF(2)	RDF(3)	RDF(4)	RDF(5)	RDF(6)
0.002734	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.013672	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.024609	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.035547	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.046484	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.057422	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

0.615234	0.540811	0.564891	4.022502	0.739344	1.501958	1.068465
0.626172	0.672651	1.111772	5.120167	0.790802	1.385397	0.972081
0.637109	0.634921	1.712764	4.512433	0.841274	1.251989	0.931392
0.648047	0.446414	1.956896	2.803530	0.833626	1.228469	0.916413
0.658984	0.240700	1.638298	1.154588	0.789623	1.240598	0.908882
0.669922	0.276131	0.961988	0.368920	0.695483	1.268800	0.952154
0.680859	0.874147	0.394502	0.087306	0.642893	1.195413	0.977327
0.691797	1.570092	0.124580	0.017123	0.682074	1.104096	0.991864

ORIENTATIONAL ORDER PARAMETERS Y(L,M) AVERAGED OVER 200 CONFIGURATIONS. SITE NUMBER 3

	0	1	2	3	4	5	6	7	8	9	10	11	12
0	0.2821	-0.0356	0.0000	0.0314	0.0000	-0.0272	0.0000	0.0234	0.0000	-0.0202	0.0000	0.0176	0.0000
1	0.0000	-0.0018	-0.0022	0.0000	0.0032	0.0000	-0.0036	0.0000	0.0037	0.0000	-0.0036	0.0000	0.0035
2	-0.1806	0.0000	-0.2981	0.0304	0.0000	-0.0227	0.0000	0.0180	0.0000	-0.0146	0.0000	0.0120	0.0000
3	0.0000	-0.0014	0.0000	0.0041	0.0034	0.0000	-0.0040	0.0000	0.0040	0.0000	-0.0038	0.0000	0.0036
4	0.1480	0.0000	0.1401	0.0000	0.2629	-0.0253	0.0000	0.0177	0.0000	-0.0132	0.0000	0.0101	0.0000
5	0.0000	0.0024	0.0000	0.0020	0.0000	-0.0060	-0.0039	0.0000	0.0041	0.0000	-0.0039	0.0000	0.0035
6	-0.1249	0.0000	-0.1011	0.0000	-0.1146	0.0000	-0.2143	0.0193	0.0000	-0.0129	0.0000	0.0091	0.0000
7	0.0000	-0.0031	0.0000	-0.0030	0.0000	-0.0022	0.0000	0.0074	0.0038	0.0000	-0.0038	0.0000	0.0034
8	0.1063	0.0000	0.0779	0.0000	0.0763	0.0000	0.0893	0.0000	0.1623	-0.0132	0.0000	0.0084	0.0000
9	0.0000	0.0035	0.0000	0.0035	0.0000	0.0031	0.0000	0.0020	0.0000	-0.0082	-0.0036	0.0000	0.0033
10	-0.0914	0.0000	-0.0614	0.0000	-0.0545	0.0000	-0.0556	0.0000	-0.0655	0.0000	-0.1145	0.0076	0.0000
11	0.0000	-0.0037	0.0000	-0.0037	0.0000	-0.0034	0.0000	-0.0028	0,0000	-0.0015	0.0000	0.0084	0.0035
12	0.0794	0.0000	0.0492	0.0000	0.0401	0.0000	0.0371	0.0000	0.0382	0.0000	0.0448	0.0000	0.0757

ORIENTATIONAL ORDER PARAMETERS Y(L,M) AVERAGED OVER 200 CONFIGURATIONS. SITE NUMBER 4

	0	1	2	3	4	5	6	7	8	9	10	11	12
0	0.2821	-0.2249	0.0000	0.2001	0.0000	-0.1697	0.0000	0.1436	0.0000	-0.1222	0.0000	0.1051	0.0000
1	0.0000	0.0026	-0.0099	0.0000	0.0117	0.0000	-0.0116	0.0000	0.0110	0.0000	-0.0101	0.0000	0.0091
2	-0.3124	0.0000	-0.2982	0.1919	0.0000	-0.1411	0.0000	0.1064	0.0000	-0.0817	0.0000	0.0637	0.0000
3	0.0000	-0.0057	0.0000	-0.0064	0.0173	0.0000	-0.0160	0.0000	0.0138	0.0000	-0.0115	0.0000	0.0093
4	0.2671	0.0000	0.2368	0.0000	0.2635	-0.1612	0.0000	0.1069	0.0000	-0.0733	0.0000	0.0513	0.0000
5	0.0000	0.0059	0.0000	0.0100	0.0000	0.0109	-0.0226	0.0000	0.0178	0.0000	-0.0134	0.0000	0.0099
6	-0.2268	0.0000	-0.1745	0.0000	-0.1868	0.0000	-0.2156	0.1265	0.0000	-0.0767	0.0000	0.0478	0.0000
7	0.0000	-0.0053	0.0000	-0.0090	0.0000	-0.0139	0.0000	-0.0150	0.0250	0.0000	-0.0170	0.0000	0.0114
8	0.1935	0.0000	0.1324	0.0000	0.1239	0.0000	0.1386	0.0000	0.1640	-0.0919	0.0000	0.0506	0.0000
9	0.0000	0.0045	0.0000	0.0077	0.0000	0.0115	0.0000	0.0168	0.0000	0.0179	-0.0242	0.0000	0.0145
10	-0.1665	0.0000	-0.1021	0.0000	-0.0851	0.0000	-0.0835	0.0000	-0.0953	0.0000	-0.1160	0.0608	0.0000
11	0.0000	-0.0037	0.0000	-0.0065	0.0000	-0.0093	0.0000	-0.0129	0.0000	-0.0182	0.0000	-0.0189	0.0207
12	0.1446	0.0000	0.0797	0.0000	0.0594	0.0000	0.0520	0.0000	0.0521	0.0000	0.0600	0.0000	0.0761

ORIENTATIONAL ORDER PARAMETERS Y(L,M) AVERAGED OVER 200 CONFIGURATIONS. SITE NUMBER 5

	0	1	2	3	4	5	6	7	8	9	10	11	12
0	0.2821	0.2605	0.0000	-0.2322	0.0000	0.1975	0.0000	-0.1673	0.0000	0.1425	0.0000	-0.1223	0.0000

1	0.0000	-0.0008	-0.0037	0.0000	0.0036	0.0000	-0.0028	0.0000	0.0020	0.0000	-0.0014	0.0000	0.0010
2	-0.3127	0.0000	-0.2983	-0.2213	0.0000	0.1619	0.0000	-0.1212	0.0000	0.0921	0.0000	-0.0708	0.0000
3	0.0000	0.0021	0.0000	0.0011	0.0053	0.0000	-0.0037	0.0000	0.0021	0.0000	-0.0011	0.0000	0.0005
4	0.2660	0.0000	0.2386	0.0000	0.2636	0.1845	0.0000	-0.1209	0.0000	0.0818	0.0000	-0.0564	0.0000
5	0.0000	-0.0013	0.0000	-0.0020	0.0000	-0.0004	-0.0051	0.0000	0.0026	0.0000	-0.0010	0.0000	0.0003
6	-0.2249	0.0000	-0.1756	0.0000	-0.1905	0.0000	-0.2153	-0.1434	0.0000	0.0859	0.0000	-0.0531	0.0000
7	0.0000	0.0004	0.0000	0.0004	0.0000	0.0009	0.0000	-0.0014	0.0035	0.0000	-0.0013	0.0000	0.0003
8	0.1910	0.0000	0.1331	0.0000	0.1269	0.0000	0.1440	0.0000	0.1634	0.1036	0.0000	-0.0572	0.0000
9	0.0000	0.0004	0.0000	0.0008	0.0000	0.0008	0.0000	0.0006	0.0000	0.0037	-0.0015	0.0000	0.0002
10	-0.1634	0.0000	-0.1024	0.0000	-0.0876	0.0000	-0.0880	0.0000	-0.1019	0.0000	-0.1156	-0.0698	0.0000
11	0.0000	-0.0010	0.0000	-0.0015	0.0000	-0.0016	0.0000	-0.0016	0.0000	-0.0018	0.0000	-0.0057	-0.0002
12	0.1411	0.0000	0.0797	0.0000	0.0616	0.0000	0.0557	0.0000	0.0574	0.0000	0.0674	0.0000	0.0767

AVERAGE PARTICLE POSITIONS AND RMS DEVIATIONS

1	-0.83351725E+00	-0.58628266E+00	-0.50082247E+00	0.14202537E-01	0.10685587E-01	0.15147869E-01
9	0.49892811E+00	-0.58391728E+00	0.16660782E+00	0.16765781E-01	0.11500624E-01	0.12924539E-01
17	-0.16826078E+00	0.41106822E+00	0.83114013E+00	0.16714720E-01	0.84399942E-02	0.15247243E-01
25	-0.83662502E+00	-0.91517312E+00	-0.16834562E+00	0.13741198E-01	0.12259206E-01	0.15856259E-01
33	0.50353395E+00	-0.91678092E+00	0.50244771E+00	0.10609922E-01	0.15089063E-01	0.83015304E-02
41	0.16483859E+00	0.57990495E+00	-0.83298883E+00	0.11552814E-01	0.10752303E-01	0.13647366E-01
49	-0.49517374E+00	-0.42347770E+00	0.50020274E+00	0.14657787E-01	0.18422416E-01	0.10016447E-01
57	0.83684845E+00	-0.83535289E-01	-0.50212130E+00	0.10780643E-01	0.13590928E-01	0.13719806E-01
65	0.16514858E+00	0.91502944E+00	0.16420051E+00	0.19031200E-01	0.15732923E-01	0.13523146E-01
73	-0.83507015E+00	-0.25535694E+00	-0.99803604E+00	0.13215039E-01	0.12097671E-01	0.12367193E-01
81	0.50545763E+00	-0.25170509E+00	-0.33578828E+00	0.17461902E-01	0.14133891E-01	0.10161392E-01
89	-0.16843725E+00	0.74423083E+00	0.34058946E+00	0.12495550E-01	0.12751971E-01	0.15798092E-01
97	-0.82682630E+00	-0.25755641E+00	-0.36701672E-02	0.16751932E-01	0.13177847E-01	0.13296891E-01
105	0.50143644E+00	-0.25444809E+00	0.66706910E+00	0.24193982E-01	0.14995333E-01	0.12640501E-01
113	0.16569719E+00	0.24579520E+00	-0.10025345E+01	0.14904043E-01	0.99483118E-02	0.12676852E-01
121	-0.49726543E+00	-0.75866153E+00	0.33224561E+00	0.17641985E-01	0.14404707E-01	0.15138341E-01
129	0.83357875E+00	-0.75559940E+00	-0.66363742E+00	0.17342280E-01	0.14783291E-01	0.11050461E-01
137	0.16465472E+00	0.24452826E+00	-0.53764551E-02	0.14332357E-01	0.17219966E-01	0.14765446E-01

ANALYSIS OF CRYSTAL STRUCTURE

BASED ON 3 2 3 ENFOLDING

NUMBER OF BASIS SITES IN UNIT CELL = 8

SITE	NAVG	SX-COORD	SY-COORD	SZ-COORD	X-RMS ERR	Y-RMS ERR	Z-RMS ERR
1	18	0.250003	0.413240	0.749053	0.022527	0.012565	0.020875
2	18	0.250292	0.079726	0.250468	0.021727	0.012590	0.019976
3	18	0.750631	0.579783	0.249178	0.021642	0.013437	0.020692
4	18	0.750669	0.913407	0.749764	0.023481	0.013130	0.019511
5	18	0.250303	0.746503	0.000242	0.022851	0.013214	0.021808
6	18	0.250489	0.746922	0.500363	0.022203	0.013617	0.021267
7	18	0.748866	0.246231	0.000220	0.023209	0.013959	0.019997

8 18 0.749337 0.246372 0.500144 0.021366 0.013599 0.019742

BRAGG PLANE PROJECTION

L M N	STR.FAC	L M N	STR.FAC
0 0 6	71.8378	0 0 6	71.6729
0 4-6	18.1946	0 4-6	71.5500
0 4-3	53.7403	0 4-3	0.0002
0 4 0	18.0757	0 4 0	71.9321
0 4 3	53.9138	0 4 3	0.0002
0 4 6	17.8776	0 4 6	71.6606
0 8-6	17.5405	0 8-6	71.2930
0 8-3	54.0233	0 8-3	0.0008
0 8 0	17.7497	0 8 0	71.7289
0 8 3	53.8846	0 8 3	0.0010
0 8 6	17.8765	0 8 6	71.5131
3-6-6	71.6192	3-6-6	71.5020
3-6 0	71.7534	3-6 0	71.7481
3-6 6	71.5643	3-6 6	71.3423
3-2-6	18.0227	3-2-6	71.5663
3-2-3	53.8735	3-2-3	0.0000
3-2 0	17.8990	3-2 0	71.8680
3-2 3	54.0267	3-2 3	0.0000
3-2 6	17.6933	3-2 6	71.5167
3 2-6	17.7443	3 2-6	71.4955
3 2-3	53.9743	3 2-3	0.0002
3 2 0	17.9466	3 2 0	71.8525
3 2 3	53.8145	3 2 3	0.0003
3 2 6	18.0693	3 2 6	71.5565
3 6-6	71.5503	3 6-6	71.2903
3 6 0	71.7303	3 6 0	71.7015
3 6 6	71.5872	3 6 6	71.4611
6-8-6	17.7291	6-8-6	71.0828
6-8-3	53.6380	6-8-3	0.0002
6-8 0	17.6013	6-8 0	71.3024
6-8 3	53.7699	6-8 3	0.0001
6-8 6	17.3893	6-8 6	70.8742
6-4-6	17.8275	6-4-6	71.1984
6-4-3	53.5555	6-4-3	0.0000
6-4 0	18.0217	6-4 0	71.4735
6-4 3	53.3757	6-4 3	0.0000
6-4 6	18.1396	6-4 6	71.0991
6 0-6	71.4166	6 0-6	71.1799
6 0 0	71.5688	6 0 0	71.5102
6 0 6	71.3985	6 0 6	71.1906
6 4-6	18.0314	6 4-6	71.0272
6 4-3	53.4619	6 4-3	0.0010
6 4 0	17.9123	6 4 0	71.4120
6 4 3	53.6276	6 4 3	0.0011

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 6 4 6   17.7124 6 4 6   71.1476
 6 8-6   17.4829 6 8-6   70.7413
 6 8-3   53.6279 6 8-3    0.0021
 6 8 0   17.6872 6 8 0   71.1794
 6 8 3   53.4837 6 8 3    0.0023
 6 8 6   17.8120 6 8 6   70.9703

TIME ELAPSED SINCE JOB START =   2123.77368164 SECONDS
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