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NOTATION (Used for data input)

Throughout the manual the following notation is used.

- F The user must supply a floating point number in F format (Note that E format is not permitted).
- I The user must supply an integer.
- A The user must supply a character constant. Only the first four characters will be interpreted.
- F,I In some parts of the input dataset, the user has a choice of a real number or an integer.
- <...>Optional parameters are enclosed in angle brackets.
- *Italic script* will be used for items in the printed output which depend on the input dataset.

INTRODUCTION

This document describes the data input to the DMAREL computer program. An outline of a typical calculation will now be described. Normally the user will use the preprocessor NEIGHBOURS to write an input file template. This manual does describe how to write an input file for DMAREL without using NEIGHBOURS, although the user will not be able to use symmetry in this case. Data describing the unit cell is first read in. All data must be supplied in orthonormal coordinates rather than conventional crystallographic coordinates. Next atom atom potentials are read in which model the crystal structure. The perfect lattice is then modelled using this potential.

The most expensive part of the calculation in terms of computer time is usually the calculation of the gradients of the energy. These are calculated at every iteration of the energy minimisation. The minimisation uses a Hessian update algorithm, hence the second derivative matrix need only be calculated and inverted once. The matrix inversion step may be expensive for large unit cells This is because the inversion increases as N^3 , whereas the gradient and matrix calculation increase as approximately N^2 .

PRELIMINARY COMMENTS

DATA INPUT

DMAREL uses a free format input processor. Each line of data is read in as characters, which make up a number of data fields separated by one or more spaces. By default 80 characters per line are read in, although

this may be reduced using the IREC directive. The characters are then interpreted as literal (character string) constants, integers or real numbers. Literals are input as a string of characters of which at least one must be alphabetic. There cannot be any embedded spaces in the constant. Only the first four characters will be interpreted by the program. This is important when assigning names to atoms, as names of different atoms must differ in the first four characters of the name for the name to be unique. For determining which short range potential to use, only the first two characters are used.

Integer constants are input as a signed or unsigned integer, which again must not contain any embedded spaces.

Real constants may only be input in the F format, and the E format is prohibited. A real constant will therefore consist of an optional sign, followed by a floating point number containing a decimal point. Again there should be no embedded spaces, and the . should always be included.

There is no end of record error message, so that attempting to read past the end of a line will not cause an error. If the program tries to read a literal constant and there are no more data fields in the record, four blank characters are input. Similarly for an integer the value 0 is input and for a real number the value 0.0.

Error Messages

INPUT ERROR TYPE 1

The input processor encountered an invalid character in an integer data field.

INPUT ERROR TYPE 2

The input processor encountered an invalid character in a real data field.

These are both non-fatal errors, the program may carry on in order to try to find further errors.

END OF INPUT DATASET ENCOUNTERED. PROGRAM TERMINATING

This is a fatal error - the input dataset is too short.

THE INPUT PROCESSOR

The DMAREL input dataset consists of a number of steps each containing one or more directives which together form the main menu of the program. Each directive consists of a four character keyword. Each of these directives may have data read in from the same record, or may instruct the program to read in further records before the next directive. These further records may consist of data, or they may be sub-directives instructing the program to choose one of several paths from a separate menu. For example, the potential input step has one directive, POTE, which instructs the program to read in potential information from subsequent records. The potential information is read in using a separate menu and records containing the data. The potential input menu contains a directive ENDS which instructs the program to return to the main menu. Care is needed in ordering the directives not to put a directive in the wrong place, for example a directive from the

main menu when a sub-directive from the potential input menu is expected. Any errors detected in the input processor may not necessarily cause the program to stop immediately to allow inexperienced users to find several errors in one run. A blank record is ignored if it is encountered when a directive from the main menu was expected, but not elsewhere. The steps in a DMAREL job are outlined in table in the order in which they should be run, together with the directives from the main menu used in each step. A number of the directives are redundant but are kept for compatibility or future developments. The main menu directives MOLE and STAR PLUT both have large sub-menus of directives.

Table: JOB STEPS IN A DMAREL JOB.

JOB STEP	DIRECTIVES	COMMENTS
TITLE	TITL	Optional
DYNAMIC MEMORY SETUP	DIME	Redundant
CUTOFFS	CUTO, RDMA	Mandatory
DEFAULT PARAMETER CHANGES	IREC, DUMP, PRIN,	Optional
	ACCU, ACCM,	
	CHGC, SCAL, CLUS	
	SYMM, FDAT, ZVAL	
UNIT CELL SETUP	LATT	Mandatory.
	BASI	Order of directives
		must not be varied.
POTENTIAL INPUT	POTE	Mandatory
	ENDS	
MOLECULE INPUT	MOLE	Mandatory
	ENDS	
UNIT CELL	THBO	For future development
THREE-BODY SETUP	ENDS	
UNIT CELL	TORS	For future development
TORSION SETUP	ENDS	
PERFECT LATTICE	STAR PLUT	
CALCULATION		
STOP	STOP	

Redundant options	REDU, WRDU, FREE	
	PLDU, PLRE	
	NOIO, SMIV, JOBT	
	GAME, BLEN, PT13	
	TEST, TEMP, RANG	
	INFO, DEFS	
	CUBI, HEXA, REGI	
	OPTI, THER, DEFE	
	REST, REGN, DBAS	
	RESE, REWI, PLOT	

The order of the job steps should not be varied, although variation from this order is permitted in certain cases. Firstly, some of the directives to change default parameters may be more conveniently placed later in the dataset. Where this is so it will be discussed in the section on the individual directives, and the default directives should otherwise always be placed where indicated. Secondly, the title step may appear more than once, anywhere in the sequence given above.

Error Messages

UNIDENTIFIED DIRECTIVE FOUND IN INPUT DATA. THE INPUT LINE IS AS FOLLOWS.

This error does not cause the program to stop immediately. Further errors will be sought before the program stops. Check that the directive has been spelt correctly. Also this error message can arise if the input dataset is in the wrong order, and the input processor attempts to process either data or a directive from one of the sub-menus as a directive from the main menu.

SYMMETRY

This section is intended to briefly describe how symmetry is used in DMAREL. Firstly we will discuss some of the problems that can arise if symmetry is not used.

If no iterations are carried out there will be no problems. However, if perfect lattice iterations are carried out a number of problems can arise. In principle, the perfect lattice calculation will conserve the space group symmetry of the input unit cell. In practice, rounding errors can permit the symmetry to change, although this rarely happens. Secondly, the perfect lattice relaxation is always carried out keeping the first molecule centre of mass fixed. This is to remove the translational invariance of the force constant matrix. The fixing of the first molecule centre of mass has important consequences for the symmetry. For example, this position may be related to a second by a two-fold axis. Relaxing the perfect lattice will relax these two positions keeping the first one fixed, so that the two-fold axis will move. It is possible that this two-fold axis initially passes

through the point group origin, but will not after relaxation. A symmetry-constrained DMAREL relaxation will be carried out by including the keyword SYMM, however NEIGHBOURS must be used to write the symmetry information file.

CUTOFFS

The short range interactions which are calculated in DMAREL are controlled by two cutoffs, CUTPOT and RDMA

The cutoffs are used with the range parameters on the input potentials. The potentials may be input over a number of ranges, although usually only one range is used. The parameter defining the ranges is intended primarily as a separation of two ranges and not as a cutoff of the potential. Therefore the maximum range of the potential is always overridden by the value of CUTPOT. Thus if the maximum range is greater than CUTPOT, then interactions will only be calculated out to CUTPOT. If the maximum range is input as a value less than CUTPOT, its value is redefined and set to a value larger than CUTPOT.

JOB STEPS IN DMAREL

TITLE SECTION

The title step has only one directive, TITL.

TITL

Operands None

This directive instructs the program to read in and print a heading on the line printer output. Subsequent records will be read in and printed out exactly as input. The title is terminated with a record with the single word ENDS, which returns control to the main menu of the program. TITL directives may appear anywhere where a main menu directive can appear, but cannot be embedded in data.

DYNAMIC MEMORY ALLOCATION

The dynamic memory section has only one directive, DIME, which must appear immediately after the title. It is currently not used.

DIME

Operand type I

Operand name MAXCOR

The DIME directive instructs the program to call the dynamic memory allocation subroutine.

Printed output

The dynamic memory routine produces output both when it is called, and later in the program when messages related to memory size are printed.

LENGTH OF ARRAY ISPACE IS *Int1* WORDS

Error messages

An error message is produced if the perfect lattice step does not have sufficient memory to run. The message is

THIS DATASET NEEDS ISPACE = *Int* WORDS

Recompile the program with the array ISPACE increased to the indicated size *Int*

DEFAULT PARAMETER CHANGES

All of these directives are optional. They may be subdivided into three classes.

Printed output	DUMP, PRIN
Program control	IREC, ACCU, ACCM, CHGC, SCAL, CLUS, SYMM, FDAT, ZVAL

PRINTED OUTPUT

DUMP

Operand type	I
Operand name	IDUMP

This is used in conjunction with the PRIN directive discussed below. IDUMP may have values 1 or 2. IDUMP = 1 produces output which may be useful if an error is suspected in the input dataset. IDUMP = 2 produces output useful for diagnostic purposes only.

PRIN

Operand types	A	I	[A I]
Operand names	APRINT	MPRINT	

The APRINT name defines certain sections of the program for which additional printed output is required. The integers MPRINT define exactly what is printed. There are currently 17 print options for DMAREL. Each of these will now be described in detail

LATT**0**

No output

> 0

The reciprocal lattice vectors are printed in the output.

Default 0

BASI**0**

Print:

Basis species as input

Origin of the basis

> 0

In addition, print:

The basis species after shift of origin

The basis species after sorting into internal program order

< 0

Suppress printing of the basis species

Default 0

REG1 REG2 RECI SYMM CLAS STRU MATR ENGY POTE PHON EPRS

These switches are redundant in DMAREL

PLUT

MPRINT is a 5 digit integer, with each digit controlling a different section of the perfect lattice calculation. Numbering the digits from the right (units digit) to left the digits have the following values and meanings.

Digit 1**0**

No output

1

List the contributions to the lattice energy and the atom forces before the first iteration and after the last iteration.

2

List the contributions to the lattice energy after each iteration.

Digit 2

As for digit 1 but listing the elastic constant tensors.

Digit 3**0**

No output

Digit 4**0**

No output

1

List the force constant matrix and gradient vector before the first cycle and after the last cycle.

2

List the force constant matrix and gradient vector on every cycle of the perfect lattice iteration.

3

List the gradient vector only before the first cycle and after the last cycle

4

List the gradient vector only on every cycle

The force constants are scaled in internal program units. To convert to $(\text{eV } \text{\AA})^{-2}$ they must be multiplied by $14.3997584/RLAT^3$, where RLAT is the lattice constant. The gradients must be scaled by $14.3997584/RLAT^2$.

Digit 5

0

No output

1

Currently not used, formerly used to print the Madelung and short range energies of each particle. (Use CCLS instead)

Default 00011

MINI

0

No output

1

Print information about progress of the minimisation.

Default 0

BOND

This APRINT option is retained for future use, it is only relevant for a system with three-body force constants.

0

No output

1

Print the three-body bonds found in the unit cell.

Default 0

TORS

This APRINT option is retained for future use, it is only relevant for a system with torsion force constants.

0

Do not print the torsion angles found in the unit cell.

1

Print the torsion angle information

Default 0

MOLE

This APRINT option is used in DMAREL to control output from the MOLE directive.

0

Do not print molecular bonding information.

1

Print molecular bonding information

Default 1

GEOM

0

No output
1
Print molecular local axis information
Default 1

PROGRAM CONTROL

IREC

Operand type I
Operand name IRECL

The input processor reads 80 characters per card image by default. IRECL should be less than 80, and gives the number of characters read in per record.

ACCU

Operand type F
Operand name ACCLAT

ACCLAT is the limit below which numbers are taken as being equal. The default set in the program is 1.0E-06. ACCLAT is also used at various other points in the program for testing small quantities.

ACCM

Operand type F
Operand Name ACCMAD

This directive changes the accuracy to which the Ewald sum is carried out. The default is 1 part in 10^{**6} (Default value of ACCMAD = 1000000.0). Setting a larger value of ACCMAD may change the perfect lattice properties slightly. It should also be noted that a larger value of ACCMAD will set a larger lattice sum cutoff.

CHGC

Operands None

The programs checks that the unit cell is neutral and will stop if this is not so. Including the directive CHGC forces the program to continue with a non-neutral cell. DMAs generated by SCF programs often have a small residual charge, so this directive should be included.

ADDITIONAL INPUT/OUTPUT

The table gives a list of the additional FORTRAN unit numbers used by DMAREL. Output is produced by default to fort.8, fort.12, fort.13, fort.15, and fort.16.

Table: ADDITIONAL FORTRAN UNIT NUMBERS USED BY PROGRAMS

DIRECTIVE	UNIT	NATURE OF I/O	USE
STAR PLUT	8	FORMATTED WRITE	Provides an updated set of lattice and basis vectors from the perfect lattice relaxation
Default	12	FORMATTED WRITE	Summary file written to fort.12
Default	13	FORMATTED WRITE	Final cell written to fort.13
Default	15	FORMATTED WRITE	Final output in FDAT format
Default	16	FORMATTED WRITE	Final output in SHELX format
CCLS	17	FORMATTED WRITE	Output close contact list to fort.17
SYMM	20	FORMATTED READ	Read the symmetry information file fort.20 written by NEIGHBOURS
R2ND	30	FORMATTED READ/WRITE	Temporary file used for restart runs.

UNIT CELL SETUP

This section reads in the unit cell. Three directives must be given in the order (For DMAREL)

CUTO, LATT, BASI

CUTOFFS

CUTO

Operand types	F	F	F	F
Operand names	RLAT	CUTPOT	CUTSHL	ACCTH
Operand types (continued)	F	< F >		
Operand names (continued)	CUTTH	KMAX		

RLAT

This gives the lattice constant in Å. (See LATT and BASI directives and the examples following). Certain quantities are input in units of RLAT, referred to as lattice units.

CUTPOT

This gives the short range potential cutoff in lattice units. CUTPOT should not be equal to an interatomic distance in the crystal. This is because the test in the perfect lattice calculation may find one bond but leave out a symmetry related bond, giving perfect lattice tensor properties of the wrong symmetry. Usually it is safe just to ensure that CUTPOT does not equal an integral number of lattice vectors. (i.e. that CUTPOT is not an integer).

CUTSHL

This is not used by DMAREL

ACCTH

This operand retained for future use, but is not used at present. Its value is ignored if the calculation does not use three-body forces. It gives the maximum permitted deviation of a bond angle from the value input on the BOHA sub-directive of the POTE directive. This maximum deviation is applied in the perfect lattice step to check that no spurious three-body interactions have been generated by the THBO directive.

CUTTH

This operand retained for future use, but is not used at present.

KMAX

This operand retained for future use, but is not used at present. It gives the maximum magnitude of a phonon wavevector used for a calculation.

Printed output

C-vector magnitude= *RLAT* Angstroms Cut off for short range potentials = *Cutpot* Angstroms

RDMA

Operand Type F
Operand Name RDMA

This gives the cutoff in lattice units for the higher multipoles.

SCAL

Operand Type F
Operand Name SCALQQ

The charge and multipole interactions will be scaled by the factor SCALQQ

SYMM

Operands None

Instructs DMAREL to read in the symmetry input file fort.20 which was written by NEIGHBOURS.

FDAT

Operands None

Instructs DMAREL to read in the symmetry input file fort.20 which was written by NEIGHBOURS, but not to switch on symmetry for this run. This option is useful for producing a final relaxed structure dataset from a run with no symmetry.

ZVAL

Operand Type I

Operand Name ZVAL

ZVAL is the user defined number of formula units per cell, used to calculate energies in kilojoules per mole. If ZVAL is not supplied, DMAREL will try to read it from the fort.20 file.

LATTICE VECTOR INPUT

LATT

Operands none

This directive is required. The LATT directive instructs the program to call the lattice vector input routine. Usually the calculations described below will be carried out by the preprocessor NEIGHBOURS. This reads in three records. The format of each record is

3F

Each record refers to one lattice vector, and gives the orthonormal \mathbf{x} , \mathbf{y} , \mathbf{z} coordinates of the lattice vectors.

The orthonormal lattice vector components must be given to a sufficiently high precision for all the symmetry elements of the lattice point group to be found. By default, at least seven significant figures must be given, unless the ACCU directive is used. (See examples after the BASI directive).

The following section describes how to calculate orthonormal lattice vectors from the conventional crystallographic unit cell. Firstly the general case will be given, although this should normally only be used for triclinic and monoclinic unit cells. The matrix given below (the normalising matrix \mathbf{N}) defines an orthonormal coordinate system with the \mathbf{z} axis parallel to the crystallographic \mathbf{c} axis, the \mathbf{x} axis parallel to the reciprocal \mathbf{a} axis and the \mathbf{y} axis forming a right-handed set with \mathbf{x} and \mathbf{z} . The matrix is normalised so that one unit = the crystallographic c spacing. This value should therefore be used for the value RLAT on the REGI directive.

$$\mathbf{N} = \begin{matrix} 1/(\mathbf{a}^* \times c) & 0 & 0 \\ \frac{a \times (\cos \gamma - \cos \alpha \times \cos \beta)}{c \times \sin \alpha} & \frac{b \times \sin \alpha}{c} & 0 \\ \frac{a \times \cos \beta}{c} & \frac{b \times \cos \alpha}{c} & 1 \end{matrix}$$

The unit cell is defined by three cell lengths a , b , c , and by three angles α , β , γ . a^* above is the length of the reciprocal a lattice vector. A general expression for the length of a^* is

$$a^* = b \times c \times \sin \alpha / V$$

$$V = 2 \times a \times b \times c \times \sqrt{\sin s \times \sin(s - \alpha) \times \sin(s - \beta) \times \sin(s - \gamma)}$$

$$s = (\alpha + \beta + \gamma) / 2$$

Whilst this matrix will work for any crystal, care is needed if comparison is to be made with perfect lattice tensor properties. (Elastic and dielectric constants). These will have been measured with respect to an orthogonal coordinate system which is not necessarily the same as that given above. Reference to the experimental papers may be necessary to find out the coordinate system used to measure the tensor properties. The above matrix should be used for triclinic and monoclinic crystals. For tetragonal, orthorhombic and cubic crystals a simpler matrix is used, which defines \mathbf{x} parallel to \mathbf{a} instead of \mathbf{a}^* .

$$\mathbf{N} = \begin{matrix} a/c & 0 & 0 \\ 0 & b/c & 0 \\ 0 & 0 & 1 \end{matrix}$$

For trigonal and hexagonal crystals, \mathbf{x} is again defined parallel to \mathbf{A} giving the matrix

$$\mathbf{N} = \begin{matrix} a/c & -a/2c & 0 \\ 0 & \sqrt{3} \times a/2c & 0 \\ 0 & 0 & 1 \end{matrix}$$

The normalising matrix \mathbf{N} defined above will transform any vector defined in crystallographic units into

orthonormal coordinates. The vector may be a unit cell vector or a basis atom vector. If the unit cell is primitive, (P), the unit cell vectors in crystallographic coordinates are simply given by the identity matrix.

$$L = \begin{matrix} & a & b & c \\ \begin{matrix} 1 \\ 0 \\ 0 \end{matrix} & 1 & 0 & 0 \\ & 0 & 1 & 0 \\ & 0 & 0 & 1 \end{matrix}$$

Multiplying this by the normalising matrix N forms the orthogonal lattice vectors $O = N \bullet L$. Hence the columns of the normalising matrix given above are the lattice vectors needed by DMAREL. Note that the input to DMAREL and the printed output from DMAREL give the lattice vectors in rows, so the normalising matrix given above will be transposed.

If the unit cell is centred, then the centred lattice vectors should be used. It is recommended that this is always done. The non-primitive cell may be used, and the same answers will be produced. However there will be more basis atoms per unit cell if this is done, and the perfect lattice calculation will take correspondingly longer to run. The centred lattice vectors in crystallographic units may conveniently be taken as the columns of the matrices L given in table . (Other choices are possible).

Table: LATTICE VECTORS FOR CENTRED CELLS

Centring type		A			B			C	
A		1			0			0	
		0			1			1/2	
		0			0			1/2	
B		1			0			1/2	
		0			1			0	
		0			0			1/2	
C		1			1/2			0	
		0			1/2			0	
		0			0			1	
I		-1/2			1/2			1/2	
		1/2			-1/2			1/2	
		1/2			1/2			-1/2	
F		0			1/2			1/2	
		1/2			0			1/2	
		1/2			1/2			0	

R		2/3			-1/3			-1/3	
		1/3			1/3			-2/3	
		1/3			1/3			1/3	

The orthonormal lattice vectors required by DMAREL are then formed by the matrix product $\mathbf{O} = \mathbf{N} \bullet \mathbf{L}$. Again the matrix \mathbf{O} must be transposed to be input to DMAREL.

Printed output

The lattice vectors are always printed by default. They are printed in rows, with the $\mathbf{x}, \mathbf{y}, \mathbf{z}$ components of each lattice vector in each row. If PRIN LATT MPRINT with MPRINT=1 is used, the reciprocal lattice vectors are also printed, again in rows.

Error messages

ERROR - THE LATTICE VECTORS ARE COPLANAR

This is a fatal error. The program decided that the lattice vectors are coplanar by working out the volume of the unit cell, which is equal to the determinant of the lattice vector matrix. This is tested to see if it is greater than ACCLAT (see ACCU directive).

ERROR - LATTICE VECTOR N INCORRECTLY READ.

A fatal error, there is a format error on the Nth lattice vector input record.

BASIS ATOM INPUT

DATA INPUT

BASI

Operands none

The BASI directive instructs the program to call the basis atom input routine. Usually the calculations described below will be carried out using the preprocessor NEIGHBOURS. This reads in further records, which have one of three possible formats

Card format 2A 3F < I >

	Species label	species coordinates	Optional molecule number
Card format	A	3F	
	CENT	Point group origin	
Card format	A		
	ENDS		

Only one CENT and ENDS record is permitted. The CENT record defines the basis origin. This record is not required for DMAREL, it may be omitted, in which case the basis origin is taken as the point 0.0 0.0 0.0. The ENDS record must be the last record, and instructs the subroutine to return to the main menu of directives.

There may be any number of species records up to a maximum of 500 (this includes the CENT record if present). The species label consists of two A4 fields (separated by a space). The first A4 field contains a species name, which must be unique for each atom type. (For example: NA+ CL- AL3+). The first two characters of the species name define the atom type for the short range potentials. If the third character is I, this indicates that the atom is part of a molecule related by an inversion centre to another molecule in the system. The second field contains the word CODA indicating that the species is an atom with a distributed multipole. Similar comments apply about the precision as for the lattice vectors, namely the coordinates must be given to at least 7 significant figures unless the ACCU directive has been used. The optional molecule number is used to indicate to which molecule it belongs. A value of zero, or leaving out the parameter all together, implies that intramolecular potentials will not be applied to this species, and is used for isolated ions. Isolated ions should be put at the end of the list, NEIGHBOURS will do this automatically.

The distributed multipoles must be given for the atoms.

Operand type	A I
Operand name	LEVEL ORDER

The record following the atom coordinates must begin with the keyword LEVEL or DUPL. Use LEVEL the first time an atom is encountered, use DUPL for duplications. LEVEL is followed by an integer indicating the pole order of the multipole on this atom, 0 for charge only up to 4 for hexadecapole. The ion charge is given in units of $|e|$ (The charge on the electron). The multipoles are then given in atomic units. The format is

Operand type	F
	F F F
	F F F F F
	F F F F F F F
	F F F F F F F
	F F

Operand name	CHARGE
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The operands are one charge, three dipole, five quadrupole, seven octopole and nine hexadecapole moments in the usual order. This will usually be input from the Punch file in NEIGHBOURS.

It should be noted that adding or subtracting a lattice vector, or an intergal multiple of a lattice vector, to a

basis vector will have no effect on the program. In other words, basis atoms need not all be in the same unit cell.

The basis species will be sorted into an internal program order, but this will normally be done by NEIGHBOURS. The order into which they are sorted is determined by a number of rules.

1. All atoms in molecules come before free ions.
2. All species of the same type are sorted together.

The Ewald parameter η is also calculated at this point, according to the formula

$$\eta = \left(\frac{\pi^3 \times NCOR}{V^2} \right)^{1/6}$$

where

NCOR = Number of atoms in the unit cell

VC = Volume of the unit cell in (lattice units)³.

This is used with the parameter ACCMAD (see ACCM directive) to define the cutoffs in direct and reciprocal space for the Ewald sums.

$$\text{Direct space cutoff} = f/\eta$$

$$\text{Reciprocal space cutoff} = f \times \eta / \pi$$

$$f = \sqrt{\log ACCMAD}$$

Printed output

THE BASIS SPECIES ARE AS FOLLOWS ALL QUANTITIES ARE IN LATTICE UNITS
NO. ORTHOGONAL COORDINATES LABEL MOLECULE

index x y z Label molecule

Origin of basis

The basis species and basis origin are printed as input by default. PRIN BASI -1 will suppress printing of the basis species. PRIN BASI 1 will print additionally the basis species after sorting and after the point group origin vector has been subtracted from them.

CUTOFF VALUE FOR DIRECT LATTICE SUM = X LATTICE UNITS

CUTOFF VALUE FOR RECIPROCAL LATTICE SUM = Y RECIPROCAL LATTICE UNITS

VALUES OF THE CONSTANTS USED IN THESE SUMMATIONS ARE $Z1$ $Z2$

This message is printed by default. The constants $Z1$ and $Z2$ are η and $\pi/(\eta^2 \times V)$.

Error messages

ERROR - LATTICE VECTORS NOT DEFINED BEFORE CRYSTAL BASIS

A LATT directive has been omitted or placed out of order, it should occur before the BASI directive.

ERROR - MAXIMUM OF *MAXBAS* BASIS SPECIES EXCEEDED

This error does not cause the program to terminate immediately.

ERROR - UNIDENTIFIED SPECIES IN LATTICE BASIS

A species label has been found with a second A4 field which is not CODA.

ERROR - BASIS SPECIES i AND j ARE AT EQUIVALENT LATTICE SITES.

Two basis species have been found at the same lattice site. They may be at the same lattice site translated by an integral number of lattice vectors, so the coordinates are not necessarily the same.

SHORT RANGE POTENTIAL INPUT

POTE

Operands none

This directive instructs the program to call the short range potential input routine. This routine is menu-driven with a menu of sub-directives. The sub-directives fall into seven classes: species data, short range interactions, [core-shell interactions, three-body interactions, torsion interactions, restart sub-directives] and subroutine termination. Those in [] are not relevant to this version of DMAREL but are retained for future use. The table gives the sub-directives in each class.

Table: DIRECTIVES FOR THE POTENTIAL INPUT SUBROUTINE

Directive class	Directives
-----------------	------------

Species data	SPEC, ENDS
Short range interactions	BUCK, MODI, LENN, MORS,
	BUC4, SPLI, MORQ, SPRI
	COUL, VDWA, HULB, BUC7
	NONE, BSPL
Three-body interactions	BOHA, TRID, MOLD, QART,
	SIXT, BOHZ, THRH, RRHA
Four-body interactions	TOHA

The directive order for the initial call must be

Directives	Comments
SPEC	Followed by subdirectives (See below)
Others	May be given in any order
ENDS	

The limits on the numbers of potentials etc. are determined by a number of PARAMETER statements in the FORTRAN. These limits may be reset simply by changing every occurrence of the PARAMETER statement to the new limit. The variable names and default limits are given in the table.

Table: POTENTIAL PARAMETERS LIMITS

Variable	Default	Meaning
	Value	
MAXPOT	500	Maximum permitted number of potentials
MAXRNG	10	Maximum number of ranges for each potential
MAXTHB	50	Maximum number of types of three-body bond
MAXTYP	500	Maximum number of species permitted
MAXTOR	50	Maximum number of types of torsions

Printed output and error messages from this section of the program are given below. Printed output may be suppressed using the option PRIN POTE 0 in the default parameter changes.

Printed output

START OF SHORT RANGE POTENTIAL PROCESSING

This is always output by the program.

Error messages

ERROR - INVALID DIRECTIVE GIVEN IN ABOVE LINE

The line above began with an invalid directive.

ERROR - SPECIES MUST BE READ IN BEFORE POTENTIALS

The program has read in a valid potential input directive, but the species have not yet been read in using SPEC.

ERROR - ABOVE LINE CONTAINS A SPEC DIRECTIVE - ONLY ONE IS PERMITTED

Only one SPEC directive is permitted.

SPECIES DATA INPUT

SPEC

Operands none

This should be the first directive after POTE. It instructs the program to read in the ion types. The subsequent data cards have the formats

Card format	2A	F	F
	Species label	Not used	Atomic mass
Card format	A		
	ENDS		

The species label is described in the BASI directive . The atomic mass is given in atomic mass units. A maximum of MAXTYP species may be read in. Species may be given which are superfluous to this particular job. The species input terminates with a directive ENDS, which returns control to the POTE menu of directives.

Error messages

These should be self-explanatory.

ERROR - A CORE HAS BEEN GIVEN WITH ZERO OR NEGATIVE MASS

ERROR - THE SPECIES TYPE *Lab Type* IS DUPLICATED

ERROR - THE LIMIT OF *Maxtyp* SPECIES IS EXCEEDED

ERROR - A BASIS SPECIES WITH SPECIES LABEL *Lab Type* DOES NOT HAVE A CORRESPONDING SPECIES TYPE IN THE POTENTIAL INPUT

SHORT RANGE INTERACTIONS

Short range interactions need to be given between some or all of the possible ion pairs. The short range interaction is designed to be as flexible as possible, although for DMAREL only a few options will normally be used. Different ion pairs may have different short range interaction types. The short range interactions are given in one or more ranges for each ion pair, up to a maximum of MAXRNG ranges. For each ion pair, the ranges must be contiguous and there must be a range which starts at zero. Interactions which have a different analytic form in different ranges are permitted. In this case, overlapping ranges are not permitted. However it is permitted to split one of the interactions into two ranges so that a range is the sum of two potentials. The ranges, if more than one range is given, must be in ascending order. The maximum range is at present overridden by CUTPOT. (See section on cutoffs) A maximum of MAXPOT short range interactions may be given.

The general format of a short range interaction is given below. There are three types of input records. Species records indicate the start of a new two body interaction and give the two species involved. Species records begin with a 2 character keyword indicating the type of interaction involved. Species records are also used to indicate a different potential form in a new range. An interaction may have more than one species record. Range records give the parameters for the interaction in a given range. Finally an ENDS record terminates the input for this interaction. Interactions involving more than one species record should not be split up with more than one ENDS record. The format of a species record is

```

A      A A      A A      <F,I>
KEYW LABELA LABELB Additional
                        Parameters

```

Where

KEYW

is a 4 character keyword giving the potential type. These are described in detail below.

LABELA,LABELB

are species labels in the usual format.

Additional Parameters

These are required for certain of the potential types only.

The format of a range record is

```
F ...      < F >      F
Parameters Optional RMAX
              RMIN
```

Where

Parameters

These are the parameters needed to define the short range potential. The number of parameters depends on the particular potential type, defined by **KEYW** on the species record.

RMIN and RMAX

define the minimum and maximum range for this potential. RMIN may be omitted; the program knows how many parameters there are on the record and can therefore determine whether an RMIN has been given. If RMIN is omitted, the program uses the following rules to decide which value it should have.

- If it is the first range record after a species record, the minimum range is assumed to be zero.
- If it is a subsequent range, the minimum range is taken as the maximum of the previous range.

If a second species record is given, the ranges must either coincide with ranges given after the first species record or must be new ranges, contiguous with the existing ranges but extending beyond the previous maximum. Overlapping ranges are not permitted. The limits of the ranges are given in Å so that no conversion needs to be done when the data is transferred to a different substance. (cf. the CUTPOT parameter, which is in lattice units.)

Printed output

POTENTIAL BETWEEN SPECIES *Lab1 Typ1* AND *Lab2 Typ2* WITH *Nrange* RANGES

LIST OF GENERAL INTERACTIONS

This indicates that the interaction is intermolecular.

Error messages

A number of error messages will be given here as they do not depend on the keyword given on the species record.

ERROR - INVALID POTENTIAL GIVEN IN ABOVE LINE

This error message arises immediately after range records have been read in. The program expects either an ENDS record, or a new species record with a different potential type between the same two species. Neither of these two was found. Check that an ENDS record has not been omitted.

ERROR - POTENTIAL TYPE GIVEN WITH NO RANGES

A species record was input with no range records before an ENDS record or another species record.

ERROR - IN ABOVE LINE AN INVALID SPECIES LABEL WAS GIVEN ON A POTENTIAL DIRECTIVE

The labels do not match anything given after the SPEC directive .

ERROR - EACH POTENTIAL MUST BE MADE UP OF INTERACTIONS BETWEEN THE SAME TWO SPECIES. CHECK THAT AN ENDS DIRECTIVE IS NOT MISSING

A species record immediately after a range record was found, with no intervening ENDS. The species labels must be the same as on the previous species record. Most probably a new interaction was intended and an ENDS record was omitted. If a second species record between the same species was intended, check that the species labels have been put in correctly.

ERROR - THE POTENTIAL BETWEEN THE ABOVE TWO SPECIES IS DUPLICATED. CHECK THAT AN UNNECESSARY ENDS DIRECTIVE HAS NOT BEEN INCLUDED

A species record has just been read between two species for which a previous interaction has been read in. If you want to have an interaction with two different potential types, there must not be an ENDS record after the ranges of the first potential.

ERROR - IN ABOVE LINE A MINIMUM RANGE IS SUPPLIED WHICH MUST BE ZERO FOR FIRST RANGE OF FIRST POTENTIAL VALUE READ IN IS *F* CHECK THE NUMBER OF PARAMETERS NEEDED FOR THIS POTENTIAL TYPE

The program found enough parameters on a range record to expect to have an RMIN parameter, but the value read in was not zero for the first range. Check that you have got the correct number of parameters for this potential type.

ERROR - IF MINIMUM OF RANGE IS GIVEN IT MUST BE THE SAME AS AN EXISTING MAXIMUM, VALUE IS *F*.

An RMIN parameter has been read in from the current range record. This was not the first range, and the

value of RMIN read in was different from any of the previously read in values of RMAX. This makes the ranges overlapping. Split the appropriate previous range into two.

ERROR - POTENTIALS WHOSE RANGES OVERLAP MUST HAVE IDENTICAL RANGES

A second species record has been read in followed by a range record. The RMAX value on this record is less than the current maximum from the previous potential. There may also have been an RMIN read in. In either case, the next highest RMAX value read in from the previous potential does not match the current RMAX. This makes an overlapping range.

ERROR - TOO MANY POTENTIALS READ IN, MAXIMUM NUMBER OF POTENTIALS IS *MAXPOT*.

Increase the value of MAXPOT in all PARAMETER statements in the program and recompile it.

ERROR - RANGES MUST BE GIVEN IN ASCENDING ORDER

A range record has a RMAX value which is less than the previous record.

ERROR - THE MAXIMUM OF *MAXRNG* RANGES HAS BEEN EXCEEDED

Increase the value of MAXRNG in all PARAMETER statements in the program and recompile it.

The individual keywords will now be described.

BUCK

There are no additional parameters to be read from the species record. Three parameters plus RMIN (optional) and RMAX must be read from the range records. The analytic form is

$$V(r) = A \times \exp(-r/B) - C/r^6$$

The parameters A, B and C must be read from the range record. Their units are given below

- A** is in eV
- B** is in Å
- C** is in eV Å⁶

The ranges are terminated with an ENDS record or a new species record between the same species.

Example

BUCK NA+ SHEL NA+ SHEL

7895.4 0.1709 29.06 20.0

ENDS

Printed output

BUCKINGHAM POTENTIAL $V(R) = A * \text{EXP}(-R/RHO) - C/R^{**6}$

A	RHO	C	RMIN	RMAX
<i>A</i>	<i>rho</i>	<i>C</i>	<i>RMIN</i>	<i>RMAX</i>
⋮	⋮	⋮	⋮	⋮

MODI

There is one additional parameter read in from the species record. It has format I and operand name N. The analytic form of the potential is

$$V(r) = A \times \exp(-r/B) - C/r^N$$

The exponent N is read in from the MODI record. It is assumed that N remains the same for all ranges, if there is more than one. The parameters A, B and C must be read from the range record. The units of C are given below

C
is in eV Å^N

The ranges are terminated with an ENDS record or a new species record between the same species.

Example

MODI NA+ SHEL NA+ SHEL 8

7895.4 0.1709 29.06 20.0

ENDS

Printed output

MODIFIED BUCKINGHAM POTENTIAL $V(R) = A * \text{EXP}(-R/RHO) - C/R^{**N}$.

A RHO C N RMIN RMAX

A rho C N RMIN RMAX

⋮ ⋮ ⋮ ⋮ ⋮ ⋮

LENN

There are two additional parameters read in from the species record. They have format I and operand names N and M. The analytic form of the potential is

$$V(r) = A/r^N - B/r^M$$

The exponents N and M are read in on the LENN record. It is assumed that N and M remain the same for all ranges, if there is more than one. The parameters A and B must be read from the range record. The units of A and B are given below

A

is in eV Å^N

B

is in eV Å^M

The ranges are terminated with an ENDS record or a new species record between the same species.

Example

LENN CL- SHEL CL- SHEL 12 6

8560.7 30.67 5.78 20.0

ENDS

Printed output

LENNARD-JONES POTENTIAL V(R)= A/R**N - B/R**M

A B N M RMIN RMAX

A B N M RMIN RMAX

⋮ ⋮ ⋮ ⋮ ⋮ ⋮

MORS

There are no additional parameters read in from the species record. The analytic form of the potential is

$$V(r) = A \times [1 - \exp(-B \times (r - C))]^2 - A$$

This has the energy zero offset from the conventional spectroscopic definition, which defines the energy zero at the minimum. The new definition is consistent with the other potentials, which have the energy zero at infinity. The parameters A, B and C must be read from the range record. The units of A, B and C are given below

A
is in eV
B
is in Å⁻¹
C
is in Å

The ranges are terminated with an ENDS record or a new species record between the same species.

Printed output

MORSE POTENTIAL $V(R) = A * (1.0 - \exp(-B * (R - C)))^2 - A$

```
A B C RMIN RMAX
A B C RMIN RMAX
: : : : :
```

BUC4

There are no additional parameters read in from the species record. The analytic form of the potential is

$$\begin{array}{lll}
 V(r) = A \times \exp(-r/B) & \text{for } r < r_b & \\
 V(r) = \text{Fifth order polynomial} & \text{for } r_b < r < r_m & \\
 V(r) = \text{Third order polynomial} & \text{for } r_m < r < r_a & \\
 V(r) = -C/r^6 & \text{for } r_a < r < r_{max} &
 \end{array}$$

5mm

There are 6 parameters read in from the range record. These are A, B, C, r_b , r_m and r_a . Their units are given

below

A

is in eV

B

is in Å

C

is in eV Å⁶

r

are given in Å

The ranges are terminated with an ENDS record. On input, the ranges must satisfy the condition

$$r_b < r_m < r_a$$

If r_a is less than CUTPOT, the C/r^6 term will be calculated out to CUTPOT.

The polynomials are fitted so that the functions, first derivatives and second derivatives match at r_b , r_m and r_a . At r_m the potential has a minimum so that the first derivatives of both polynomials are zero. Only one ranges record is permitted for this interaction, since all of the ranges are given on the first record. Also, this potential must not overlap an existing potential.

Printed output

4 RANGE MODIFIED BUCKINGHAM POTENTIAL

RANGE 1 V(R)= A * EXP(-R/RHO),

RANGE 2 V(R) = A5*R**5+ B5*R**4 + C5*R**3 + D5*R**2 + E5*R + F5

RANGE 3 V(R) = A3*R**3 + B3*R**2 + C3*R + D3,

RANGE 4 V(R)= -C/R**6

				RMIN	RMAX
A =	A	RHO =	RHO	RMIN	r_b
A5 =	A5	B5 =	B5	C5 =	C5
D5 =	D5	E5 =	E5	F5 =	F5
A3 =	A3	B3 =	B3	r_b	r_m
C3 =	C3	D3 =	D3	E3 =	E3
				r_m	r_a

$C = C \quad r_a \quad RMAX$

Error messages

ERROR - THE FOUR RANGE BUCKINGHAM POTENTIAL AND CUBIC SPLINE MUST NOT OVERLAP AN EXISTING POTENTIAL

ERROR - ONLY ONE PARAMETERS DIRECTIVE MUST BE GIVEN WITH THE FOUR RANGE BUCKINGHAM FORM

ERROR - THE RANGES ON THE FOUR RANGE BUCKINGHAM CARD ARE NOT GIVEN IN ASCENDING ORDER

SPLI

There are two additional parameters on the species record, but they are both optional. They have format F, with operand names SMIN and SMAX. If only one F format number is given, the program interprets it as SMAX. If both are given, the program interprets them in the order SMIN then SMAX.

A cubic spline is defined in the following way. The energies E_i at n points r_i are given. The points need not be equally spaced. A cubic polynomial is then defined, polynomial P_i being between points i and $i + 1$. There are thus $n - 1$ cubic polynomials. These are defined to be equal to E_i and E_{i+1} at r_i and r_{i+1} respectively. Also P_i and P_{i+1} will have the same first and second derivatives at r_{i+1} . A quick count of the number of parameters and equations shows that two more equations are required. These are taken to be that the second derivatives of P_1 and P_{n-1} are zero at r_1 and r_n respectively. It is also possible to define two more polynomials, which are in fact linear equations, P_0 and P_n , to be extensions of the spline beyond the points r_1 and r_n .

There are two parameters read in from the range record, E_i and r_i . E_i is in eV and r_i is in Å. The interpretation of the range records for the cubic spline potential is somewhat different to the other potentials. Usually this would be interpreted as the maximum of the range RMAX. For the cubic spline, it should be the value of r at which the energy is E . A value of RMIN is not permitted on the range record for a cubic spline. The program rearranges the input data so that it defines $n - 1$ ranges each with an RMIN and RMAX. The usual convention that the potential must start at zero also applies to the cubic spline. There are two ways of doing this. Firstly, the energy at zero may be given on the first range card. The program will define $n - 1$ ranges. If the energy at zero is not known, then input $SMIN = 0.0$ on the species record and input a value for SMAX. The program will define $n + 1$ ranges, with range 1 and $n + 1$ being the linear functions P_0 and P_n defined above. A third format is permitted, in which SMAX only is supplied. The cubic spline potential cannot have other potentials defined in the same range for the same species. It may, however, have different potential types defined in other ranges. A minimum of 3 and a maximum of $MAXRNG - 1$ records defining the energy points must be given. The RMAX parameters must be in ascending order as usual. Care is needed if the ranges do not extend as far as CUTPOT. In this case the program will extend the last range out to CUTPOT. In general, however, the energy will not tend to zero as the range is extended. This may be overcome by adding extra ranges with

zero energy.

Printed output

CUBIC SPLINE POTENTIAL $V(R) = A \cdot R^3 + B \cdot R^2 + C \cdot R + D$

A B C D RMIN RMAX E(RMIN)

A B C D RMIN RMAX E

⋮ ⋮ ⋮ ⋮ ⋮ ⋮ ⋮

Error messages

ERROR - A MINIMUM RANGE MUST NOT BE GIVEN ON A CUBIC SPLINE
PARAMETERS CARD

One of the range records has three parameters on it; the program assumes that an RMIN has been given.

ERROR - FOR CUBIC SPLINE THE FIRST PARAMETER CARD HAS A MINIMUM
RANGE ON IT. THIS MUST BE ZERO FOR FIRST RANGE OF FIRST POTENTIAL

Either no SMIN has been given on the species record and the value of r on the first range record is not zero,
or SMIN has been given but is not zero.

ERROR - THE CUBIC SPLINE MUST NOT EXCEED THE MAXIMUM NUMBER OF
RANGES -1, MAXIMUM NUMBER OF RANGES IS *MAXRNG*

ERROR - THE FOUR RANGE BUCKINGHAM POTENTIAL AND CUBIC SPLINE MUST
NOT OVERLAP AN EXISTING POTENTIAL

ERROR - THE CUBIC SPLINE MUST HAVE AT LEAST 3 RANGES, THE NUMBER
INPUT IS *N*

ERROR - THE MAXIMUM FOR THE LINEAR EXTENSION OF THE CUBIC SPLINE IS
LESS THAN THE LAST RANGE

This error message occurs when SMAX is given on the species record, but the value is less than the last
RMAX given on the range records.

MORQ

There are no additional parameters read in from the species record. The analytic form of the potential is

$$V(r) = A \times [1 - \exp(-B \times (r - C))]^2 - A - \frac{D \times Q_1 \times Q_2}{r}$$

The parameters A, B, C and D must be read from the range record. Q_1 and Q_2 are the charges on the species 1 and 2. This potential is intended to permit a Morse function for nearest neighbour interactions with no Coulomb term. To achieve this the parameter D must be set equal to 1.0 The effect of this additional term is to remove the Coulomb interaction between the species 1 and 2. The units of A, B, C and D are given below

- A**
is in eV
- B**
is in \AA^{-1}
- C**
is in \AA
- D**
is dimensionless

The ranges are terminated with an ENDS record or a new species record between the same species.

Printed output

COULOMB SUBTRACTED OFFSET MORSE POTENTIAL

V(R)=A*(1.0-EXP(-B(R-C)))**2 - A -D*Q1*Q2/R

```
A B C D*Q1*Q2 RMIN RMAX
A B C D*Q1 *Q2 RMIN RMAX
: : : : : :
```

SPRI

There are no additional parameters to be read in from the species record. The analytic form of the potential is

$$V(r) = A \times (r - B)^2 - \frac{C \times Q_1 \times Q_2}{r}$$

Q_1 and Q_2 are the charges on the species 1 and 2. This potential is intended to permit a harmonic spring function for nearest neighbour interactions with no Coulomb term. The parameter B should be set equal to the bond length, and A to the spring constant. To achieve this the parameter C must be set equal to 1.0 Setting C equal to 0.0 will leave the Coulomb term in. The effect of this additional term is to remove the

Coulomb interaction between the species 1 and 2. The units of A, B and C are given below

A

is in eV

B

is in Å

C

is dimensionless

The ranges are terminated with an ENDS record or a new species record between the same species.

Printed output

HARMONIC SPRING CONSTANT BETWEEN DIFFERENT BASIS ATOMS WITH
COULOMB TERM SUBTRACTED

$$V(R) = 1/2 * K * (R - R_0)^2 - A * Q_1 * Q_2 / R$$

K R0 D*Q1*Q2 RMIN RMAX

*K R0 D*Q1 *Q2 RMIN RMAX*

⋮ ⋮ ⋮ ⋮ ⋮

COUL

There are no additional parameters to be read in from the species record. The analytic form of the potential is

$$V(r) = \frac{A \times Q_1 \times Q_2}{r}$$

Q_1 and Q_2 are the charges on the species 1 and 2. This potential is intended to permit Coulomb subtraction between nearest neighbours. To achieve this the parameter A must be set equal to -1.0 The units of A are given below

A

is dimensionless

The ranges are terminated with an ENDS record or a new species record between the same species.

Printed output

COULOMB POTENTIAL $V(R) = A * Q_1 * Q_2 / R$

```
A*Q1*Q2 RMIN RMAX
A*Q1*Q2 RMIN RMAX
  ⋮      ⋮      ⋮
```

VDWA

There is one additional parameter read in from the species record. It has format I and operand name N. The analytic form of the potential is

$$V(r) = A/r^N$$

The exponent N is read in on the VDWA record. It is assumed that N remains the same for all ranges, if there is more than one. The parameter A must be read from the range record. The units of A is given below

A
is in eV Å^N

The ranges are terminated with an ENDS record or a new species record between the same species.

Printed output

VAN DER WAALS INTERACTION V(R) = A/R**N

```
A N RMIN RMAX
A N RMIN RMAX
  ⋮  ⋮  ⋮  ⋮
```

HULB

There are no additional parameters to be read in from the species record. The analytic form of the potential is

$$V(r) = A \times \left[(1 - \eta_1)^2 + D \times \beta^3 \times \eta_2 \times (1 + E \times \beta) \right]$$

$$- F - \frac{Q_1 \times Q_2}{r}$$

Where

$$\eta_1 = \exp(-\beta)$$

$$\eta_2 = \exp(-2 \times \beta)$$

$$\beta = B \times (r - C)$$

The parameters A, B, C, D, E and F must be read from the range record. The units of A, B, C, D, E and F are given below

A is in eV

B is in \AA^{-1}

C is in \AA

D is dimensionless

E is dimensionless

F is in eV

The ranges are terminated with an ENDS record or a new species record between the same species.

Printed output

COULOMB SUBTRACTED OFFSET HULBURT-HIRCHFELDER INTERACTION

$$V(R) = A * ((1.0 - \exp(-B * (R - C)))^{**2} + (D * (B^{**3}) * ((R - C)^{**3}) * \exp(-2.0 * B * (R - C)) * (1.0 + E * B * (R - C)))) - F - QI * QJ / R$$

A B C RMIN RMAX

D E F

A B C RMIN RMAX

D E F

⋮ ⋮ ⋮ ⋮ ⋮

BUC7

There are no additional parameters read in from the species record. The analytic form of the potential is

$$\begin{aligned}
 V(r) &= A \times \exp(-r/B) && \text{for } r < r_b \\
 V(r) &= \text{Fifth order polynomial} && \text{for } r_b < r < r_m \\
 V(r) &= \text{Third order polynomial} && \text{for } r_m < r < r_a \\
 V(r) &= -C/r^6 && \text{for } r_a < r < r_{max}
 \end{aligned}$$

There are 6 parameters read in from the range record. These are A, B, C, r_b , r_m and r_a . Their units are given below

A
is in eV
B
is in Å
C
is in eV Å⁶
r
are given in Å

The ranges are terminated with an ENDS record. On input, the ranges must satisfy the condition

$$r_b < r_m < r_a$$

If r_a is less than CUTPOT, the C/r^6 term will be calculated out to CUTPOT.

The polynomials are fitted so that the functions, first derivatives, second derivatives and third derivatives match at r_b , r_m and r_a . At r_m the potential has a minimum so that the first derivatives of both polynomials are zero. Only one ranges record is permitted for this interaction, since all of the ranges are given on the first record. Also, this potential must not overlap an existing potential.

Printed output

4 RANGE MODIFIED BUCKINGHAM POTENTIAL WITH 7/4 SPLINE

RANGE 1 V(R) = A * EXP(-R/RHO)

RANGE 2 V(R) = A7*R**7 + B7*R**6 + C7*R**5 + D7*R**4 + E7*R**3 + F7*R**2 + G7*R + H7

RANGE 3 V(R) = A4*R**4 + B4*R**3 + C4*R**2 + D4*R + E4

RANGE 4 $V(R) = -C/R^{**6}$

		RMIN	RMAX
A =	A	RHO =	RHO
		RMIN	r_b
A7 =	A7	B7 =	B7
		C7 =	C7
D7 =	D7	E7 =	E7
		F7 =	F7
G7 =	G7	H7 =	H7
		r_b	r_m
A4 =	A4	B4 =	B4
		C4 =	C4
D4 =	D4	E4 =	E4
		r_b	r_m
C =	C	r_a	RMAX

Error messages

ERROR - THE FOUR RANGE BUCKINGHAM POTENTIAL AND CUBIC SPLINE MUST NOT OVERLAP AN EXISTING POTENTIAL

ERROR - ONLY ONE PARAMETERS DIRECTIVE MUST BE GIVEN WITH THE FOUR RANGE BUCKINGHAM FORM

ERROR - THE RANGES ON THE FOUR RANGE BUCKINGHAM CARD ARE NOT GIVEN IN ASCENDING ORDER

NONE

There are no additional parameters to be read from the species record. This is a dummy two-body potential which does nothing. It may be used where the true range of a potential is less than CUTPOT, and where a range needs to be put in so that the potential extends out as far as CUTPOT. This will most commonly occur for intramolecular potentials. The range record should contain the value of RMAX and (optionally) the value of RMIN.

BSPL

There are no additional parameters on the species record. The program will fit a 5th. order spline between the points. There are two parameters read in from the range record, E_1 and r_1 . E_1 is in eV and r_1 is in Å. The interpretation of the range records for the quintic spline potential is somewhat different to the other potentials. Usually this would be interpreted as the maximum of the range RMAX. For the quintic spline, it should be the value of r at which the energy is E. A value of RMIN is not permitted on the range record for a quintic spline. The program rearranges the input data. In doing this ranges are redefined and extra ranges may be added. The quintic spline should not therefore be used with any other potential functions. The usual convention that the potential must start at zero also applies to the quintic spline.

Printed output

B-SPLINE POTENTIAL. ORDER 5

SEPARATION	SPLINE PARAMETER	ENERGY, 1ST AND 2ND DERIVATIVES		
<i>R</i>	<i>A</i>	<i>E</i>	<i>G</i>	<i>W</i>
⋮	⋮	⋮	⋮	⋮

Error messages

ERROR - FOR QUINTIC SPLINE THE NUMBER OF RANGES INPUT IS *i* AND MUST BE LESS THAN MAXRNG -6 WHERE MAXRNG = *maxrng*

ERROR - THE NUMBER OF QUINTIC SPLINE KNOTS WHICH IS SET INTERNALLY IS TOO LARGE RESET MAXRNG TO *i*

The number of quintic spline points input was too large.

ERROR - SMOOT ERROR CODE *i*

User error - probably too few points.

ENDS

This directive must be the last directive used to return control to the main menu of directives. Do not confuse this use of ENDS with previous ENDS terminating a short-range potential input. In some cases 2 consecutive ENDS directives are needed.

Error messages

EXECUTION TERMINATING BECAUSE OF ABOVE ERRORS

The detection of an error does not necessarily cause an immediate stop, the program continues to try to detect as many errors as possible in one run. If you get this error, check the output for additional error messages.

INTRAMOLECULAR GEOMETRY SETUP

MOLE

Operands none

The aim of this directive is to set up a neighbour list to define which pairs of atoms will form part of a rigid unit. Atoms are considered to be neighbours if they are in the same molecule (defined by the molecule number in the basis species input) and if additional conditions defined by sub-directives given below are met. No potential will be applied between neighbours. Intermolecular potentials will be used

1. Within the same molecule between species which are not defined to be neighbours. Normally this should not be used.
2. Between different molecules with different molecule numbers.
3. Between an atom in a molecule and a atom with a molecule number of zero, which will be a free ion.

The sub-directives used to define the neighbour list are given below.

CUTM

Operand types F
 Operand names CUTMOL

CUTMOL

is the cutoff in Å used to limit intramolecular interactions. NEIGHBOURS sets this to 10 Å, which should normally be sufficient.

NBUR

Operand types I
 Operand names NEBOUR

NEBOUR

An integer giving the maximum number of intramolecular bonds between species in the neighbour list. The value should be large enough to cover the whole molecule.

NNCU

Operands none

This sub-directive instructs the program to read in nearest neighbour cutoffs between intramolecular species until terminated by an ENDS directive. The format of the subsequent records is

Card format A A A A F
 LABELA LABELB BOND CUT

Card format A
 ENDS

Where

LABELA,LABELB

are species labels in the usual format.

BONDCUT

is the cutoff in Å between two species of the given type for the species to be treated as nearest neighbours within a molecule.

The ENDS directive returns control to the main menu of sub-directives.

NFXP

Operands none

This directive is redundant in DMAREL

MOLX

This directive inputs the local axis system of the molecule.

Operand type I

Operand name NAXES

NAXES is the number of different types of molecule. There are 2 X NAXES following records.

Card format

A A A A A A I

A A A A A A I A A A I

Direction 'LINE' SPECA 'CODA' SPECB CODA NNBU1

Direction 'PLANE' SPECA 'CODA' SPECB CODA NNBU2 SPECC 'CODA' NNBU3

where Direction is one of X, Y or Z. The first record defines a local axis to lie along the line joining two species which are NNBU1'th neighbours, the second record defines a local axis lying in a plane formed by the three species, the third axis forms a right handed set. Normally the first direction will be X and the second Y. As DMAREL always works with right handed axis systems, special precautions are needed if the system contains two enantiomers. NEIGHBOURS will label all atoms which are related by a centre of symmetry with the letter 'T' as the third character of the label. It will also change the sign of all the odd-z multipole components in the distributed multipole. This has the same effect as using a left handed axis system. This will only be valid if the axis order is X LINE and Y PLANE. If another order is put in the multipole component signs will need to be altered. NEIGHBOURS always outputs this order.

ENDS

This directive returns control to the main menu of directives.

Printed output

If PRIN MOLE 1 is set, the following is output

START OF NEIGHBOUR LIST PROCESSING

CUTOFF FOR INTRAMOLECULAR INTERACTIONS SEARCH = *CUTMOL*

NEIGHBOUR LIST WILL BE SET UP OUT TO *NEBOUR* NEIGHBOURS

THERE ARE *i* NEAREST NEIGHBOUR CUTOFFS (IN ANGSTROMS)

SPECIES TYPES CUTOFF

LABELI LABELJ BONDCUT

LIST OF NEIGHBOURS

SPECIES NUMBERS MOLECULE LATTICE SPACING DISTANCE

AND TYPES VECTORS

i j LABELI LABELJ nmole la lb lc nbur r

ij

are the index of the basis species after sorting.

LABELI LABELJ

are species labels.

nmole

is the molecule number as input in BASI section.

la lb lc

give the number of lattice vector translations needed to be applied to the species *j* to bring it within the cutoff from species *i*.

nbur

gives the minimum number of species between *i* and *j* moving along bonds. In other words, *i* and *j* are *nbur*th neighbours.

r

gives the distance between the species in Angstroms.

Error messages

ERROR - POTENTIAL INFORMATION MUST BE READ IN BEFORE TWO BODY BONDS

MOLE directive must come after POTE.

ERROR - IN ABOVE LINE AN INVALID SPECIES LABEL WAS GIVEN ON A MOLECULE CUTOFF DIRECTIVE

On a line following NNCU, a species label could not be recognised.

ERROR - THE CUTOFF BETWEEN THE ABOVE TWO SPECIES IS DUPLICATED

ERROR - MAXIMUM OF *MAXBOND* BOND CUTOFFS PERMITTED

ERROR, INSUFFICIENT MEMORY TO GENERATE NEIGHBOUR LIST, PROGRAM TERMINATING

UNIDENTIFIED MOLECULE KEYWORD *KEYW* PROGRAM TERMINATING

Example

```
MOLE
NFXP
CUTM 10.0
NBUR 10
NNCU
CLR1 CODA CAR1 CODA 1.800
CLI1 CODA CAI1 CODA 1.800
CLR2 CODA CAR2 CODA 1.800
CLI2 CODA CAI2 CODA 1.800
CLI4 CODA CAI4 CODA 1.800
CLR4 CODA CAR4 CODA 1.800
NIT1 CODA CAR1 CODA 1.500
NIT1 CODA CAR2 CODA 1.500
NII1 CODA CAI1 CODA 1.500
NII1 CODA CAI2 CODA 1.500
NII3 CODA CAI1 CODA 1.500
NII3 CODA CAI4 CODA 1.500
NIT3 CODA CAR1 CODA 1.500
NIT3 CODA CAR4 CODA 1.500
NIT2 CODA CAR2 CODA 1.500
NIT2 CODA CAR4 CODA 1.500
NII2 CODA CAI2 CODA 1.500
NII2 CODA CAI4 CODA 1.500
ENDS
MOLX 2
X LINE NIT1 CODA CAR4 CODA 3
Y PLANE NIT1 CODA CAR4 CODA 3 CAR1 CODA 1
X LINE NII1 CODA CAI4 CODA 3
Y PLANE NII1 CODA CAI4 CODA 3 CAI1 CODA 1
```

ENDS

PERFECT LATTICE CALCULATION

The perfect lattice calculation step is invoked by the keywords STAR PLUT.

STAR PLUT

Perfect Lattice Relaxation Control Parameters

All of the directives are optional except the final start. The defaults are indicated.

CONP

Operands none

This instructs DMAREL to relax the lattice vectors as well as the basis positions. There are 6 independent components of the bulk strain tensor which augment the $3NBAS \times 3NBAS$ matrix of basis strain components. The relaxation of both cell and atom components is carried out simultaneously. Only one of CONV and CONP may be given; this is the default directive.

CONV

Operands none

This instructs the program to keep the lattice vectors fixed during the relaxation.

MAXI

Operand Type I
Operand Name MAXIT

This defines the maximum number of iterations which will be carried out before a dump is written. The default is zero, which calculates the lattice properties at this configuration with no relaxation.

MAXU

Operand Type I
Operand Name MAXUPD

MAXUPD gives the number of times the Hessian will be updated before it is recalculated. It is recommended that for large unit cells MAXU should not be set too small; a value greater than 100 should be used. The default is 1000, which effectively means that the properties will only be recalculated when the structure converges or the calculation stops for another reason.

MAXD

Operand type F
Operand name MAXDISP

MAXDISP is the maximum permitted displacement of a coordinate per iteration. The default is 0.05 Angstroms, which is set small for most problems. A larger value may improve the speed at which a problem converges, but may allow the problem to reach a region in which the structure is physically unreasonable.

LIMI

Operand type F
Operand name LIMIT

LIMIT gives the convergence test at which the relaxation stops with a valid minimisation. The minimisation will assume to have converged if all displacements in one cycle are less than LIM I. The default is 1.0E-06 Angstroms, which is set very small. Most problems will be satisfactory with LIM I 0.0001.

WCAL

Operand Types A
Operand Names WKEY

This forces the program to recalculate the Hessian rather than use the updating algorithm if the surface is abnormal. The default is no recalculation. The keyword WKEY can have two values, GDPO or NGCV. GDPO forces recalculation if an increase in energy is found after a Hessian update. NGCV forces

recalculation if the curvature of the energy surface is negative. If both are required, the keyword WCAL may be given twice. This keyword is very seldom needed.

ENGO

Operand Types I
Operand Names ICTRL

ICTRL is an integer which determines whether matrix properties will be calculated. It may have two values. ICTRL = 3 is the default and instructs the program to calculate matrix properties. ICTRL = 1 calculates lattice energy only. ENGO 1 in DMAREL is only useful if no relaxation is being carried out (MAXI 0).

LIMG

Operand type F
Operand name GLIMIT

GLIMIT gives the convergence test at which the relaxation stops with a valid minimisation due to energy test being satisfied. The minimisation will assume to have converged if the predicted change in energy, calculated as the scalar product of the gradient vector and displacement vector, is less than GLIMIT. The default is 1.0E-10, which is set very small. Most problems will be satisfactory with $LIMG = 0.0001 \times LIMI$.

UDTE

Operand type F
Operand name UPDATE

UPDATE fine tunes the Hessian updating algorithm. The default value is 0.0, which will allow searching to continue in a given direction for a long way before updating. This can sometimes move into unphysical regions of the energy surface and give negative curvature. Setting a larger value will force the program to choose a new direction more often and may overcome this problem. It is suggested that a value of 0.1 for UPDATE would be suitable.

CCLS

Operand Types F < II >
Operand Names RCCMAX ICCMAX ICCLS

Prints out the close contact list together with the energy subdivided by type of interaction. The information is written to fort.17 RCCMAX is the maximum separation to which information is written, ICCMAX is the maximum number of atom pairs and ICCLS is a flag. ICCLS=1 prints on the first and last cycle only, ICCLS=2 prints every 10 cycles and ICCLS=3 prints every cycle.

R2ND

Operands None

Switches on the storing or reading of the accurate second derivative matrix. Only useful if you may need to restart the run, which is seldom done.

SEIG

Operand Types

I < F F I I I I >

Operand Names LSEIG EIRNMI EIRNMX NEISTP IREPS IREPF NEINS NEINF

This will instruct DMAREL to search along eigenvector directions for energies lower than the minimum which has been located. This is most useful if there is a negative eigenvalue belonging to a symmetry class which is not totally symmetric at the valid minimum for a particular run. If LSEIG is zero (default), the search will be carried out by default only for the totally symmetric representation if one or more eigenvalue is negative. LSEIG = 1 allows the search even if these conditions are not met. If LSEIG=0, the following defaults are used; EIRNMI=-1.0, EIRNMX=+1.0, NEISTP=20, IREPS=IREPA1, IREPF=IREPA1, NEINS=1, NEINF=0. The search is done with displacements from EIRNMI to EIRNMX in NEISTP steps for representations from IREPS to IREPF (IREPA1 is the totally symmetric representation) for eigenvectors NEINS to NEINF.

NOPR

Operands None

NOPR switches off the calculation of elastic properties at the end of the calculation. (This calculation is slow as it uses numerical derivatives).

STAR

Operands none

This must be the final sub-directive in the list. It starts the execution of the perfect lattice calculation and then returns control to the main menu of directives.

Printed Output

COMMENCING WITH PLUTO CALCULATION

HESSIAN WILL BE UPDATED WHEN
 $(1.0 + UDTE * ALPHA2 / ALPHAM) * (1.0 - ABS(GD2 / GD1)) > 0.75$
 ALPHA2 = GREATEST SHIFT OF AN ION SINCE LAST UPDATE
 ALPHAM = MAXIMUM ALLOWED SHIFT PER ITERATION
 UDTE = *UPDATE* = USER DEFINED PARAMETER (DEFAULT ZERO)
 GD2, GD1 ENERGY CHANGES IN SEARCH DIRECTION

This message is written if the UDTE option is used, and it describes how the Hessian update is modified.

START RELAXATION AT CONSTANT VOLUME
 START RELAXATION TO ZERO PRESSURE

One of these messages is produced according to whether CONV or CONP (default) is given.

MAX NUMBER OF ITERATIONS = *MAXIT*
 MAX RELAXATION OF A COORDINATE PER CYCLE
 (NOTE IN LATTICE UNITS) = *MAXD*
 MAX NUMBER OF HESSIAN UPDATES BEFORE RECALCULATION *MAXU*
 ITERATION WILL TERMINATE WHEN ALL DISPLACEMENTS ARE LESS THAN *LIMIT*
 ITERATION WILL ALSO TERMINATE WHEN DOT PRODUCT OF GRADIENT
 AND DISPLACEMENT VECTORS IS LESS THAN *GLIMIT*

This message is produced if *MAXI* greater than zero is given. Note the *MAXD* parameter has been scaled by the lattice parameter before it is printed.

HESSIAN WILL BE RECALCULATED IF SURFACE IS ABNORMAL

This message is written if directive WCAL is supplied.

PERFECT LATTICE PROPERTY CALCULATION WITHOUT RELAXATION

This is written if *MAXI* 0 is given. (This is the default).

THE LATTICE ENERGY IS *e* EV

This message is always printed. According to the value of the MPRINT parameter on the PRIN PLUT MPRINT record, various other quantities may be printed, either before the first cycle and after the last cycle, or every cycle of iteration.

THE FORCE CONSTANT MATRIX IS AS FOLLOWS
 THE GRADIENT VECTOR IS AS FOLLOWS

The force constant matrix and gradient vector may be printed by setting PRIN PLUT 01000. If just the

gradient vector is required, set PRIN PLUT 03000 (first and last cycle only) or PRIN PLUT 04000 (Each cycle). There are 6*MOLS + 6 elements. The order of the elements is

x, y and z derivatives of each molecule in the sorted order. This is followed by the torsions for each molecule.

6 components of the bulk strain derivatives.

Note that there are mixed second derivatives between all three types. The elements of the matrix are not scaled to eV Angstrom units. To convert to eV Angstrom units, multiply

W or G	Position		Multiplication factor	Resulting Units
	From	To		
Gradient	1	6*MOLS	$\frac{14.3997584}{RLAT^2}$	$(eV \text{ \AA})^{-1}$
	6*MOLS	END	$\frac{14.3997584}{RLAT^3}$	$(eV \text{ \AA})^{-2}$
Matrix	1,1	6*MOLS,6*MOLS	$\frac{14.3997584}{RLAT^3}$	$(eV \text{ \AA})^{-2}$
	1,6*MOLS	6*MOLS,END	$\frac{14.3997584}{RLAT^4}$	$(eV \text{ \AA})^{-3}$
	6*MOLS,6*MOLS	END,END	$\frac{14.3997584}{RLAT^5}$	$(eV \text{ \AA})^{-4}$

ELASTIC CONSTANT TENSOR - 10**11 DYNE/CM**2

.....

ELASTIC COMPLIANCE TENSOR - 10**-11 CM**2/DYNE

.....

The elastic constant tensor is printed in units of 10 **11 Dynes cm. **-2. The rows and columns refer to the xx yy zz yz xz xy components of the tensor. Note that the values printed depend on the choice of orthonormal coordinate system The symmetry reflects that of the unit cell.

If a perfect lattice relaxation is carried out ($MAXIT > 1$), the lattice energy is printed out on each cycle of iteration. The final lattice vectors and basis positions are printed out after the final cycle of iteration. The basis positions are in the sorted order. The lattice vectors, basis species types and positions will be written to FORTRAN unit 8. This is by default for DMAREL.

Error messages

ERROR - NO ROUTE PARAMETER ON START DIRECTIVE CARD

The directive has the keyword STAR but not the keyword PLUT. Check that the keyword is correct.

ERROR - POTENTIAL FUNCTIONS NOT DEFINED BEFORE START OF PLUTO EXECUTION OR FILE INPUT

The POTE directive has been omitted or placed in the incorrect order. It should be before STAR PLUT

EXECUTION TERMINATED BEFORE START OF PLUTO CALCULATION BECAUSE OF ABOVE ERRORS

The STAR PLUT directive is one point where the program stops if it has detected a previous error. Look through the printed output for further error messages.

ERROR - THE DYNAMIC MEMORY REQUIREMENTS OF PLUTO SECTION HAS EXCEEDED THE n WORDS OF CORE AVAILABLE. PROGRAM TERMINATING.

THIS DATASET NEEDS $ISPACE = n$ WORDS

The job has insufficient memory.

UNREGCOGNISED KEYWORD *KEYW*

A keyword has been found which is not in the STAR PLUT menu.

ERROR - BASIS SPECIES NUMBERS i AND j
LABELS $label_i$ $label_j$ ARE SEPARATED BY LESS THAN CUTSHL

This error message is produced by inconsistencies between the species labels and the CUTSHL parameter. This message comes from two species lying within CUTSHL of each other in the perfect lattice relaxation. This means that the structure has moved to an unphysical geometry. Redefine MAXD to be smaller and resubmit the job.

Printed output

If the relaxation vector is sufficiently small, DMAREL will assume that a valid minimum has been found. Currently the distance used in this test is 5.0×10^{-6} lattice units, and the program terminates if all displacements of all symmetry adapted variables are less than this value.

If PRIN MINI is set to a value greater than one, the following output will be obtained.

MINIMISATION SETUP

This is printed every time the inner iterative loop is entered. Usually this will be once only on the first iteration, unless one of the Hessian recalculation options is used.

$$GD1 = F$$

This is written twice after the MINIMISATION SETUP message. The first value F is the value of G.DELTA, the second is the value of G.DELTA scaled if necessary to keep all of the elements of delta within RMAXSF. G.DELTA should be negative indicating a decrease of energy in the search direction. If the first value of GD1 is positive, the direction of the search is reversed to ensure that the energy decreases.

$$ALPHA = F1 \quad ALPHA2 = F2$$

This message occurs after MINIMISATION SETUP or after CHANGE DIRECTION. (See below). ALPHA and ALPHA2 will both be one in this case. ALPHA is the current fraction of DELTA to be applied. ALPHA2 is the total fraction of DELTA applied since the last Hessian update.

$$GD1 = F1 \quad GD2 = F2$$

This is printed every cycle except for MINIMISATION SETUP cycles. GD1 is the previous value of G.DELTA, GD2 is the value calculated at the position after the step in the search direction. If the minimisation is working correctly, the magnitude of GD2 should be less than GD1.

If $ABS(GD2/GD1)$ is less than 0.25, the following is printed.

CHANGE DIRECTION

HESSIAN UPDATE COMPLETE ... GD1 = F1 GD2 = F2 IKIND = I1 DELMAX = F3 IN
COMPONENT I2

Where

F1

is the value of G.DELTA calculated from the updated Hessian and the new search direction DELTA. (DELTA = Hessian.G).

F2

is zero.

I1

is 0 if the Davidon-Fletcher-Powell algorithm has been used to update the Hessian.(R. Fletcher and M. J. D. Powell. Computer J. 6 (1963) 16) I1 is 1 if the Broyden, Fletcher and Shanno algorithm has been used. (C. G. Broyden. J. Inst. Maths. Applns. 6 (1970) 66 and 222. D. F. Shanno. Math. Computing 24 (1970) 647.)

F3

is the maximum displacement of a symmetry adapted variable. If F3 is greater than RMAXSF the

search direction will be scaled so that the maximum displacement is RMAXSF.

I2

is the index of the variable with the maximum displacement.

GD1 = F1

ALPHA = F1 ALPHA2 = F2

These messages are described above under MINIMISATION SETUP.

If $ABS(GD2/GD1)$ is greater than 0.25 then a further search in this direction is made before an update is carried out. There are three possible options.

1. If GD2 is less than GD1 (that is more negative), the system is in a region where the potential energy surface has negative curvature. Possible causes of this are that it is close to a saddle point and is moving away from it. Another point to look out for is that two ions interacting with a BUCK short range potential have not become too close. If the Van der Waals parameter is non-zero, the R^{*-6} term eventually dominates the exponential term, leading to negative curvature in the energy surface. If this is the cause, either reduce RMAXSF or consider using the BUC4 potential instead.

Printed output

NEGATIVE CURVATURE

ALPHA = F1 ALPHA2 = F2 ALPHA3 = F3 ALPHA4 = F4 GD1 = F5 GD2 = F6 GD3 = F7
GD4 = F8

These are the ALPHA values and corresponding G.DELTA values at four points in the search direction. ALPHA is the current step in the search direction. ALPHA2 is the total step since the last Hessian update or Hessian calculation. GD1 is the G.DELTA value for ALPHA = 1.0 GD2 is the G.GELTA value for the current step length ALPHA2. ALPHA3, ALPHA4, GD3 and GD4 are ALPHA and GD values from previous iterations in this search direction.

ALPHA2 TOO LARGE TO EXTRAPOLATE

Extrapolation in this direction would change one of the variables by more than RMAXSF, therefore a matrix update is carried out. If GD2 is negative, a linear extrapolation is carried out.

Printed output

EXTRAPOLATE

ALPHA = F1 ALPHA2 = F2 ALPHA3 = F3 ALPHA4 = F4 GD1 = F5 GD2 = F6 GD3 = F7
GD4 = F8

This has the same meaning as described above. If GD2 is greater than zero, an interpolation is carried out.

Printed output

LINEAR INTERPOLATION

ALPHA = F1 ALPHA2 = F2 ALPHA3 = F3 ALPHA4 = F4 GD1 = F5 GD2 = F6 GD3 = F7
GD4 = F8

This has the same meaning as above.

If a further search is necessary in the same direction, additional printed output may be obtained.

Printed output

QUADRATIC INTERPOLATION

QUADRATIC EXTRAPOLATION

These messages indicate that the results of two previous steps are being used to interpolate/extrapolate.

THREE INTERPOLATIONS

This indicates that three interpolations failed to reduce GD2 sufficiently and an update will be carried out in any case.

Error messages

INVALID MINIMISATION - PERSISTENT NEGATIVE CURVATURE

This indicates that the energy surface has negative curvature. It may not be possible to converge this dataset, however the values of RMAXSF and MAXUPD could be changed to alter the path taken by the minimisation.

Three checks are now carried out to ensure that the minimisation is proceeding properly. See section (3.9.13) below.

PRINT ANY ERROR MESSAGES

If the number of iterations exceeds the maximum permitted, (see section 3.3.2.2) the following is printed:

WARNING - MAXIMUM NUMBER OF I1 ITERATIONS HAS BEEN REACHED