Cameron Manual

Chemical Crystallography Laboratory, Oxford

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Chapter 1

Introduction

CAMERON was designed and built in the Chemical Crystallography Laboratory, Oxford, by Lisa Pearce, Keith Prout and David Watkin. Manypeople have contributed ides for improvements, and Louis Ferrugiapioneerd a completely WINDOWS based version.

1.1   HOW TO CONTROL THE PROGRAM

The program is controlled by typing commands at the keyboard, by use of a mouse to pick items from a menu, or by using the mouse to manipulate the diagram.

1.2   Command Groups

The commands have been collected into groups (twenty-three at present). Each group contains commands and sub-commands which perform related functions or which will act as qualifiers to each other. The command processor will spot invalid combinations of commands and sub-commands and enter error mode. Once in this mode the error can be corrected.

Command groups are used to decide when the user has finished entering all the qualifiers for a particular operation. The qualifiers are assumed to be finished when a command of another group is entered. For example :-

```
XROT 20 YROT 30 VIEW LINE ALL
```

XROT, YROT and **VIEW** are all in the same group but **LINE** (a command that sets the drawing style) is not. When the command processor reaches the **LINE** command it will then execute the previous commands ie **XROT** to **VIEW.** This is useful because it means that the user does not need to input all the qualifiers on one line, and also because the user does not need to tell the computer when it has finished with an operation - the computer is able to work this out for itself. The input lines :-

```
XROT 20 YROT 30 VIEW LINE
```

and

```
XROT 20
YROT
20 VIEW
LINE
```

will produce exactly the same results.

If the user wishes to execute a group of commands without entering a command of another group this can be done by sending a blank line to the command processor (ie press the RETURN key twice).

```
XROT 20 YROT 30 VIEW <RETURN> <RETURN>
```

will execute the three commands without the need for **LINE.**

1.3   ERROR HANDLING

The command processor is able to check for some errors in the commands input by the user. The computer checks for two types of error:

```
1. Whether a command / sub-command combination is valid.
2. Whether the arguments supplied after a command are valid and also if there is
the correct number of arguments.
```

The action taken after an error depends upon the setting of the **EDIT** flag. If EDIT is OFF, only an error message is displayed. If EDIT is ON, the faulty input can be edited. Once an error has been detected the user can take action and modify the input line so that as many commands as possible can be processed. (If error checking is not carried out at this level, the detection of an error while executing a command will cause that command - and possibly its sub commands - to be lost.)

The user is given three options once an error has been detected.

Abandon
Do not execute any more commands not yet executed.

Edit
The action taken by choosing the second option will depend on the nature of the error. If a word has been input that the computer has not recognised the user will be asked to enter an alternative word. If <return> is used then the word is replaced by a blank space - it is effectively deleted from the input line. If too many arguments are supplied the user is given the opportunity to delete the excess arguments. Alternatively if arguments are missing the user will be asked to input them.

Help
Help information is supplied if the user requests it. This will say what arguments, if any, are required by the current command. Also, if any sub commands are valid in the context of the error these are listed.

For example, the input line

```
XROT 10 YROT ZROT 15 VIEW
```

contains an error - an argument is missing after **YROT.** The program will give the user three options :-

```
Abandon      Don't execute any of the commands
Edit         The user can supply the needed argument
             and the new line is then processed.
Help         This will display the help information
```

```
   This command requires one numeric argument - the angle of rotation in degrees.
```

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1.4 The HELP facility

The CAMERON **HELP** facility can be entered in one of two ways, either once an error has occurred (as described above) or by requesting it directly. This second way of accessing HELP is achieved by entering **'HELP'** or '?' at any point in the input line. If a command follows **'HELP'** / '?' then information is given on this command - otherwise information is given on the previous command (if any). If no HELP is available (because the command is not recognised) then the user is supplied with general HELP information. The only difference between 'HELP' and '?' is in the detail of the information supplied. Each command comes with a help information line. Entering '?' will provide the user with the information line for the command on which you have requested HELP and a list of the sub-commands that are valid at this point. Entering 'HELP' gives the same information except that the help line for each of the sub-commands shown is also listed. 'HELP' will therefore provide the user with more detailed information than '?' will.

Once the HELP information has been read the user may 'Continue' or 'Abort'. The later two options are the same as for Error Handling and are described above. 'Continue' simply removes the word 'HELP' or '?' (and any following words) from the input line and the user can carry on as before.

1.5 Mouse Activation

The Mouse can be used to pick out atoms (and elements if a KEY is present). In some cases this is much quicker than typing on the keyboard - especially if the user does not know the names of the atoms concerned. The mouse cursor (an arrow) is present once an appropriate output device has been chosen.

For some commands the mouse is used for functions other than atom/element picking. In such cases - eg text positioning and labelling - the mouse is activated by typing MOUSE as a separate command.

1.6 General Input Syntax

When the atoms are in their initial state (ie no symmetry operators have been applied) they are referred to by their normal atom or element names. With commands that allow elements to be affected eg COLOUR, BALL you may use a '*' to refer to ALL atoms. For example CONNECT O * 0.0 3.0 will find all bonds between oxygen and any other atom within 3 angstroms. A '*' can also be used to refer to GROUP names (see DEFGROUP later).

Once pack operations have been carried out the atoms are identified differently. During PACK and ENCLOSURE the user is provided with information similar to :-

```
2 additional symmetry generated units.
```

The atoms generated will be referred to by suffixing their packnumber eg O1_2. These numbers can be shown by using LABEL GENERATED. Therefore, consider an asymmetric unit which contains N1 and O2. The following will be available after packing:-

```
N1_1     the single atom
N1       all N1 atoms in the packed structure
N        all the nitrogen atoms
N_2      all the nitrogen atoms with pack number 2
*_1      all the atoms with pack number 2
```

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These pack numbered atom identifiers are produced by mouse clicking on the atoms concerned. The symmetry operation used to generate the atoms can be found from INFO PACKNUMBER. The operators are also written to the CRYSTALS listing file

When CAMERON is parsing the commands input it checks to see whether the next work on the line is a command or not. Only the first 4 characters of each word are significant. Therefore, the processor will not know the difference between the command COLOUR and the file COLOUR.PST. If you require the later then it must be enclosed in quotes - eg COPY "COLOUR.PST".

Chapter 2

How To Get Started

There is a basic 'startup' procedure that can be followed in order toget a picture on to the screen.The following steps are required :-

```
1)      Load in a spacegroup if required2)      Load in the unit cell dimensions3)      Load in the atomic
```

This can be accomplished with the following commands, which areillustrated for a compound which has a spacegroup P 21, unit cellparameters a=6.0, b=7.0, c=8.0, alpha=90, beta=115, gamma=90. The atomiccoordinates are held in a "list5" type file NIGEL.L5.

```
SPACEGROUP P 21INPUTCELL 6 7 8 90 115 90LIST5 NIGEL.L5DEVICE VGABALL ALLFILLVIEW
```

From here the view direction can be controlled via XROT, YROT, ZROT orCURSOR. If you require a picture of all the atoms in the unit cell, and the unit cell also displayed,the commands are :-

```
PACK CELLINCLUDE CELLVIEW
```

Chapter 3

Data Input

At present data is read from CRYSTALS generated LIST5 files and CSSRfiles (see the CRYSTALS manual).

3.1 Input of CRYSTALS List 5 files

These files do not contain information on the dimensions of the unit cell. It is therefore necessary to use CELL to enter this information prior to the reading of the list 5 file.

INPUT

CELL The syntax of this sub-command is :-

`INPUT CELL a b c alpha beta gamma`

ie we require six arguments - cell dimensions in angstroms and angles in degrees. Their values are assigned as shown above.

LIST5 This command requires as its argument the name of the file that contains the atomic coordinates. The syntax is :-

`LIST5 filename.L5`

NB The LIST5 command will not be accepted without the previous command CELL.

CSSR
CSSR files are input by using INPUT CSSR. As with LIST5 files above it is advisable to input the symmetry information before inputting the atomic coordinates.
Related commands : OBEY, OUTPUT

Chapter 4

Outputting Data

OUTPUT
CAMERON outputs data in CRYSTALS LIST5 and CSSR format.

LIST5 This outputs a crystals list5. It must be followed by a filename. Thelist5 will contain LIST1 unit cell information at the end - such a filecan be re-read by CAMERON with no problem.

CSSR

FRACT

*ORTH*These subcommands are needed to specify the coodinate type for the CSSRfile ie orthogonal or fractional. The command is followed by thefilename of the output file.

```
Example:OUPUT CSR FRACT mydata.css
```

Related commands : INPUT

Chapter 5

Editing The Atom List

The user is able to edit the names and elemental types of the atoms inthe current list. The following commands are available -

RENAME
The syntax is:

```
 RENAME at1 at2     or: RENAME el1 el2.
```

Arguments are entered inpairs - the first is renamed to the second - and must be like with like.i.e. you cannot rename an atom to an element or vice versa.

RETYPE
This allows the user to change the element of a list of atoms.

*ATOMS*The syntax is -

```
RETYPE element ATOM at1 at2 at3
```

Chapter 6

Obeying Files

OBEY

If required the user is able to hand over control of CAMERON to anexternal file. This is particulary useful if a set of operations is tobe carried out on a number of pictures because the file need only begenerated once and then it can be used over and over again. At thepresent time CAMERON is able to read files is its own format - ie inwith the same syntax as the commands input at the keyboard - or it canread a SNOOPI.INI file as output by CRYSTALS. The syntax is :-

```
OBEY nnn.nn
```

Note that any commands entered after OBEY (on the same line) areignored. This is to allow for possible errors in the OBEY file - errorswill cause the OBEYed file to be closed. OBEY files may themselvescontain the names of other files to be OBEYed.

Related commands : LOG

Chapter 7

Archiving And Retrieving Views

The user can archive the present structure view on disk or retrieve a previously archived view from disk. At present only structure views residing in the same directory as the crfilev2.dsc (the working directory) can be retrieved. Equally well, views can only be archived in the working directory. As an alternative to the line commands, the user may choose the commands that are available in the pull-down menu 'File'. The following commands are available -

ARCHIVE
The syntax is:

```
ARCHIVE "foo.foo"
```

Note that the quotes (") are necessary to avoid confusion with non-existing sub-commands to this command. The filename must not exceed 12 characters.

RETRIEVE
The syntax is:

```
RETRIEVE "foo.foo"
```

Note that the quotes (") are necessary to avoid confusion with non-existing sub-commands to this command. The filename must not exceed 12 characters.

Chapter 8

Graphical Output Devices

The user has to specify a graphical output device before the commandVIEW can be used. This is done with the command SCREEN. Note that if thetitle screen file CAMERON.SRT is present the screen is automatically setto VGA.

SCREEN
The following devices are currently supported:-

VGAThis sends the output to a VGA monitor eg to a PC graphics screen.

EGAThis sends the output to an EGA monitor.

SIGMAThis sends the output to a SIGMA terminal.

TEKThis is used for VAX terminals with Tektronics 4010 emulation.

HARDCOPY
If hardcopy output is required the user must specify a separatedevice which is then drawn to using COPY. Those available are :-

POSTSCRIPTThe graphical output is sent to a file in POSTSCRIPT format so that itcan be printed on a postscript printer.

ENCAPPOSTThe graphical output will be sent to a file in the same way as with-POSTSCRIPT, the onlydifference is that the resulting file will be in Encapsulated form sothat it can be incorporated into other packages eg Word Perfect (using the Graphics range of commands).

CPOSTThis generates a file in Colour Postscript (Level 1) format.

CENCAPThis generates an colour encapsulated postscript file.
Related commands : VIEW, COPY

Chapter 9

View Direction Control

One of the most important features of a graphics package is theeasewith which a required molecular view can be obtained. CAMERONcontains alarge number of options which allow the user to control the viewdirection.

9.1 BASIC CONTROL

Five commands are available to control the view direction by applying rotations to the molecule. These rotations are applied cumulatively - rotating about the x axis by 20 degrees then by -10 degrees will result in an overall rotation of 10 degrees *relative to the starting point.*

XROT
This command is used to apply a rotation of n degrees about the
x-axis which lies horizontally across the screen. The syntax is:

```
XROT n
```

YROT

ZROT
These two commands are identical to XROT except for the axis about which the rotation is carried out. The y-axis lies vertically up the screen and the z-axis is perpendicular to the screen.

ROT
This command is a 'shorthand' for the previous three commands as it allows you to apply three successive rotations by entering only one command. The syntax is :-

```
ROT x y z
```

Note that the order of rotation is: rotate about x then y then z. The order of rotation is important - YROT 10 XROT 5 ZROT 15 will NOT produce the same result as ROT 5 10 15 as the rotation matrices are non-commutative.

CURSOR
This command allows the user to control rotation with the cursor keys. Each time a key is struck a rotation of 5 degrees is applied about the relevant axes. After each key stroke the molecule

is rotated and then re-drawn. To speed up this process the molecule is drawn in line style during the CURSOR rotation and is not scaled. The set-up prior to CURSOR is restored once rotation is terminated. The keys used are:

```
Rotation about the x-axis

Positive        up arrow
Negative        down arrow

Rotation about the y-axis

Positive        left arrow
Negative        right arrow

Rotation about the z-axis

Positive        Delete key (PC)
Negative        End key (PC)
```

Any other key stroke will terminate the CURSOR control and draw the resultant picture.

9.2   ORIENTATION COMMANDS

More specific orientation of the molecule can be achieved by relating the view direction to the position of certain atoms within the picture.

PLANE
In some cases it is useful to be able to define a PLANE and then set the view direction to be perpendicular to it. The syntax of this command is :-

```
PLANE at1 at2 at3 ...
```

At least 3 atoms must be used to define the plane (element names will not be accepted). If more than 3 are used then the program calculates the best plane through the atoms and projects onto this.

ALL PLANE ALL will generated a 'best view' of the current structure.

FACE
Alternatively you may want to view onto a particular crystallographic face of the unit cell. The syntax for this command is:

```
FACE h k l
```

where h k and l are the Miller indices of the FACE in question.

ALONG
It is possible to define the view direction as that looking down an interatomic direction. The direction is specified by inputting :-

```
ALONG at1 at2
```

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As with PLANE atoms not elements must be used as the arguments. Note that the view direction is calculated as that looking down the at1 - at2 direction ie at1 is the closest of the two. The reverse view will be obtained by requesting ALONG at2 at1. ALONG also has a sub-command associated with it:

AXIS

It is possible to define the view direction as looking along a particular unit cell axis. The syntax of the command is:

```
ALONG AXIS x
```

where x is A, B or C.

VERTICAL

HORIZONTAL

These two commands are similar to ALONG except that the at1 - at2 direction is oriented up (VERTICAL) or across (HORIZONTAL) the screen as required.

AXIS

The AXIS sub command may be applied to the HORIZONTAL and VERTICAL commands. This rotates the diagram around the z axis so that the required axis is HORIZONTAL or VERTICAL as specified. This is particularly useful when generating hard copy output.

BISECT

This command requires three arguments, at1 at2 and at3. It will generate a view direction looking along the bisector of the at1-at2-at3 angle. The syntax is:

```
BISECT at1 at2 at3
```

where at2 is the apex atom.

9.3 Other related commands

IVIEW
The 'title' command of this group of commands is VIEW. IT IS A VERY IMPORTANT COMMAND. This requires no arguments as causes a picture to be output to the current output device (see SCREEN). The picture is generated according to all of the parameters that are set up prior to its use. For example:

```
XROT 10 VIEW
```

will rotate the molecule by 10 degrees about x and then draw a picture.

```
VIEW XROT 10
```

would draw the picture first and then carry out the rotation. This rotation would not be observed until the next VIEW is entered.

COPY

COPY is the equivalent command for hardcopy output. COPY must be followed by a filename to which the output will be send. HARDCOPY must have been used prior to this to specify the output type. The filename may be one that has already been used in the current run of CAMERON in which case the user is given an option to append the information.

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MATRIX
This command allows the user to save the current view matrix.

FILE This is followed by a filename. If the file exists (and it is of the correct format) then any matrices contained within it are available and any matrices stored are appended to the file.

STORE This stores the current matrix. It is followed by a piece of text (in quotes "text") to act as a description for the matrix. On storage a number is assigned to the matrix which can be used to retrieve it later.

RETRIEVE This command obtains a view matrix from the file set up with MATRIX FILE. This command must be followed by the number of the matrix required. Note that these matrices depend on the unit cell parameters and are specific to a particular structure. They may be used for other structures but this will have very strange results. IF this happens an operation such as ALONG AXIS C will recalculate a correct matrix.

LIST This outputs a list of the descriptions and numbers of the matrices currently stored.

STEREO
This generates output in the form of stereo pairs.

DEGREE The angle of rotation between the stereo pairs is given by using the DEGREE command.

NOSTEREO
Reverts output back to normal.

9.4 PHOTOGRAPHS

PHOTO

ON

OFF These commands are used to control the PHOTO facility. VIEW displays the user with information about the current scale and displays the mouse cursor once it has finished. PHOTO ON turns off this and waits for a key press before proceeding. This allows the user to obtain a 'clean' screen for photographs to be taken.
Related commands : SCREEN, HARDCOPY

Chapter 10

Include And Exclude

The commands INCLUDE and EXCLUDE are very useful as theycontrol whichatoms are drawn at any one time. The syntax for both of thecommands isvery similar as they are effectively the reverse of each other.

INCLUDE

EXCLUDE
These commands may be entered on their own and be follow byatom orelement names. The syntax is :-

```
nnCLUDE at1 at2 el1 el2
```

Once an atom has been EXCLUDED from the picture it is not drawnand itis not included in any calculations eg PACK or ENCLOSURE.

ALLThe ALL sub-command is a 'blanket' command that applies theIN/EXCLUDEoperation to ALL of the atoms in the current view. Therefore ifwe wantto exclude more atoms than we want to include we can use EXCLUDEALL toget rid of all of the atoms and then add in those we want byusingINCLUDE.

GROUPThe command DEFGROUP is available to define groups of atoms thatare tobe referred to as a whole. The IN/EXCLUDE command can be usedwith GROUPto remove or atoms all of the atoms in the group in the pictureasrequired.

FRAGMENTThe user can specify atoms to be IN/EXCLUDEd by defining groups of atomsas fragments. A fragment is defined by a single atom, and consists ofall the atoms linked to it by the current CONNECTIVITY TABLE. That is,if atoms are excluded from the picture the bonds ARE NOT broken andFRAGMENT will use bonds involving excluded atoms in its calculations. The usercan select this atom by typing or by clicking on it with the mouse.ie. EXCLUDE FRAGMENT C1 will exclude C1, any atoms joined to C1, anyatoms joined to those atoms etc.

CELLIt is often useful to see how the atoms being drawn relate to theunitcell. IN/EXCLUDE CELL is used to control the inclusion of theunit cell(in the LINE style) on the picture.

AREAChoosing INCLUDE or EXCLUDE AREA in the PC version allows the user to draw a polygonal area with the mouse. The polygon is created by clickingwith the left button on the

position required for the vertices. The polygon is closed by clicking close to the initial position. The mouse cursor is changed to a cross during polygon creation and to an arrow when you are close enough to the initial point for closure to occur. Hitting the <return> key or clicking with the right mouse button will abort the operation.

SELECT The select option is equivalent to EXCLUDE ALL followed by INCLUDE AREA. The polygonal area is chosen in the same way as described above and all atoms not within that area are excluded.

10.1 Further related commands

For pictures with more than one 'type' of constituent atom three more commands will prove to be useful.

MASK

UNMASK
The MASK command has the same syntax as EXCLUDE ie.

```
(UN)MASK at1 at2 el1 el2 ...
```

It is used to remove atoms from current INCLUDE operations - ie atoms that have been MASKed will not be included when using INCLUDE ALL. For example the user could MASK out solvent molecules from a diagram leaving the 'basic' asymmetric unit to be worked on. UNMASK can be used to re-include the required atoms. The sub commands ALL and GROUP are available for use with both MASK and UNMASK.

SWITCH
The SWITCH command causes any atoms that are EXCLUDEd from the picture to be INCLUDEd and vice versa. This command can be used in conjunction with MASK as any MASKed atoms WILL NOT be included in the picture after a SWITCH operation.

Consider an asymmetric unit containing an anion, a cation and some solvent. The user could MASK out the solvent atoms. EXCLUDE the anion and obtain pictures of the cation atoms. The SWITCH command then allows the user to examine the anion without having to INCLUDE and EXCLUDE atoms, and the solvent atoms remain excluded throughout.

10.2 Generation of Dummy atoms

DUMMY
In certain circumstances it may be useful for the user to be able to generate new 'dummy' atoms from the initial atomic coordinates. One example of this is a compound that contains a cyclopentadienyl ring. The bonding in such a system can either be represented as five M - C bonds or as a single bond to the ring's centre. The syntax for the command is:

```
INCLUDE DUMMY d
```

where d is the name of the created atom. This must then be followed by a sub-command which defines the atoms position.

COORDS This specifies the atoms coordinates in unit cell fractions. The syntax is:

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```
COORDS x y z
```

CENTROID Alternatively, the atoms position can be defined relative to others already in the molecule. At least TWO atoms must be entered to define new atoms position and it is placed at the CENTROID of their coordinates. The syntax is:

```
CENTROID at1 at2 at3 ...
```

ALL A further sub-command is available so that the new atom is placed at the centroid of all of the atoms in the molecule. This will prove particulary useful when trying to alter the spacegroup of a structure eg to convert from P 1 to P -1 as the centre of inversion will lie at the newly generated dummy atom whose coordinates are output once they have been calculated.

10.3 Example

To create a dummy atom in the centre of a cyclopentadienyl ring you would use:

```
INCLUDE
DUMMY d1
CENTROID C1 C2 C3 C4 C5
```

Chapter 11

Drawing Style Control

The user is able to choose from three different drawing styles.Theseare:

LINE

BALL

ELLIPSE
The basic syntax for style control is:

```
XXXX at1 at2 el1 el2
```

where XXXX is LINE, BALL or ELLIPSE as required. The user mayspecifyatoms eg C1, C2 and/or elements eg C O to be drawn in the XXXXstyle.The user may therefore have all three styles present at any onetimewithin the picture. Alternatively the ALL may be usedtoconvert the drawing style of all the atoms present to XXXX.The initial drawing style used is LINE.

The ELLIPSE drawing style is only available if the user hasinput datathat contains information on the temperature factors (isotropicoranisotropic) of the atoms concerned. The ellipse drawing stylerepresents atoms by their thermal ellipsoid. Note that negative eigen values are reset at input to .001* the next largest.If the informationavailable is U[iso] only, a circle is plotted whose radiusis scaled according to its value.

ALL

FRAGMENT

GROUP
These subcommands can be used to specify which atoms are to be affected by the drawing style command.

Several other commands are available in addition to the basicstylecommands.

11.1   LINE commands.

There are no extra commands following LINE.

11.2   BALL commands.

RADII The user can specify the drawing radius (in angstroms) of a specified atom or element. The syntax is:

```
BALL RADII C 0.8 N1 1.1
```

which will draw all C atoms with a radius of 0.8 angstroms, and the N1 atom with radius of 1.1 angstroms.

DEFAULT This sets all the radii to their initial covalent values. The syntax is:

```
BALL RADII DEFAULT.
```

COVALENT

IONIC

VANDERWAALS This sets the radii of the specified atoms/elements to the appropriate values. The syntax is:

```
BALL RADII COVALENT N
```

The further subcommand ALL can be used - BALL RADII IONIC ALL - to set all atoms if required.

FILL

UNFILL These are header commands and are used to specify whether the circles drawn in the BALL style are to be filled with colour or not. No arguments are required by these commands.

11.3   ELLIPSE commands

TYPE
ELLIPSE may be followed by the sub command TYPE which enables the user to control the type of ellipse used to represent the atom. The syntax is:

```
ELLIPSE TYPE at/els/all n.
```

Type 'n' can take any of four values:

```
1 - bounding ellipse only.
2 - bounding ellipse and principal ellipses.
   This is the default representation.
3 - as 2 but excluding the principle axes.
4 - as 2 but with shading.
```

ALL ALL can be used followed by a number to set the ellipse type of all atoms in the drawing.
Note that any use of ELLIPSE TYPE will set all the atoms referred to ellipse type even if they were previously in LINE or BALL. Hence,

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```
ELLIPSE TYPE C 2  will have all carbon atoms drawn in type 2 form.
ELLIPSE TYPE ALL 4 will have all atoms drawn in type 4 form
```

NEGATIVE

The NEGATIVE sub command requires one argument. If atoms are input with negative temperature factors the atoms temperature factor is reset using the value specified by ELLIPSE NEGATIVE u. The default value of u is 0.01.

PROBABILITY

This is used to specify the size of the ellipsoid probability envelope displayed. It is followed by a percentage value.

Chapter 12

Connectivity Control

It is important that the user has complete control over thebonds displayed in a drawing. The CONNECT group of options is acomplicated one but has been designed so as to provide to userwith afully flexible set of commands.

12.1 CONNECT

CONNECT is used in one of two ways, either on its own or with a modifying sub-command.

CONNECT
The syntax for this command is:

```
CONNECT X Y dmin dmax
```

This will create two lists of atoms (one from X and one from Y which may be atoms, elements or * as required) and uses these lists when calculating connectivity. dmin and dmax are in angstroms. The distances between all combinations of the atoms in the two lists are determined. If distances any lie within the specified dmin -> dmax range (and the bonds do not already exist) they will be added into the connectivity lists. To connect up CU1 O bonds for example you could use:

```
CONNECT CU1 O 0.0 2.0
```

which would create one list - containing Cu1 only - and another list - containing all of the oxygen atoms - and then search for inter-list bonds. In this way, if any O - O bonds exist within the given range they will NOT be found. Note that if you require connections to be calculated between atoms of the same type you use:

```
CONNECT X X dmin dmax.
```

ALL CONNECT ALL requires two arguments dmin and dmax. The result is identical to CONNECT above except that ALL of the atoms are included in the calculation.

```
CONNECT ALL 0.0 2.0
```

will draw all bonds that fall within the 0.0 - 2.0 angstrom range.

DEFAULT CONNECT DEFAULT requires no arguments. This command does two things:

```
1)      Reset all of the connectivity radii
        to their initial values
2)      Calculate the connectivity according
        to these radii.
```

It is effectively a 'start again' option as it removes any changes in bonding that have been introduced with the JOIN, REMOVE etc options.

RADII This is a sub-command of CONNECT and comes immediately after it. It requires the following arguments:

```
CONNECT RADII X r
```

where X is the name of an atom or element and r is its new connectivity radius. The connectivity of this atom/element is then redetermined.

COVALENT

IONIC

VANDERWAALS These subcommands set the specified atoms to appropriate connectivity radii eg CONNECT RADII IONIC N. The further subcommand ALL can be used to set all atoms.

HBONDS This command enables the user to search for hydrogen bonds within the structure. The syntax is :-

```
CONNECT HBONDS dmin dmax X Y
```

dmin/dmax is the range for searching (in angstroms), X/Y are atoms/elements to be included in the search. For a H-bond to be valid it must be bonded to one of the atoms in the list X,Y etc AND be within the range of another of the atoms. For example, if we are searching for H-bonds involving oxygen atoms:

```
CONNECT HBONDS 0.0 2.5 O
```

will achieve this. There may well be eg C - H - O linkages within the range but only O - H - O ones will be registered. In this way we can filter the search and set a large value for dmax so that all the H-bonds are discovered without obtaining spurious information. The bond style used for H-bonds is dotted.

INTER
This option is intended to be used after a PACK or ENCLOSURE operation. This will find connections between atoms which have DIFFERENT packnumbers - ie. between assymetric units or between different GROUPS if PACK or ENCLOSURE GROUP has been used. The bonds are in the DOTTED style when generated. The syntax is:

```
CONNECT INTER O C 0.0 3.0
```

as for CONNECT itself.

FULL

DOTTED
The CONNECT command can also be used if bonds already exist to alter the style. There are three options:

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```
CONNECT DOTTED at1 at2
CONNECT DOTTED at1 el1
CONNECT DOTTED el1 el2
```

These change the style of the single bond at1-at2, the style of any el1-at1 bonds and the style of any el1-el2 bonds respectively. Note that in the latter case, el1 and el2 may be the same element ie you can make all C-C bonds dotted.

JOIN

DOTTED

FULL

Another connectivity header command is JOIN. This is a more specific command which is used to make a new bond. The syntax is:

```
JOIN DOTTED at1 at2
JOIN FULL al1 at2
```

This will create a new bond between at1 and at2 of the specified type.

REMOVE

This is the reverse command to JOIN. It will break the bond between the specified atoms. The syntax is:

```
REMOVE at1 at2
```

DISCONNECT

This command is the reverse of CONNECT.

```
DISCONNECT C O 0.5 1.5
```

will get rid of any C-O bonds that are OUTSIDE the range 0.5 - 1.5 angstroms.

ALL DISCONNECT ALL removes all of the connectivity information.

GROUP DISCONNECT GROUP is intended primarily for use with disordered structures although other uses can be envisaged. For example a substituent may be 'flipping' between two sites generating very short distances between atoms in different groups. It is not possible to DISCONNECT these bonds since some of the distances may appear to be 'normal'. To get over this, each disordered part is defined as a group (See DEFGROUP) and DISCONNECT GROUP is used to remove any bonds that exist between them. The syntax is:

```
DISCONNECT GROUP group1 group2
```

ATOM

This command deletes ALL bonds involving the specified atom. The syntax is:

```
DISCONNECT ATOM at1
```

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12.2 Miscellaneous CONNECT commands

There are three other commands which either relate to connectivity or to how the bond is represented on the output device.

TAPER

This controls the bond tapering. It has an initial value of 2.0. Increasing this increases the tapering of the bonds. This tapering is useful as it introduces a 3-D effect into the drawing. If tapering is not required then entering:

```
CONNECT TAPER 0.0
```

will achieve this.

THICKNESS

This command controls the thickness (radius) of the bonds in angstroms. It requires one argument, whose default value is 0.02.

```
CONNECT THICKNESS 0.04
```

will double the radius of the bonds as drawn.

TOLERANCE

This sets the tolerance used when determining whether or not a bond exists. The formula used is:

```
If  dist < ( C1 + C2 ) * tol  then a bond exists
```

where C1 and C2 are the connectivity radii of the atoms in question. The initial value of 'tol' is 1.1 ie the interatomic distance has to be no more than 10% greater than the sum of the two connectivity radii for a bond to be found. The syntax for the command is:

```
CONNECT TOLERANCE n
```

Chapter 13

Control Of Colour

Within CAMERON it is possible to control the colour of eachindividualatom and bond and also the colour of the labels.

COLOUR
This is the header command for colour control - it may befollowed byatom/element names if required. The syntax is:

```
COLOUR C BLUE N YELLOW ...
```

The atom/elements are entered in pairs together with the colour name.A list of the current colours can be obtained by using 'INFO COLOUR'. There are two setsof colournames - those for normal colour and those for greyscale eithermay be used interchangeably as once the colour type is altered thecolours are translated accordingly.

```
COLOUR ALL colour
```

Colours all the atoms the given colour

GROUP
This sets the colour of all of the atoms in a given group. The syntaxis:

```
COLOUR GROUP groupname colourname
```

*FRAGMENT*COLOUR FRAGMENT n col will set the colour of all atoms in the fragment attached to atom n.

*BACKGROUND*Sets the background colour.

*TEXT*Sets the colour of the title and other annotation text.

MENUTEXT

*BUTTON*Selects the colours of the text and buttons in menu mode.

LABCOLOUR
This sets the colour of the labels and requires a singleargument - thename of the new colour.

BONDS

Altering the colour of bonds is a more complicated procedure.It isfollowed by atoms/elements that define the bond and a colourname.These arguments are therefore entered in threes. For example, tomakeall carbon carbon bonds colour blue and all CU1 to oxygen bondscolour yellowyou would use:

```
COLOUR BONDS C C BLUE CU1 O YELLOW
```

*ALL*There is a further sub-command ALL which changes the colour ofALL ofthe bonds eg:

```
COLOUR BONDS ALL PINK
```

makes all bonds colour PINK.

GROUP
This sub-command requires arguments in pairs - the group nameand thenew bond colour:

```
COLOUR BONDS GROUP g1 LGREY
```

colours all bonds BETWEEN atoms in group g1 (both atoms in a bondmust be inthe group for its colour to be altered) to colour LGREY.

13.1   Example

To have a picture with the following requirements:

```
All C atoms colour BLUE
All N atoms colour PINK
Cu1 colour YELLOW
All Cu1 - O bonds colour LGREY
All bonds between atoms in group g1 colour RED
All other bonds colour GREEN
All labels colour PURPLE
```

the commands would be:

```
COLOUR C BLUE N PINK CU1 YELLOW
BONDS ALL RED
(do this first)
BONDS CU1 O LGREY
GROUP g1 GREEN
LABCOLOUR PURPLE
```

BACKGROUND
The default background colour is WHITE but this can be changed as required by the COLOUR BACKGROUND colour command.

DEFAULT
The default colours for the elements are as defined in the PROP.CMN file -

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```
B - ORANGE
Br,Cl,F,I - LGREEN
C - GREEN
D,H - LGREY
N - BLUE
O - RED
P - PURPLE
S - YELLOW
SI - DGREY
```

These colours can be recovered if altered by using COLOUR DEFAULT which returns ALL atoms to their original colours.

NORMAL

GSCALE

These sub-commands allow the user to see how the hardcopy greyscale picture will look. COLOUR GSCALE changes the screen colours to the equivalent greyscale colours. The colour names GREYn (n=1,14) can be used to specify colour changes if required as COLOUR N PURPLE makes little sense on a greyscale picture.

```
BLACK      BLACK
BLUE       GREY1
GREEN      GREY2
ORANGE     GREY3
RED        GREY4
CYAN       GREY5
MAGENTA    GREY6
LGREY      GREY7
GREY       GREY8
LGREEN     GREY9
LBLUE      GREY10
LRED       GREY11
PINK       GREY12
PURPLE     GREY13
YELLOW     GREY14
WHITE      WHITE
```

Chapter 14

Atom Labelling

LABEL

NOLABEL
The LABEL and NOLABEL commands control the atom labelling. Theyareset up in an identical way to INCLUDE and EXCLUDE and the syntaxisidentical:

```
LABEL C1 C2 ONOLABEL C H1LABEL ALLNOLABEL ALLLABEL GROUP g1 ....
```

are all valid. Note that atoms will not be labelled if they arenot included in the picture.

MOUSE
All atoms will be labelled if the LABEL command has been used forthem. The label positions can be altered using the mouse if required.Note that label positions are recalculated if atoms are included orexcluded or a change in the view direction has occurred. Therefore, it isadvisable that the 'final' view is obtained before labels are positionedwith the mouse.

Mouse labelling is controlled as follows. The user clicks on aposition on the screen (once the message Mouse Labelling activated hasbeen seen). If this position is over a label then the label is replacedby a box of the same size as the label. A red cross is drawn over theatom that the label refers to to aid identification. The mouse is thenused to position the TOP LEFT HAND CORNER of the label by a secondclick. Alternatively, hitting the N key (for Nolabel) will remove thelabel altogether.

If the mouse is clicked on an atom which is NOT labelled then a labelwill appear at the atom centre, this label can then be moved asdescribed above.

If at any time the user wishes to view the current picture without releasing the mouse, this can be done by hitting the 'V' key.

GENERATED

INITIAL
These commands relate to the pack number display while labelling.Atoms are assigned a pack number after PACK or ENCLOSURE. This number isthen displayed as eg N1_5. These numbers are used to refer to atoms andelements as required. INITIAL (the default) will just display N1 whileGENERATED shows N1_5.

CELL Controls the cell labelling.

FRAGMENT Allows the user to set labels for a given fragment.

FONT

This sets the point size of the font to be used in hardcopy output. It requires one argument.

DEFAULT This resets the point size to its default value.

TEXT

POSITION This allows the user to annotate a picture. The syntax is:

```
TEXT "text string" POSITION x y
```

The text must be in quotes. x and y are the position of the text in percentages from the top left hand corner of the diagram. After the text is processed it is assigned a number.

NUMBER The NUMBER command can be used to move a text item after it has been created by using TEXT NUMBER n POSITION x y.

Chapter 15

Other Picture Controlling Commands

There are a few other commands in CAMERON which deal with control of the type of picture being used.

MAXIMISE

This command is related to the VIEW commands PLANE, ALONG, VERTICAL etc. In these commands the view direction does not define all of the degrees of freedom of the molecule. It is possible to rotate the molecule further so that as much of is as possible is shown on the screen.

ON

OFF

These two commands switch maximisation calculations ON and OFF. These calculations are slow - especially for large molecules so they are included as an option.

SCALE
DFIX
DUNFIX

These two commands allow the user to control the calculation of picture scale. SCALE FIX sets the scale to its current value and does not recalculate it, irrespective of changes in the number and position of atoms in the picture. SCALE UNFIX reverts to scale calculations.

SET

SCALE SET is followed by a number, the value of the scale to be used for all subsequent pictures. This can be altered with another SCALE SET command or by issuing SCALE UNFIX.

Chapter 16

Symmetry Input

16.1 Input of symmetry operators

CAMERON is a crystallographically oriented program and hence many of its functions require the use of symmetry operators. There are two methods of inputting the symmetry operators, inputting the Spacegroup symbol and inputting the individual operators themselves.

SPACEGROUP

The SPACEGROUP command is followed by the symbol, which must contain all UPPER CASE letters. If the symbol is in a non-standard setting then the full symbol must be entered. For example P 21 will be interpreted as P 1 21 1 which is the standard setting. If P 21 1 1 is required then the "1's" must be entered to force the choice of unique axis.

The syntax of the command is:

```
SPACEGROUP X X X X
```

where X are "fields" of the symbol, with spaces between fields ie entered as P 21 and NOT P21. The program will then output the operators that have been calculated for the symbol . Note that if a centre of inversion is present the inverted operators will NOT be shown. Also the operators generated from the centring vectors - eg 1/2 1/2 1/2 for body centring - will NOT be shown. The complete list of operators used for packing etc can be found by entering INFO SYMMETRY.

SYMMETRY

The input of symmetry operators can be done "by hand" if required. There are several steps and sub-commands available to do this.

OPERATORS

This sub-command MUST be entered even if only the x y z operator is to be included. The syntax is :-

```
SYMMETRY OPERATORS x y z -x y+1/2 -z ...
```

with the operators being entered with the translational part in fractional form (1/2 , 1/3 , 1/4 , 2/3 , 1/6 , 5/6 are recognised) which must come after the x/y/z as required. The fractional part must be linked to the x/y/z part with a + or - sign. Note that NO spaces are allowed within each part of the operator. This is so that ambiguities cannot arise.

CENTRE

This command is used to introduce a centre of inversion into the symmetry information it must be followed by a centring letter (P,A,B,C,I,F,R) or the command VECTORS.

NOCENTRE
This command is used to specify that there is no centre of inversion - the centring vectors are the specified by letter or by using VECTORS.

VECTORS
This command enables the user to introduce centring vectors into the symmetry operators eg for body centring use :-

```
VECTORS 0 0 0 1/2 1/2 1/2
```

USE

NOUSE These commands allow the user to omit certain symmetry operators from the packing calculations. The command is followed by the operator numbers (found using INFO SYMMETRY) of the operators needed.

ALL This may be used to USE/NOUSE all of the operators. Note that using NOUSE ALL without following it with USE n will result in no atoms being generated after a pack operation!

16.2 Example of Space Group Input

In order to end up with the Spacegroup F m m m we require :-

```
SPACEGROUP F M M M
```

or

```
SYMMETRY OPERATORS
X Y Z  -X -Y Z  -X Y -Z  X -Y -Z
CENTRE
VECTORS
0 0 0
0 1/2 1/2
1/2 1/2 0
1/2 0 1/2
```

16.3 Other symmetry related operations

SETUNIT
This command causes the atoms that are to be included in the current picture to be set as the asymmetric unit. Their data then replaces that of the initially input atoms and they are used as the asymmetric unit from now on. This is useful if, for example only half of a molecule is present in the asymmetric unit. The other half can be generated with ADD and then SETUNIT is used to treat all of the atoms as the basic "building block". SETUNIT is a DANGEROUS command in that it cannot be undone - UNPACK will NOT reverse the operation. Therefore the user is prompted for confirmation before the command is executed. The syntax is simply SETUNIT.

ENANTIO

This command inverts the hand of the atoms in the asymmetric unit. Note that the operator applied is :-

```
-1  0  0
 0 -1  0
 0  0 -1
```

and no spacegroup changes that may be required are made.

SPECIAL

ON

OFF Controls the special position calculations that occur during packing to eliminate duplicate atoms. By default this is ON.

Chapter 17

Crystal Packing Commands

There are two methods of crystal packing available, PACK andENCLOSURE. Both use ALL of the symmetry operators in theSpacegroup togenerate all of the atoms that lie within a user-defined volume.Thecommands ADD and MOVE are available if single symmetry operatorsarerequired. The difference between the two commands lies in themethod ofvolume definition.

17.1 PACK

The PACK command allows the user to define a volume to be filled relative to the unit cell. One of two-sub commands is required to define this volume.

CELL
PACK CELL will cause the program to generate all the atoms that lie within the unit cell. This is the default option if no range for packing is input.

WINDOW
PACK WINDOW allows the user to define the volume in terms of the unit cell axes. It is followed by three pairs of numbers.

```
PACK WINDOW xmin xmax ymin ymax zmin zmax
```

The values of xmin etc are relative to the unit cell origin. Therefore to define a volume of which contained all of the x axis, all of the y axis and the first half of the z axis we would use:

```
PACK WINDOW 0.0 1.0 0.0 1.0 0.0 0.5
```

If more than one unit cell is required negative numbers and numbers exceeding one may be used.

One more sub-command may be entered after the WINDOW or CELL commands. If this command is omitted then the option chosen in the last PACK command will be used. If this is the first time PACK is used then CUT is the default option. Three sub-commands are available:

CUT CUT will generate all the atoms that lie within the defined volume. ie. the generation is "cut" at the boundary.

COMPLETE COMPLETE is most useful for molecular crystallographers. It will generate all the asymmetric units that have ANY ATOMS lying with the defined volume.

CENTROID CENTROID is similar to COMPLETE except that it calculates the centroid of the asymmetric unit (as though all of the atoms have equal weight) and includes only those which have their centroid within the defined volume. This is particulary useful for molecular crystallographers as it creates a picture without the "odd atoms" at the edge of the unit cell.

17.2 Dealing with connectivity

There are three other qualifying commands that apply to PACK:

INTRA

INTER

KEEP
These deal with the treatment of connectivity calculations once the PACK has been carried out.

INTRA
This qualifiers means that the connectivity will be calculated within each newly generated asymmetric unit only. Any changes to the bonding - eg with JOIN, REMOVE, CONNECT, COLOUR BONDS - will be undone. This is the fastest option.

INTER
In this case connectivity is calculated once all of the atoms have been generated - therefore if any intra-unit bonds exist they will be found.

KEEP
This is the default option. Connectivity is copied from the unit used to do the packing - this includes colour and style changes if any - into the bond info of the new atoms. This is done for each asymmetric unit as it is generated and is slower than INTRA as it requires more comparisons to be carried out.

17.3 EXAMPLES

Therefore, to create a picture containing all of the complete molecules within a cube of side equal to 2 unit cells we need :-

```
PACK
WINDOW 0.0 2.0 0.0 2.0 0.0 2.0
COMPLETE
```

Or alternatively,

```
PACK
WINDOW -1.0 1.0 -1.0 1.0 -1.0 1.0
COMPLETE
```

17.4 ENCLOSURE

The enclosure command is more flexible than PACK as it enables the user to choose the "origin" for the atom generation. The first task is to specify this origin which is either a point in the unit cell or an atom.

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17.5   Choice of enclosure "origin"

ATOM
   If we wish to generate the atoms around Cu1 in order to examine the coordination environment for example we can use:

```
ENCLOSURE ATOM CU1
```

POINT
Alternatively we can choose the centre of the unit cell:

```
ENCLOSURE POINT 0.5 0.5 0.5
```

   The POINT sub-command can be used if an atom does not lie at the point in question eg if we are examining a "hole" within a structure.

17.6   Type of volume to be used

There are three different ways of defining the volume of enclosure:

SPHERE
This will generate a sphere of enclosure about the origin. The syntax is:

```
SPHERE r
```

   where r is the radius in angstroms of the sphere.

ANORTHIC
   This is used to generate an ANORTHIC box ie a box whose sides are parallel to the unit cell axes. As this box is directly related to the unit cell its dimensions are given in fractional coordinates. The syntax is:

```
ANORTHIC -x +x -y +y -z +z
```

   Therefore, to generate an anorthic box with sides extending one quarter of a unit cell in all six directions from the defined origin we use:

```
ANORTHIC 0.25 0.25 0.25 0.25 0.25 0.25
```

ORTHOGONAL
   This is used to generate a box whose sides are perpendicular to each other. The z axis lies along the current view direction and the x and y axes lie across and vertically up the screen respectively. The dimensions of this box is defined in a similar way to the ANORTHIC box except that they are given in angstroms. For example, to generate a box that is 4.0 angstroms wide in x, 1 in y and 0.5 in z we would use:

```
ORTHOGONAL 2.0 2.0 1.0 1.0 0.25 0.25
```

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It is important to note that this volume is related to the CURRENT view direction. The VIEW ALONG AXIS command can be used to orient the picture prior to carrying out this command if required.

CUT

COMPLETE

CENTROID As with PACK a further sub-command can be used if desired to define the type of boundary handling used. CUT, COMPLETE and CENTROID have the same meanings as described above for PACK.

INTRA

INTER

KEEP These sub commands have an identical meaning to those described for PACK above.

17.7 EXAMPLE

To generate all the atoms that lie within a sphere of radius 5.0 angstroms about a CU1 atom we use:

```
ENCLOSURE
ATOM CU1
SPHERE 5.0
CUT
```

To generate all the asymmetric units that have any atoms within a box of side 0.5 units around the unit cell centre we use:-

```
ENCLOSURE
POINT 0.5 0.5 0.5
ANORTHIC 0.25 0.25 0.25 0.25 0.25 0.25
COMPLETE
```

And to generate all the atoms that lie inside a box centred on the point 0.25 0.25 0.25 and of sides x=1.0 y=2.0 and z=3.0 angstroms :-

```
ENCLOSURE
POINT 0.25 0.25 0.25
ORTHOGONAL 0.5 0.5 1.0 1.0 1.5 1.5
CUT
```

17.8 PACKING MORE COMPLICATED STRUCTURES

The PACK and ENCLOSURE commands always work on the initial data- unless a SETUNIT command has been issued. In some cases however, it is more useful for the user to be able to deal with certain sections of the structure separately. This is most likely to occur where there is more than one distinct unit in the asymmetric unit. This is dealt with by the command GROUP.

GROUP
GROUP can be used directly after both PACK and ENCLOSURE. The syntax is:-

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```
PACK GROUP groupname CELL ...
or
PACK GROUP groupname WINDOW ...
etc
```

This causes the groups to be packed individually, the CENTROID, COMPLETE and CUT commands are applied to the group and not to the asymmetric unit as a whole. Packs are cumulative, unless a PACK/ENCLOSURE is done without the GROUP sub command in which case the previously generated atoms are overwritten. Groups are defined with the command DEFGROUP.

If required, more than one groupname can be packed at once - they are all treated separately. All groups can be packed in turn if PACK GROUP * is used.

17.9 UNPACK

This command causes all atoms generated via PACK or ENCLOSURE to be removed from the calculations, drawings etc. It has no sub-commands. It also works with ADD and MOVE generated data.

Chapter 18

Add And Move - Further Symmetry Related Commands

The PACK and ENCLOSURE commands already detailed allow the usertoapply all of the symmetry operators in the spacegroup to theinitialset of atoms in order to get a fully 'packed' result. In somecaseshowever, the user may wish to apply only one symmetry operatoror toapply ones that are not present in the spacegroup. The ADD andMOVEcommands allow this.

18.1   ADD

The ADD command allows the user complete control over the symmetry operator used to generate new atoms. The first task of the user is to generate a list of those atoms to be used in the symmetry generation later. One of the following sub-commands is required :-

ATOMS
The names of atoms to be included in the pack list are specified here. Element names can also be used if required.

ALL
ALL refers to the atoms that are in the current list. If any atoms have been generated by previous PACK , ENCLOSURE or ADD commands then these will all go into the list.

INITIAL
ADD INITIAL means that the only atoms to go into the ADD list are those that were initially input.

GROUP
This is followed by a group name. The group must have been previously been defined by the command DEFGROUP.

Once the ADD list has been created the user must then supply the symmetry operators which will act on the atoms in this list to generate the new atoms. The symmetry input is in two parts.

OPERATOR The symmetry operator may be input in decimal or fractional form eg

```
x y+1/2 z
```

```
-0.333-x -y -z
ETC
```

Decimal translations may come before or after the axis symbol. The fractions 1/2, 1/3, 1/4, 2/3, 1/6 and 5/6 are accepted by the
program, but **must** appear **after** the x/y/z character. There must be spaces between the three parts but NO SPACES within the operator ie

```
X + 1/2 -Y  Z
```

will produce an error as it is not possible to tell whether you mean X+1/2, -Y, Z or X, +1/2-Y, Z. This strict input syntax is used to eliminate any ambiguities.

TRANS Translations can also be applied if required. The translations are applied in unit cell fractions. The syntax is :-

```
TRANS x y z
```

18.2 EXAMPLES

To generate an atom at x+1/2 y z from an atom at x y z we can use

```
ADD
ATOMS C1
OPERATOR X+1/2 Y Z
```

or we could use

```
ADD
ATOMS C1
TRANS 0.5 0 0
```

The OPERATOR and TRANS commands can be used together if required. We can apply a symmetry operator followed by a translation. This reduces the errors that may occur when trying to combine the two things into one symmetry operator.

The use of INITIAL versus ALL is illustrated below. Start with :-

```
ADD
ALL
TRANS 1 0 0
```

which gives us a molecule at x y z and another at x+1 y z. Follow this with :-

```
ADD
ALL
TRANS 0 1 0
```

and we get four molecules, x y z , x+1 y z , x+1 y+1 z and x y+1 z. Following it with :-

```
ADD
INITIAL
TRANS 0 1 0
```

Gives us three molecules, x y z, x+1 y z and x y+1 z.

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18.3 MOVE

The syntax for this command is identical to that for ADD. Therefore the commands available are :-

ATOMS

ALL

GROUP

INITIAL
Which must be followed one (or both) of :-

OPERATOR

TRANS
The MOVE command applies a symmetry operator and/or a translation to all of the atoms held in the list defined by the ATOMS/ALL/GROUP/INITIAL commands. Unlike ADD therefore, the same number of atoms are present at the beginning and end of the operation.

Chapter 19

Distance And Angle Calculations

CAMERON allows the user to calculate distances , angles andtorsion angles.

DISTANCE
In order to perform a distance calculation two atoms lists must begenerated. The first list is used as a 'starting atom' and the secondlist is for 'target atoms'. Distances will be calculated between atomsin separate lists BUT NOT within the lists themselves. The list may begenerated in two ways:-

```
DISTANCE N O
```

generates two lists - both of which can all the N and all the O atoms.In this case N-O, N-N and O-O distances will be found.

FROM

TOThese subcommands allow to specify different starting and target atoms.

```
DISTANCE FROM N TO O
```

will only calculated N-O distances. Note that the distance arguments maybe either atoms or elements as required.

RANGEThis sets the minimum and maximum ranges for displayed distances. Thesyntax is :-

```
DISTANCE RANGE dmin dmax
```

distances are given in angstroms. If only TWO atoms are present in theatom list then the distance will be outputted irrespective of the range.However, as the full calculation will be carried out first there may bea time delay while the calculation proceeds.

19.1   Method of Calculation

The distances output make use of the symmetry operators in order to find distances within the given range. The starting atom coordinates are NOT ALTERED but those of the target atoms are. The symmetry operators (and any suitable translations) are used to move the target atoms around. The output produced is:-

```
N1_0      O2      2.323
Operator x y z Translations 0 0 1
N1_0      O2_4    1.114
Operator -x y+1/2 -z Translations 0 0 -1
```

These show the N1 to O2 distances. The first distance relates to an O2 atom which does not currently exist. The operator and translations shown can be used with ADD to generate the atom if required. The second distance is to an atom (O2_4) which does exist. ie. if no pack number is given for the second atom it is not present in the current list.

ANGLE

TORSION

These commands are used to find angles and torsion angles between atoms that are in the current list. They are entered in sets of three (or four) as required.

Chapter 20

Information On Data Held Within The Program

CAMERON holds a number of pieces of information while it is runningand in some cases it is useful for the user to be able to access thisinformation.

INFORMATION
This command is followed by a sub-command which specifies the type ofinformation wanted.

CELLOutputs the unit cell parameters.

ATOMSOutputs the names of atoms stored within the program. It produces twolists - one of atoms currently included and one of atoms currentlyexcluded from the picture.

COLOURThis outputs the colour names that are available.

SYMMETRYThis command outputs the symmetry operators currently stored.

GROUPOutputs a list of the currently defined groups and their members.

PACKNUMBERSOutputs the symmetry operator and translation associated with a given packnumber. The syntax is INFO PACKNUMBER n1 n2 n3.

Chapter 21

Group Definitions

For complicated structures it is sometimes useful to defineGROUPS ofatoms which can be referred to as a whole later. EXCLUDE,INCLUDE,COLOUR BONDS etc can all be used with the GROUP sub-command.

DEFGROUP

This is the main header command and is followed by the name ofthegroup. Note that it is not possible to have group names thatbegin withGROUP itself - g1, g2 are valid names but group1, group2 are not.Up totwelve characters are allowed to define the group name.

ATOMS

This is followed by a list of atoms/elements to be included inthegroup.

GROUP

It is possible to have an atom as a member of up to threegroups atonce. You can therefore add groups into other groups (see Example).

FRAGMENT

The user can include atoms in a group by defining a fragment. Thefragment definition requires a single atom. Any atoms joined to it, andany atoms to those etc are made part of the group.

DELETE

You can also remove atoms from groups if required.

21.1   Example

Consider an molecule that contains a tri-phenyl phosphine. A use of the DEFGROUP command would be :-

```
DEFGROUP PHENYL1
ATOMS C1 C2 C3 C4 C5 C6
DEFGROUP PHENYL2
ATOMS C11 C12 C13 C14 C15 C16
DEFGROUP PHENYL3
ATOMS C21 C22 C23 C24 C35 C36
DEFGROUP PPH3
ATOMS P
GROUP PHENYL1 PHENYL2 PHENYL3
```

If you then realise that there are two phosphorus atoms in the molecule P1 and P2 you can use :-

```
DEFGROUP PPH3 DELETE P2
```

to remove P2 as it is not a member of the tri-phenyl phosphine group.

Chapter 22

Miscellaneous Commands

RESET

This command allows the user to begin again without having to exit and reload CAMERON. All current flags will be set to their initial states. Note that if a CAMERON.INI file is present it will not be obeyed after aRESET command. The screen will be set to VGA automatically (as on startup) if a CAMERON.SRT file is present.

LOG

The LOG command is used to generate a log of the CAMERON session, thismay be OBEYed later if required.LOG must be followed by a filename. If a file is already in use for alog file then the log information will be transferred to the new file.

EDIT

ON

*OFF*This sets the edit option which is used when an error is found in an input line. If edit is on (the default) then the user is prompted as described in Chapter 1. If not the computer will bleep and put up the message "Error: Automatic Abandon", ignore any unexecuted commands and wait for a new input line.

MENUS

ON

*OFF*The user is able to control the program via push button menus at the side of the screen (PC only). These can be turned on or off as required.When the menus are active the user can input commands as normal by typing - they will appear in a box at the bottom of the screen.

ISSUE

This allows the user to execute a single system command. This command should be enclosed in quotes if it is longer than one word or if it corresponds to a CAMERON command.

PRINT

This allows the user to print a hardcopy file. The file will be closed if it is currently attached to CAMERON via a COPY command. **NOTE** that the print job will be very slow - it may be quicker to close down CAMERON first.

Chapter 23

How To Stop The Program

END
  The command END will cause the program to finish.

Chapter 24

Menu Definition File

The labels on the menu buttons and the actions they invoke are in the file cameron\button.cam.

The first line gives the number of columns and the number of lines in the menu.After this, adjacent pairs of lines give the text to appear on the button, and the CAMERON commands to be obeyed by the button. The pairs of lines are given first for column 1, then column 2 etc.

Chapter 25

Some Useful Ideas

To produce black and white illustrations for papers,try

```
colour c blackcolour h blackcolour n blackcolour o blackcolour bond all whiteball all unfilball h fillcolou
```

To hack up a packing diagram, cutting out most and just keeping a bit,try (all on one line)

```
EXCLUDE ALL INCLUDE AREA
```

Then use the mouse to draw round the bit you want to keep.

Chapter 26

Cameron Manual