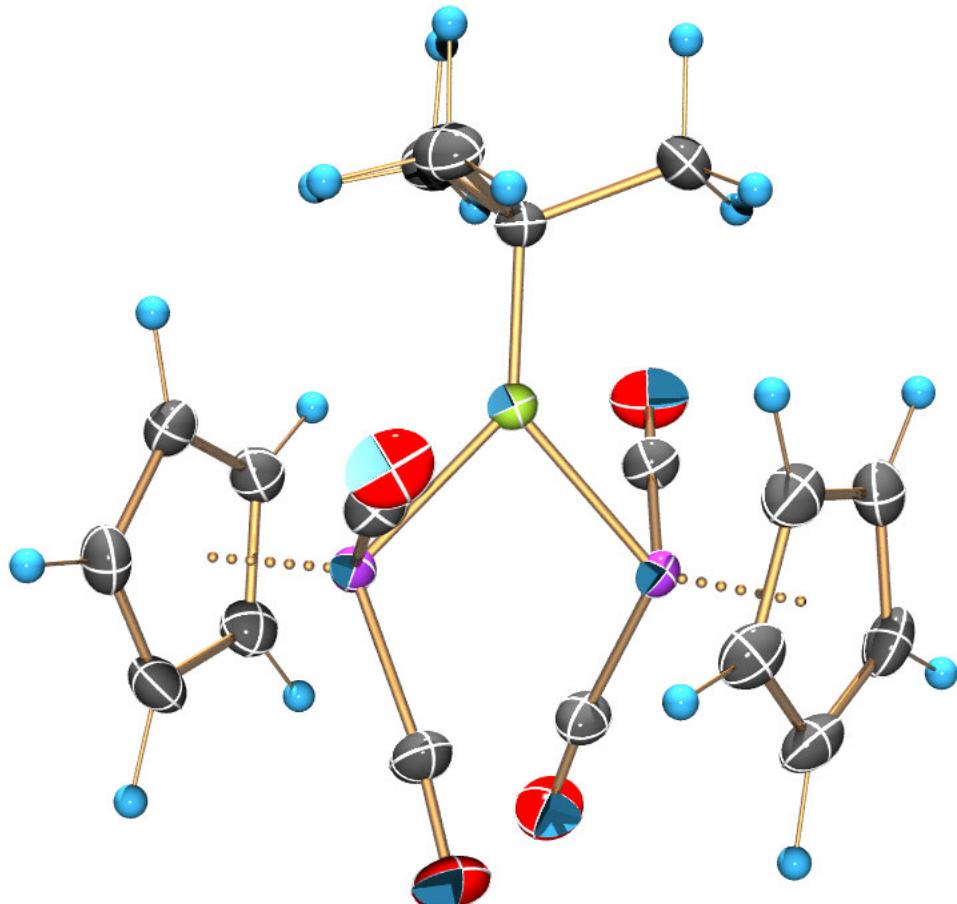


Ortep-3 for Windows

Version 2.0

A current version of *Ortep-3 for Windows* is available from :

<http://www.chem.gla.ac.uk/~louis/software/ortep3>



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1. INTRODUCTION

*Ortep-3 for Windows*¹ is an implementation of *ORTEP-III*² which incorporates a Graphical User Interface (GUI) to make the production of thermal ellipsoid plots much easier. Most of the commonly used features of *ORTEP-III* are directly available from the GUI, and all the facilities present in *ORTEP-III* are also available in *Ortep-3 for Windows*. The main GUI facilities are:

- *Ortep-3 for Windows* can directly read most crystallographic ASCII file formats that contain information on the positional and anisotropic displacement parameters. Currently supported formats are SHELX, GX, CIF, SPF, XD, CSSR-XR, CSD-FDAT, GSAS, Sybyl MOL, XYZ (various), PDB, Rietica-LHPM, FULLPROF, AIMPAC-WFN, Chem3d-Cartesian, GAMMES-UK input and ICSD. In addition, *Ortep-3 for Windows* will accept any legal *ORTEP-III* instruction file.
- Up to 996 atoms may be present in the asymmetric unit, and up to 2000 atoms may be drawn. Covalent and van der Waals radii for the first 105 elements are stored internally and are read from the external file *atomcols.def*, which may be modified by the user. All bonds are calculated automatically from these covalent radii. Any individual bonds may be selected for removal, or for a special representation.
- Several style-templates are supplied, but the graphical representations of thermal ellipsoids for any element or selected sets of atoms can be individually set. All the possible graphical representations of thermal ellipsoids in *ORTEP-III* are also available in *Ortep-3 for Windows*. Over 120 different colours are stored internally and an unlimited number of colours may be defined. All graphic objects may be drawn in any colour.
- The GUI provides a mouse labelling routine. Any number of selected atoms may be labelled, and any available Windows font may be used for the labels. The font attributes, e.g. italic, bold, colour, point-size etc can also be selected via a standard Windows dialog box.
- The HPGL and PostScript Graphics drivers from *ORTEP-III* provide standard graphic metafiles, and it is also possible to get high quality graphics output by printing directly to an attached printer. The screen display may be saved as BMP metafiles, and may also be copied to the clipboard for subsequent use by other Windows programs, e.g. word processing or graphics processing programs. Colour is available for all these output modes.
- High quality raster images are available using the *Raster3d* or *POV-Ray* formats. Several representations are available from the *POV-Ray* interface, including thermal ellipsoids (standard ORTEP, RMSD and MSD surfaces) and van der Waals surface plots.
- A simple text-editor is provided, so that input files may be modified without leaving the program. The *ORTEP-III* instruction file which is written by the GUI (and which corresponds to the currently displayed picture) may be saved at any time for future use or modification.
- Symmetry expansion of the asymmetric unit to give complete connected fragments may be carried out automatically, or the user may define a single seed-atom for symmetry expansion of a single fragment.
- Unit cell packing diagrams are produced automatically.

- A number of options are provided to control the view direction. The molecular view may be rotated or translated by button commands from the tool bar, and views normal to crystallographic planes may also be obtained.

1.1 NEW FEATURES IN VERSION 2

The creation of Version 2 has involved a complete rewrite of the GUI code. The GUI retains virtually all the useful features of Version 1, and the layout has remained very similar. New features are :

- The viewpoint may be rotated in real time by mouse dragging. If more than 100 atoms are displayed, the drawing mode switches to line-style while dragging.
- Dynamic allocation of memory is implemented for all the GUI functions, so that no arbitrary limits on special atom or bond treatments etc are imposed. Unfortunately it was not possible to apply dynamic allocation for the core *ORTEP-III* graphics driver, but the maximum number of atoms in the asymmetric unit has been increased to 996.
- Much more text output is now given and is displayed in a separate window, the OrtepConsole Window (which is opened as a minimised Window on the taskbar).
- Many more parameters are permanently stored and updated in the INI file *ortep.ini*, so that most user preferences are retained between sessions. The orientation and mouse labels for the currently displayed illustration can be stored when the program is closed, and restored automatically on reloading *Ortep-3 for Windows*.
- The *POV-Ray* interface has been improved, so that the ray traced image is a much closer representation of the screen drawing.
- An automatic searching for H-bonds is introduced. The H atoms must be in the model.
- An entirely new screen display is used for routines that use mouse selection of atoms or bonds. Side panels provide an explanation of how each task may be accomplished.
- The mouse labelling has been improved, to comply more closely with Acta Cryst requirements regarding symmetry labelling.
- The screen display can be saved in bitmap files in various formats, and with much higher resolution than the monitor resolution.
- In UnitCell drawings, the cell outlines for the *a*, *b*, and *c* axes are automatically colour code as RGB (red, green & blue) respectively

In this manual, computer programs like *Ortep-3 for Windows* are shown in italic bold, directories like the **working directory** are shown in bold red and ORTEP parameters like **BondSearchDistanceMax** are shown in bold green. File names such as *ortep.ini* are shown in italic Times Roman font. The program name *ORTEP-III*² refers to original program of Burnett & Carroll, while *Ortep-3 for Windows* refers to the combination of the GUI and the graphics driver *ORTEP-III*.

2. HOW ORTEP-3 FOR WINDOWS WORKS

*Ortep-3 for Windows*¹ uses the current release of *ORTEP-III*² (version 1.0.3, dated January 2000) as the drawing engine, with very little change. Some of the arrays have been increased in size, and some features which are rendered redundant by the GUI (*e.g.* the line editor and command line menus) have been removed.

Major features of the GUI are the mouse labelling routine (see 5.4.2), interactive GEOM (see 5.8.4), and some extra output facilities (see 5.1.6, 5.1.7, 5.6.6 - 5.6.8). The GUI is essentially an editor that writes input files for *ORTEP-III*, and makes production of ORTEP pictures substantially easier. In most instances it is not necessary for the user to understand how *ORTEP-III* works, although if some less common features are required, *e.g.* the drawing of critical net illustrations, then it will be necessary to prepare an *ORTEP-III* instruction file manually (or modify one produced by *Ortep-3 for Windows*). *Users should be aware however that the program ORTEP-III requires FORTRAN fixed format instructions, and any format error in the instruction file may result in a program crash or obscure failure.* The complete *ORTEP-III* manual is available on the Web.³

Each drawing of a new structure is initiated by opening a new coordinate file (from the FILE menu item). Opening a new file has the following results:

- The selected coordinate file is first checked for the file-format. The decision as to the file-format is made on the basis of the *contents* of the file, rather than the filename extension. If there is an error in reading the file, or if the program does not recognise the file format, a message to this effect is issued to the OrtepConsole Window, and the program is ready to read another coordinate file.
- If the coordinate file is successfully read, then the style is reset to the default style **Default**, the contents mode is set to **Use Asymmetric Unit**, and a number of other options are reset to their standard conditions.
- If the selected coordinate file is an *ORTEP-III* instruction file, the user is offered a choice. The file may be treated as other coordinate file formats, with all the *ORTEP-III* drawing instructions ignored. Alternatively, the file may be interpreted *directly*. If this latter option is chosen, then most of the facilities of the GUI are by-passed, the only ones available being the PostScript and HPGL metafile output (FILE menu), the mouse labelling routine (LABELS menu) and all items from the GRAPHICS menu. Note that *ORTEP-III* is downwards compatible, and will accept instructions from previous versions of ORTEP.
- On the other hand, if the selected coordinate file is NOT an *ORTEP-III* instruction file, the program then writes its own internal *ORTEP-III* instruction file that is subsequently interpreted and displayed on-screen. All facilities of the GUI are then available to modify the ORTEP picture. Once a suitable view is obtained, hardcopy graphic output may be produced in a variety of ways.

3. ORTEP PARAMETERS

Many of the parameters required by the GUI and *ORTEP-III* have sensible default values embedded in the program. These values may be modified dynamically by selecting the menu item **Change ORTEP Parameters** in the **STYLES** menu (see 5.3.2). A parameter box is then displayed, which allows the user to scan all the modifiable parameters and enter any new desired value. Changes made in this way are stored permanently in the file *ortep.ini*, which is read every time the program is loaded. A full list of all **ORTEP Parameters** is given in Table 6.1 at the end of this manual.

4. GENERAL INFORMATION ON ORTEP-3 FOR WINDOWS

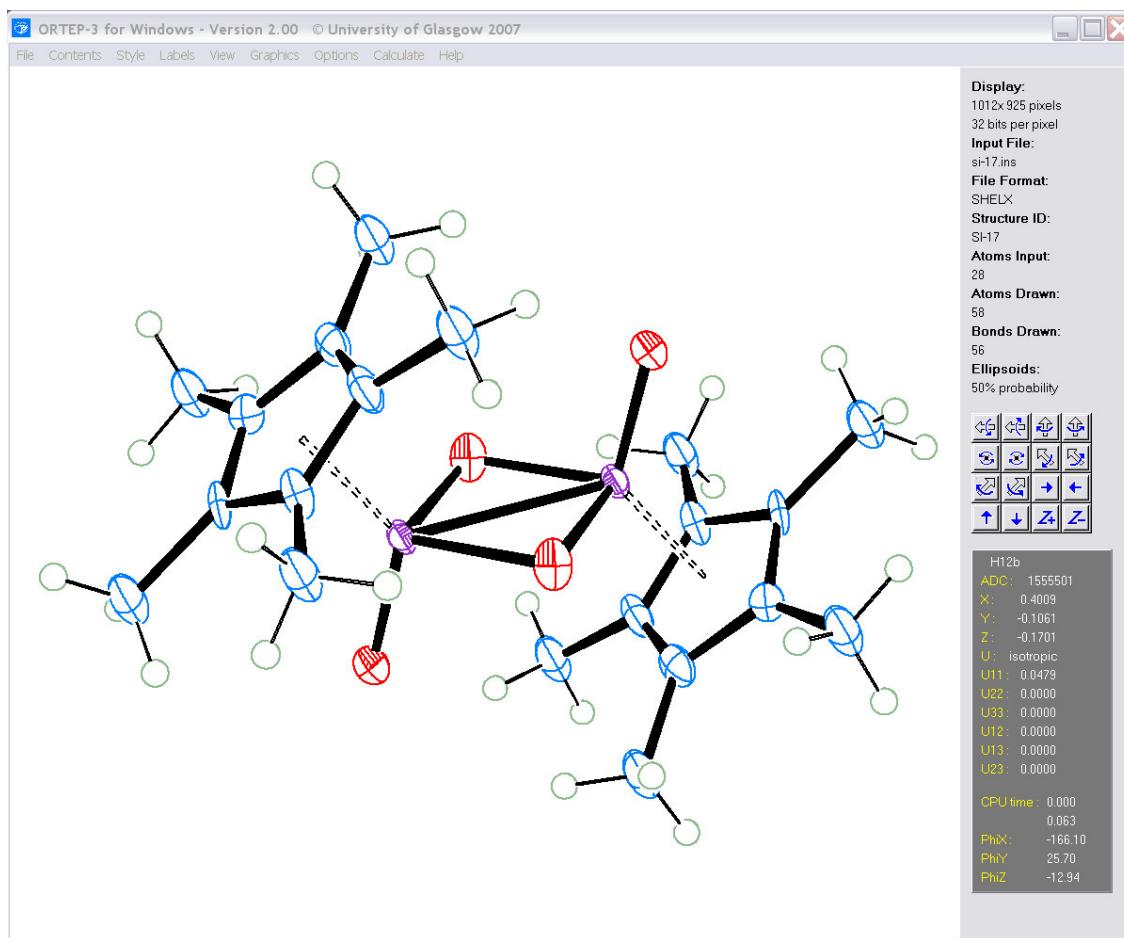


Figure 1. The standard display screen for *Ortep3 for Windows*. When this standard side panel with the tool bar is displayed, the viewpoint may be rotated by mouse dragging.

The GUI for the new version of *Ortep-3 for Windows*, shown in Figure 1, is similar to that for previous versions of the program. The maximum allowed number of atoms in the asymmetric unit has been increased to 996, while the number of atoms that may be drawn remains 2000, so that unit cell packing diagrams are

more complete. ORTEP is primarily designed for producing publication-quality thermal ellipsoid plots of small molecules. It is relatively slow, and not really suited for macromolecular structures (there are many other excellent packages which do this). However, it is an excellent “visualisation tool” for crystallographic analysis, since the ellipsoid representation of the anisotropic displacement parameters provides an instant visual check on the quality of the crystal structure refinement. Unusually elongated or flattened thermal ellipsoids are almost invariably an indication of a serious problem in the structure refinement.

4.1 ATOM LABELS

While *Ortep3 for Windows* does not explicitly prescribe any format for atom labels, it is *strongly recommended* that the atomic label in the input data file should consist of the chemical symbol followed by a character string where at least the first character is a non-alphabetical character (preferably an integer representation), e.g. "H100". The non-alphabetical character string may optionally be enclosed in brackets, e.g. "H(100)". Atom labels are used to determine the atomic type for several of the input formats, where this information is not obtainable in another way, and are used to identify the unique set of atoms. They are stored internally without brackets, with a maximum of 10 characters. *It is very important that each atom has a unique label.* All atom labels are checked when the coordinate file is read, and if any duplicate labels are found, a warning is issued. Several of the mouse-selection options will not be available in this case.

The labels created by the mouse labelling routine (mouse labels) are a separate set of labels, and may have an additional symmetry designator code, which is added after a trailing underscore (e.g. "H100_ii"). The symmetry designator code may either be a Roman numeral (the default - and mandatory for *Acta Cryst* journals) or Arabic numeral, the choice being determined by the setting of General Preference #8. Within the actual *ORTEP-III* driver program however, atom labels are restricted to a maximum of 6 characters, so if labels are drawn using the ORTEP graphics driver, no symmetry designators are added. Once the mouse labels have been set, it is possible to manually edit the label strings using the menu item **Edit Mouse Labels**. The symmetry designator codes may then be changed to any desired character string. These mouse labels are stored as 22-character strings, to allow for long symmetry designator codes. Note that changing the mouse label string DOES NOT change the atom label string used to identify the atom.

4.2 BONDS

Bonds are automatically calculated in *Ortep-3 for Windows* using the stored covalent radii, which are stored internally and read from the file *atomcols.def*. A bond is considered to exist between two atoms if the distance between them is greater than the ORTEP parameter **BondSearchDistanceMin** and less than the sum of their covalent radii plus the ORTEP parameter **BondToleranceFactor**.

$$r(A-B) \geq \text{BondSearchDistanceMin} \text{ and } r(A-B) \leq r(A) + r(B) + \text{BondToleranceFactor}$$

The ORTEP parameter **BondSearchDistanceMax** defines an upper limit for any possible bond distance. The internally stored covalent radii for elements may be

modified using the **Set Element Style** menu item in the **STYLES** menu, and the three ORTEP parameters may be modified in the normal fashion (see page 6). A judicious choice of the values for these parameters should allow unusually long or short bonds to be displayed, or not displayed, as required. The file *atomcols.def* contains the covalent and van der Waals radii and is always read (if present) when the program is loaded. The **Set Element Style** menu item does not permanently store changes to the atom radii - if permanent changes are required, then the file *atomcols.def* must be manually modified.

By default, all bonds (except those to H atoms) are drawn with the same “standard” style. This style may be altered using the menu item **Set Bond Style**. In addition, individual bonds, or sets of bonds, may be given a special style or may be eliminated from the illustration altogether, using the menu items **Selected Bond Style** and **Delete Selected Bond** respectively.

4.3 COLOURS

Ortep-3 for Windows allows a large choice of colours. Over 120 colour names and their corresponding RGB triplet values are stored internally, see Table 6.4. The exact appearance of these colours will depend on the colour-depth of your monitor, which should be at least 256 colours. The use of 16-bit colour or better is recommended. Note that case is important in declaring colour names, e.g. “SkyBlue” is not the same as “Skyblue”. Additional colours may be defined (or re-defined) in the file *rgbcols.def*, which is located in the **home directory** (see 4.11). The default colours for each atomic species are given in the file *atomcols.def*, also located in the **home directory**.

4.4 ERROR MESSAGES

Error messages from *Ortep-3 for Windows* are usually provided via the OrtepConsole Window. In some cases, a message box is displayed. When the program starts, the OrtepConsole Window is opened as a minimised Window on the task bar, and can be maximised in the usual way. If this Window is closed, a new instance will be created whenever the next text message is issued by *Ortep-3 for Windows*.

4.5 MENU ITEMS

Several of the menu items in *Ortep-3 for Windows* are toggles or are ganged. If several menu items are ganged, they form an exclusive set of options, of which only one may be active at any time. If a toggled or ganged menu option is active, this is indicated by a check (✓) mark in front of that item. For instance, if the user wishes to have brackets around the atomic labels, then the **Brackets on Labels** menu item from the **LABELS** menu must be selected. Once this is done, this item will become active and have a check mark in front. If a coordinate file is already loaded, a new picture will then be drawn, with brackets round all labels. If the user wishes to remove these brackets, the **Brackets on Labels** menu item must be clicked again, causing the control to become inactive.

4.6 MOUSE SELECTION AND LABELLING OF ATOMS

Several menu items rely on selection of atoms by using left mouse-button clicks. In this case, the standard side-panel shown in Figure 1 disappears, and is replaced by a panel with a brown-grey background on the right side of the screen. This indicates that the screen is now in *interactive/select mode* and mouse dragging of the viewpoint, and all other menu items, are deactivated. These *interactive/select* panels all have an "Exit" button that returns the screen to standard *display mode* (the ESC key or a middle mouse-button click has the same effect).

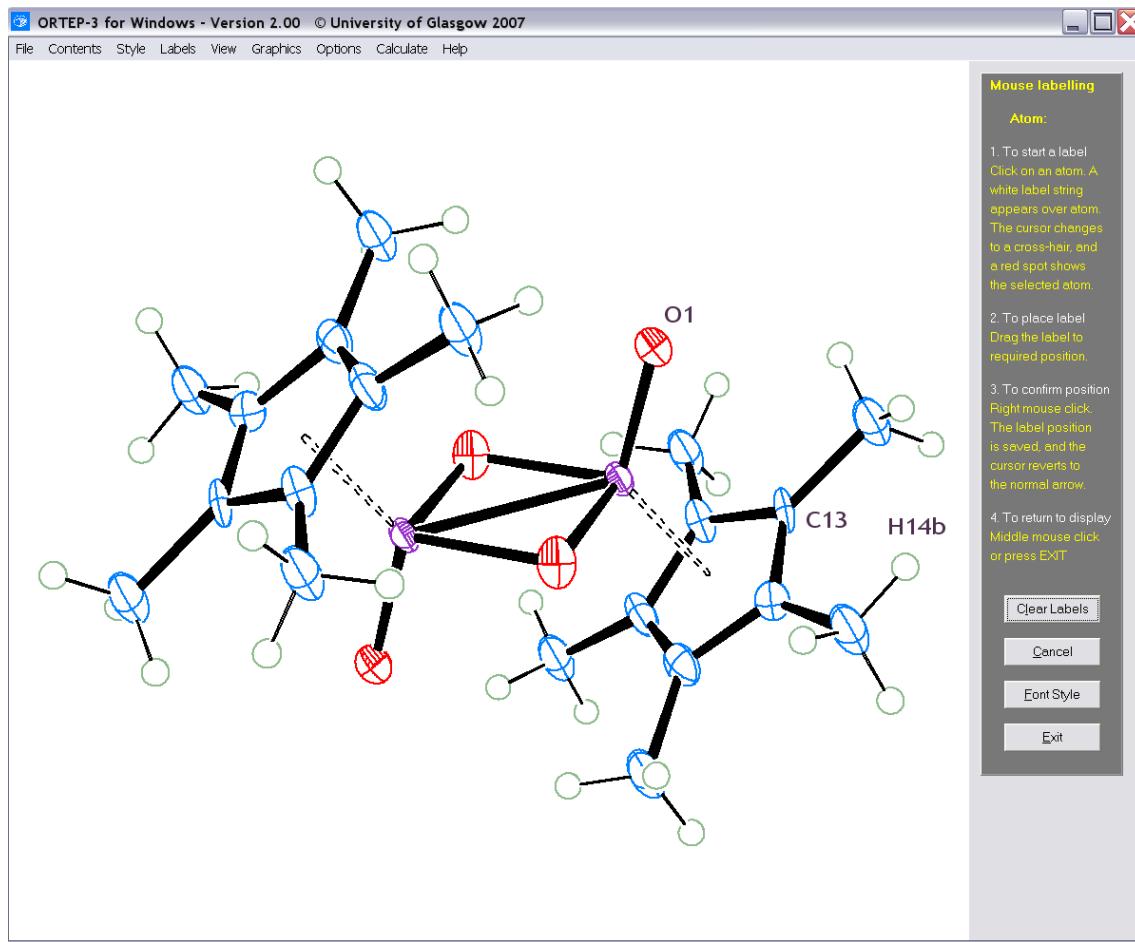


Figure 2. The *interactive/select* screen mode for *Ortep3 for Windows*, this example showing that for mouse labelling. When a side panel of this type is displayed, all other menu items and mouse dragging are inoperative.

The specific actions of the mouse buttons are given in the panel and depend on which selection mode is activated. It is generally possible to reverse an incorrect selection. If duplicate atom names are found in the input file, then many of the mouse selection options are unavailable. This is because the name is used in the search routines.

The mouse labelling routine in *Ortep-3 for Windows* is a service provided by the GUI (see 5.4.2) and is independent of *ORTEP-III*. There are two types of font available for the mouse labels, the font supplied by the GUI (the Graphics font), and the font embedded in *ORTEP-III* itself (the ORTEP font). The choice of which

to use is basically a cosmetic one. Only a limited set of fonts are available for PostScript or HPGL hardcopy output. If the graphics screen is directly printed, then either font may be used. The characteristics of each are:

- **ORTEP font:** There is only one character set available (see *ORTEP-III* manual for details). The size of characters and the colour of the font may be altered using the **Select Graphics Font** menu item in the same was as the GUI font. *If this font is used, the symmetry designators are not attached to the labels (see last paragraph of 5.4.2).*
- **GUI (or Graphics) font:** Any available Windows font may be used. The font size and other attributes are set by the FONT dialogue box obtained from the **Select Graphics Font** menu item (under **Graphics** menu). These Windows fonts are not available for Postscript or HPGL output, or saved *ortep_*.ort* files.

4.7 SYMMETRY OPERATORS

Unlike most crystallographic programs, *ORTEP-III* does not automatically take into account either lattice centring or centres of symmetry, so these operators must either be included implicitly in the asymmetric unit, or as explicit symmetry operators in the *ORTEP-III* file written by the GUI. No more than 96 symmetry operators are allowed in *ORTEP-III*. This number is sufficient to cover the multiplicity of the general site for all space groups, *except* the following four cubic space groups (225-228) :

Fm-3m , Fm-3c , Fd-3m and Fd-3c

for which this number is 192. The program *Ortep-3 for Windows* automatically expands the symmetry operations given in the input coordinate file to include explicitly any lattice centring or centre of symmetry. In general, an input coordinate-file format (like SHELX) will only include a minimal set of symmetry operations (*i.e.* omit those related by a lattice translation or inversion centre). The CIF format is unusual in that it requires ALL symmetry operators to be present. The order of the symmetry operations generated by *Ortep-3 for Windows* is as follows:

- the set of symmetry operators from the input file in the given order (including the identity operator first)
- if the structure is centric, the centrosymmetrically related operators, in the same order as (i)
- if not primitive then lattice translations for all operators in (i) {and (ii) if present} are added. For *F*-centred lattices, the order of added lattice translations is (1/2,1/2,0) then (1/2,0,1/2) then (0,1/2,1/2).

The symmetry operators used by *Ortep-3 for Windows* may be displayed using the menu item **List Symmops** in the **CALCULATE** menu (see 5.8.3). In the present version, if the input file has a full set of operations (*e.g.* CIF), then only the first 96 symmetry operators are accepted. If such a format is used for any of the above four space groups, then it is suggested that the lattice type is declared as Primitive, and all the lattice translations are included explicitly in the asymmetric

unit. Symmetry operators relating to the F-lattice translations should then be removed.

4.8 TOOL BAR and TOOLS

A number of operations are provided by the tool-bar (at the side of the graphics screen in standard display mode). There is a help facility on all of these to explain their purpose. All rotations and translations are provided by this tool bar. The default rotation increment angle is 10° but this may be altered. Two general operations are also available from mouse clicks on the graphics window when the screen is in standard display mode :

- a left mouse click near an atom will display that atom name, position and thermal parameter(s) in the status window.
- a right mouse click will bring up a pop-up menu. This allows the user to modify some commonly used parameters such as the ellipsoid probability.

4.9 HARD COPY GRAPHICS OUTPUT

There are three methods of obtaining hardcopy output from *Ortep-3 for Windows*

- as standard vector graphic metafiles in HPGL and PostScript format (**Write HPGL File** and **Write PostScript File** see Section 5.1.4),
- by saving the graphics screen in various ways (see Sections 5.6.6 - 5.6.8). Full details of both methods are given in these Sections. The ORTEP parameter **PlotLineWidthA4/DJS** controls the drawn linewidth for the HPGL, PostScript and **PrintGraphicsScreen** options. The default values give a good solid line. The corresponding parameter for the graphics screen is **ScreenLineWidth**, and this parameter is also used for the direct screen copies, *i.e.* **Copy To Clipboard** and **Export BMP**.
- as rendered raster images. There is an interface from *Ortep-3 for Windows* to the rendering packages **Raster3D**⁴ and **POV-Ray**⁵. The latter in particular can provide excellent presentation-quality graphical images. See Sections 5.1.6 and 5.1.7.

4.10 CUSTOMISATION OF ORTEP-3 FOR WINDOWS

There are a number of ways of customising the defaults in *Ortep-3 for Windows*. This can be carried out dynamically (see p. 6), but if the user finds that a different default is normally required, then a better way is to modify the values in the *ortep.ini* file, which is found in the same directory as the program executable. All the ORTEP parameters may be changed in this way

See Table 6.1 for full details of all ORTEP Parameters.

4.11 SYSTEM FILES AND DIRECTORIES

There are three directories used by *Ortep-3 for Windows*, the **program directory**, the **home directory** and the **working directory**.

The **program directory** is where the program executables *ortep3.exe*, *OrtTextServer.exe*, *editor.exe*, *wgxsy01.exe* and required DLL's are installed. This directory may be on a non-local networked drive and does not require write access.

The **home directory** is the directory pointed to by the environment variable **ORTEP3DIR**. It is where the system files *ortep.ini*, *atomcols.def*, *rgbcols.def* and the licence file *Ortep3-licence* are located. This directory MUST have write access by the user. If you do not know how to set environment variables, see the FAQ page

<http://www.chem.gla.ac.uk/~louis/software/faq/q1.html>

The **program directory** and the **home directory** can be the same directory (in fact the installation program assumes they are), and in this case, the directory must have the same access properties as the **home directory**. In addition to the above named files, there are two ASCII output files which are always written by *Ortep-3 for Windows* to the **home directory**, *OrtepListing* (the listing file from *ORTEP-III*) and *OrtepInstructions* (the *ORTEP-III* instruction file written by the GUI). They are usually of little interest, and are always overwritten. If there is an unexpected failure however, these files may be examined. If the current illustration has atoms other than those in the asymmetric unit, another ASCII file *OrtepDrawing* is also written to the **home directory**. This contains the symmetry designations for all drawn atoms, and is useful for the purposes of labelling for Acta Cryst publication. All these files may be opened directly from the *Ortep-3 for Windows* GUI.

Finally, the **working directory** is the one containing the current coordinate file and this directory must also have write access for the user. If the user has activated General Preference # 4 ("Save the current viewpoint and mouse labels"), then a file called *OrtViewMatrix* is written when the program is closed, or a new input file is opened. On start up, *Ortep-3 for Windows* will automatically start in the last used **working directory**, and if the file *OrtViewMatrix* is present, this will also be read to restore the last used viewpoint and set of mouse labels. The General Preference #3 ("Use automatic file naming for all ORTEP output files") is a very important one. If it is activated (checked) then all other output files written by *Ortep-3 for Windows* will be placed in the **working directory**. They will be given unique names, which ensures that no file is overwritten. These files include all the output graphics, .POV, .BMP, .EPS etc. If General Preference #3 is NOT activated, then all these files are written to the **home directory**, with names which ensure they will always be overwritten, e.g *ortep.pov*, *ortep.bmp* etc. So if you wish to save these files, ensure that General Preference #3 is activated (checked)!

5. FULL DETAILS OF THE GUI FACILITIES

5.1. FILE MENU

5.1.1 Open File

As explained above, this menu item must be selected when a new structure file is to be input. The routine performs a simple check on the contents of the selected file, to determine the file-format, and hence the subsequent action to be taken. The following common atomic/crystallographic coordinate file-formats are currently supported: SHELX, GX, CIF, SPF, CSSR-XR, CSD-FDAT, GSAS, Sybyl MOL, XYZ (various), PDB, Rietica-LHPM, FULLPROF, AIMPAC-WFN, Chem3d-Cartesian, GAMMES-UK input, ICSD and XD. In addition, *Ortep-3 for Windows* will accept any legal *ORTEP-III* instruction file. The file extension is NOT used in this check, so that the filters given in the **Select Molecular Coordinate File** dialog box are for guidance only, and indicate the most common extensions given for these file types.

Regardless of the file-format, only the first 996 atoms read are stored by *Ortep-3 for Windows*, any extra ones being ignored. If no atoms are found in the file, the program issues a message to this effect to the OrtepConsole Window. All file-formats are read automatically, but if there is a failure, the user may find the following information useful in tracking down the source of the problem. If there is a simple syntax error in the input file, the **Edit Input File** option (5.1.2) may be used to modify this file without leaving *Ortep-3 for Windows*. After editing is finished, the **Open Coordinate File** menu item will need to be re-selected.

5.1.1.1 SHELX format file.

The following instructions, with the correct information, are ESSENTIAL for success in reading a SHELX file.

TITL
CELL lambda (not used) a,b,c,alpha,beta,gamma
SFAC
UNIT
LATT
SYMM
FVAR
Atom cards

All other legal SHELX instructions are ignored.

5.1.1.2 GX format file.

The following instructions, with the correct information, are ESSENTIAL for success in reading a GX file.

TITLE
CELL a,b,c,alpha,beta,gamma

CONTENTS (at least one element type)
LATT (if not centrosymmetric and primitive)
SYMM (if not triclinic)
ATOM cards

All other legal GX instructions are ignored

5.1.1.3 CIF format file.

The presence of a DATA_ statement triggers recognition of a CIF file-format. The following data items are ESSENTIAL (in each data_ block) for success in reading a CIF file. Note that the CIF format requires that all symmetry operators be explicitly given (including lattice translations and centres of symmetry).

```
data_
_cell_length_a
_cell_length_b
_cell_length_c
_cell_angle_alpha          (if missing 90° assumed)
_cell_angle_beta           (if missing 90° assumed)
_cell_angle_gamma          (if missing 90° assumed)
_symmetry_equiv_pos_as_xyz (if missing space group P1 assumed)
```

a loop with the following data

```
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

and possibly

```
_atom_site_type_symbol
_atom_site_U_iso_or_equiv
```

PLUS another loop containing the data items (if _atom_site_U_iso_or_equiv is not present. If no U^{ij} information is present, a default U_{iso} of 0.05 Å² is assumed)

```
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
```

The following data item will also be used, but is not mandatory.

```
_atom_type_symbol
```

All other (standard or non-standard) CIF data items are ignored. Any logical error in the construction of the CIF (as detected by the input routines of CIFtbx) will immediately terminate input. Any CIF file written by SHELX or PLATON should be suitable for *Ortep-3 for Windows*.

5.1.1.4 SPF (PLATON/PLUTON) format file.

It is vital that the **ATOM** instruction *precedes* the corresponding thermal parameter **UIJ/BIJ/U/B** instructions for each individual atom. The following instructions are ESSENTIAL for success in reading an SPF file.

TITL

CELL (wavelength) a,b,c,alpha,beta,gamma

LATT (if absent P C - primitive, centrosymmetric - assumed)

SYMM (if not triclinic)

ATOM

and one of the following for each **ATOM** card

UIJ or **BIJ** or **U** or **B**

5.1.1.5 CSD-FDAT format file.

All structures will be extracted, and the user will then be presented with a dialog box to select the structure to display. In the current version of *Ortep-3 for Windows* only one structure may be selected for viewing at any one time. This same option applies to multi-structure CIF and MOL2 files.

5.1.1.6 GSAS format file.

In the current version, only information on the *first* phase is extracted.

5.1.1.7 ORTEP format files.

Ortep3 for Windows will read any ORTEP instruction file. The user is offered two choices when reading this format. The ORTEP drawing instructions may be interpreted directly, effectively by-passing the GUI. Alternatively, the user may extract just the crystallographic information from the file, and ignore all ORTEP drawing instructions. In the latter case, the full facilities of the GUI are available, but it is *very important* that the atom labels in the ORTEP file follow the recommendations outlined in 4.1. Any blank or uninterpretable labels will result in that atom being ignored.

5.1.1.8 Sybyl MOL format files.

The first line should contain the number of atoms and the word “MOL” in Fortran format (i4,1x,a3). Since no anisotropic displacement parameters are available, the default style for this format is PLUTO.

5.1.1.9 XYZ Angstrom coordinate format files.

There should be two header lines before the atomic coordinates. Either of these should contain a single entry in free format, the integer number of atoms. The content of the other line is immaterial, but should not be blank. If two lines

containing a single integer are found, the second one is used. If the number of atoms found does not tally with this number, an error is assumed. The atom coordinates should be entered one on each line, and will be read in free format. The first field should either be a character string representing the element type, or an integer representing the atomic number. The remaining three fields should contain the Angstrom coordinates. A cubic unit cell of 1 Å is assumed. Since no anisotropic displacement parameters are available, the default style for this format is PLUTO.

5.1.1.10 Rietica-LHPM and FULLPROF format files.

These two formats commonly used for powder diffraction/Rietveld analysis. They have not been as extensively tested as the other formats and some problems may remain.

5.1.1.11 Brookhaven PDB format files.

The only data interpreted are those on the ATOM, HETATM and ANISOU cards, all other cards are ignored. The atom-naming scheme is important since an unrecognised atomic type will cause this routine to fail. This input is NOT intended for real protein structures (ORTEP is limited to 996 atoms) but it now a commonly used format for small molecules and hence included in *Ortep-3 for Windows*.

5.1.2 Reload File

The currently selected data file is re-read and the standard defaults are re-applied.

5.1.3 Recent Files

Previously opened data filenames (up to 30) are stored in *ortep.ini*, and may be opened with this menu item.

5.1.4 Edit Input File

A simple text editor is provided in *Ortep-3 for Windows* so that the input file may be edited without leaving the program. Although there are facilities in the GUI for omitting specified atoms, it is often simpler and less frustrating to prepare an input file that only contains the atoms required. For instance, when only *some* of a set of symmetry equivalent atoms is required, there is no option but to prepare an edited input file, since the **Exclude Selected Atom** and **Delete Bond** routines in the present version of *Ortep-3 for Windows* will remove ALL symmetry equivalents. The usual Cut, Paste, Copy, and cursor-insertion editor functions are provided. Naturally, this editor may be used for any text file.

5.1.5 Edit Instruction File

The **ORTEP-III** instruction file *OrtepInstructions*, which is written by the GUI to the **home directory**, is opened in a text editor. Expert users may wish to make changes to this file, and then run the **ORTEP-III** program directly from this file ("Run ORTEP Direct" under the Options menu, section 5.7.3). Note that this file is read in

FORTRAN fixed format, so you need to know what you are doing ! Note also that any action of the GUI will write a new *OrtepInstructions* file and overwrite the edited version.

5.1.6 Edit Listing File

The **ORTEP-III** output file *OrtepListing*, which is written to the **home directory**, is opened in a text editor. Expert users may wish to examine this file, but in general it is not of much interest.

5.1.7 Edit Drawing File

The output file *OrtepDrawing*, which is written to the **home directory**, is opened in a text editor. The menu item is greyed out unless this file exists - the file is ONLY written if the current illustration uses symmetry operators other than the base one (e.g. if a cell packing diagram or structure expansion is drawn). It lists all symmetry operators used to plot all atoms, and example contents are

```
This file lists all the unique symmetry operations (including translations)
which are used for the current drawing. The space group operations are :
```

```
1. x,y,z
```

```
2. -x,y+1/2,-z
```

```
Symmetry operation (i) -x,y+1/2,-z with translations 1.0 0.0 0.0
```

```
Designator codes :: ORTEP : 65502 CIF : 2_655
```

```
-1.00000 0.00000 0.00000 1.00000
```

```
0.00000 1.00000 0.00000 0.50000
```

```
0.00000 0.00000 -1.00000 0.00000
```

```
Full symmetry operator (IT format) : 1-x, 1/2+y, -z
```

```
Atoms plotted using this symmetry operation are :
```

```
C1 C11 C2 C21 C3 C31 C4
```

At the end of this file, a summary list of all symmetry operators codes used, with their Roman numerals is given. This is in the exact format required by Acta Cryst C/E, so this table may be directly pasted into a manuscript (or CIF) for a figure legend.

```
Acta Cryst format for figure legends :
```

```
Symmetry codes:
```

```
(i) 1-x, 1/2+y, -z ;
```

```
(ii) -x, 1/2+y, -z ;
```

```
(iii) 1+x, y, z ;
```

5.1.8 Write ORTEP3 file

Selecting this menu item will save the current **ORTEP-III** instruction set. If General Preference #3 is activated (Auto file naming), then a file called *ortep_*.ort* (where * is a unique number) will be written to the current **working directory**. Otherwise, a file called *ortep.ort* is written to the **home directory**, where it may be overwritten.

NOTE that this file may NOT be compatible with the standard release of *ORTEP-III* (mainly because a much larger number of trailer cards are allowed in *Ortep-3 for Windows*).

5.1.9 Write HPGL / PostScript File

Selecting these menu items will write an HPGL or PostScript format metafile, corresponding to the currently displayed picture. If General Preference #3 is activated (Auto file naming), then a file called *ortep_*.hpg* or *ortep_*.eps* (where * is a unique number) will be written to the current **working directory**. Otherwise, a file called *ortep.hpg* or *ortep.eps* is written to the **home directory**, where it may be overwritten. If the option **Mouse Labelling** is active, then atom labels close to the positions shown on the screen display will be also drawn. If the **Underscore on Labels** option (see 5.4.4) is *NOT active* and the **Mouse Labels** (GUI font) is active, then the symmetry indicator characters will be drawn as *superscripts*. The user may choose to write either monochrome or colour HPGL/PostScript files. The background colour for HPGL/PostScript files is ALWAYS white, and any graphical object drawn in white on screen (e.g. bonds) will be drawn as black in the HPGL/PostScript file.

5.1.10 Write SHELX / XYZ File

The atomic contents of the screen *as currently displayed* are written in SHELX or XYZ formats. If General Preference #3 is activated (Auto file naming), then a file called *shelx_*.ins* or *ortep_*.xyz* (where * is a unique number) will be written to the current **working directory**. Otherwise, a file called *shelx.ins* or *ortep.xyz* is written to the **home directory**, where it may be overwritten. If the originally loaded coordinate file was a SHELX file, then the non-atomic instructions from this file will be copied verbatim to the new file (except for sequence dependent instructions such as AFIX and MOLE which will be removed), otherwise a basic SHELX header is written. The order of atoms follows that in the ATOMS array of ORTEP-III, and will usually be different from that input. Up to the maximum number of 2000 atoms may be listed. This option is useful if the atomic parameters for some portion of the structure (or a set of symmetry equivalent atoms) are desired.

5.1.11 Write Raster3D File

This option is only available if *Ortep-3 for Windows* detects that a current version of **WinGX** is also installed. The atomic contents of the screen *as currently displayed and in the current orientation* are written to the file *raster3d.dat*, which is a pseudo-PDB type file suitable for input to the **Raster3D** suite of programs.⁴ The location of this file depends on the setting of General Preference #3. The **Raster3D** GUI will then appear, allowing the user to customise the rendered drawing.

5.1.12 Write POV-Ray File

The contents of the screen are written to a **POV-Ray**⁵ scene description file. If General Preference #3 is activated (Auto file naming), then the POV-Ray scene

description file called *ortep_*.pov* (where * is a unique number) will be written to the current **working directory**. Otherwise, a file called *ortep.pov* is written to the **home directory**, where it may be overwritten. If the **POV-Ray** program is installed as a plugin (and if General Preference #7 is activated), the file is then rendered to give a raster image file *ortep_*.png*. Colour information about the atoms, background, lettering etc is also passed to this file, so that a ray traced picture corresponding to the exact current screen illustration may be obtained, see Figure 4. There is a choice as to the representation of atoms in the **POV-Ray** picture, standard ORTEP type thermal ellipsoids, RMSD or MSD (PEANUT type) surfaces, ball-and-stick models, van der Waals surfaces or rod representation. This file is rendered by the freely available ray-tracing program **POV-Ray**, which is obtainable as an executable for a number of different platforms.⁵ Version 3.5 of **POV-Ray** (or higher) is required for the files written by this program. The scene description language of **POV-Ray** is highly complex and flexible. Manual editing of the file written by *Ortep-3 for Windows* will often be necessary to obtain a desired final graphic.

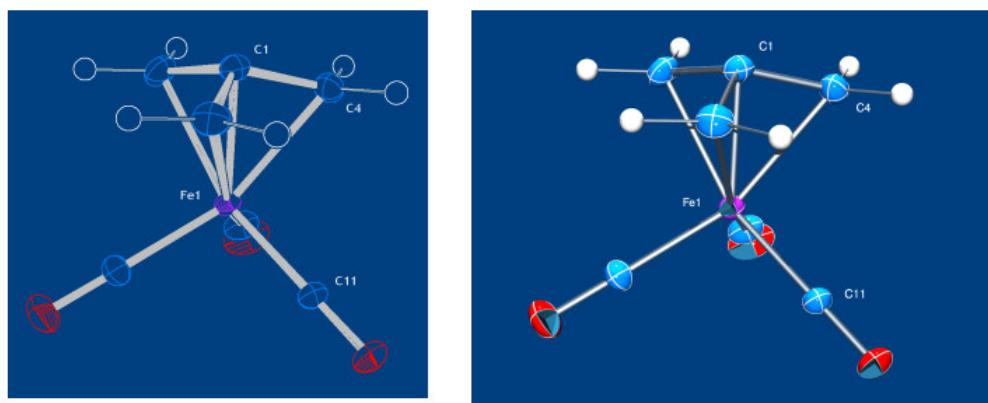


Figure 4. An illustrative screen display and the corresponding **POV-Ray** picture.

Some care has been taken to make the scene description file easy to modify. Most of the variables (apart from the individual atomic positional parameters, quadric coefficients used to describe the thermal ellipsoids and coordinates of bonds) are declared in the header at the top of the file and need only be modified in this one place. Each bond is recalculated from the interatomic distances when the **POV-Ray** file is written, and excluded bonds will be omitted in the **POV-Ray** picture. Since each bond is clearly annotated in the file, it is a relatively easy matter to delete unwanted bonds. An example of such a header is shown below :

```
#include "colors.inc"
#include "textures.inc"
#include "metals.inc"
#declare Bond_Texture      = texture {
                           pigment {color Black }
                           finish { Metal } }

#declare HBond_Texture    = texture {
                           pigment {color Black }
                           finish { Metal } }

#declare Texture_C         = texture {
                           pigment {color SkyBlue }
                           finish { Shiny } }

#declare Texture_H         = texture {
                           pigment {color Green }
                           finish { Shiny } }

#declare Texture_N         = texture {
```

```
                pigment {color BrightGold }
                finish { Shiny } }
#declare Texture_O      = texture {
                           pigment {color Firebrick }
                           finish { Shiny } }
                           = 0.05;
#declare HBond_Radius   = 0.02;
#declare Bond_Radius    = 0.02;
#declare Radius_C       = 0.77;
#declare Radius_H       = 0.32;
#declare Radius_N       = 0.70;
#declare Radius_O       = 0.66;
#declare Radius_Scale   = 0.33;
#declare Bond_Truncate  = 0;
#declare View_Distance   = 36.5;

global_settings { assumed_gamma 2.2 ambient_light rgb < 1, 1, 1 > }
camera {
    location < 0.0 , 0.0 , View_Distance >
    angle     20.0
    up        < 0.0 , 1.0 , 0.0 >
    right     <-1.33, 0.0 , 0.0 >
    look_at   < 0.0 , 0.0 , 0.0 >
}
background { color SteelBlue }
light_source { < 0.0, 0.0, 100.0 >
               color red 2.0 green 2.0 blue 2.0 }
```

The textures (*i.e.* colours and finishes) of each atomic type and the standard bonds and bonds to H atoms may be modified by editing each entry

```
#declare Texture_C      = texture {
                           pigment {color SkyBlue }
                           finish { Shiny } }
```

Note that case is important in all declarations, *e.g.* "SkyBlue" is not the same as "Skyblue". In this example a ball and stick representation is being described and the radius of atomic types (in Å) and the bonds may be set individually and the overall scale set by:

```
#declare Radius_N      = 0.70;
#declare Radius_O      = 0.66;
#declare Radius_Scale  = 0.33;
```

ORTEP style thermal ellipsoids may be drawn as plain ellipsoids, ellipsoids with the boundary ellipses or cutout ellipsoids. Bonds are normally drawn from atomic centre to atomic centre. Since the ellipsoids or other atomic representations are solid objects in the **POV-Ray** world, this is normally invisible, but in the case of cutout ellipses these "interior bonds" may become visible. There is an option to truncate all bonds to cutout ellipsoids at the ellipsoid surface (which is how **ORTEP-III** draws bonds) but as this increases the rendering time by a factor of 3-5 it is available as an option. The easiest way to use this facility is to deselect Truncate bond in the **POV-Ray** Interface GUI (actually you need do nothing since this is the default) and when the required illustration is ready a final rendering can be made with this option set on by modifying the scene description file and declaring the variable Bond_Truncate to have any value other than zero. *e.g.*

```
#declare Bond_Truncate = 1;
```

The view distance is set automatically but is not always correct. To zoom in, declare View_Distance with a smaller value, to zoom out, with a larger value.

```
#declare View_Distance = 36.5;
```

The global settings will not normally need adjustment, but the user is encouraged to read the (unfortunately very extensive) ***POV-Ray*** documentation to find out more about the ***POV-Ray*** scene description language.

5.1.13 Exit ORTEP3

Quit ***Ortep-3 for Windows*** program. No confirmatory prompt is given. The current settings will be saved in the file *ortep.ini*, and if General Preference #4 is activated, the current viewpoint and mouse labels (if any) will also be saved in the current **working directory**.

5.2. CONTENTS MENU

The items from this menu control the contents of the illustration, *i.e.* those atoms to be drawn. By default, and for all new coordinate data sets read in, the **Use Asymmetric Unit** mode will be made active. The menu items **Use Asymmetric Unit**, **Grow Fragment** and **Unit Cell Contents** are ganged, so that only one may be active.

5.2.1 Use Asymmetric Unit

If this option is active, the entire asymmetric unit forms the contents of the illustration, unless some atoms have been specifically excluded by other options (see 5.2.6 - 5.2.11). This mode is the default mode for displaying a new structure.

5.2.2 Grow Fragment

If this mode is active, a symmetry expansion of incomplete fragments which are situated about crystallographic symmetry elements is performed. The **auto-mode** is generally most effective; all atoms in the input file are treated as seed atoms, which results in the symmetry expansion of ALL the incomplete fragments in the asymmetric unit. Alternatively, the user can select **User-define**, which will prompt for a specific seed atom and search radius. This will result in the symmetry expansion of the fragment containing this seed atom, with other non-connected fragments being ignored. If the structure is polymeric, then this process will continue until the atoms array is filled (this may take a while to complete, as 2000 atoms can now be drawn !!)

5.2.3 Unit Cell Contents

This menu item draws the unit cell contents. The **auto-mode** will result in an illustration with the entire contents of one unit cell, and where all molecules, which have at least one atom within the unit cell, are completed. If the structure is polymeric, then this process will continue until the atoms array is filled. The **user-define** mode allows the user to specify how many unit cells in all three directions are required. These will be centred about the midpoint of the primary unit cell. In this mode it is also possible to choose whether all molecules are completed, and whether the cell outline is drawn. The default action is identical

to **auto-mode**. Selecting the **Unit Cell Contents** option will automatically switch off all labels.

5.2.4 Sphere of Enclosure

All atoms within a sphere of user defined radius, about a user defined atom, are included in the illustration. This option does NOT expand all fragments, and hence allows the drawing of polymeric or infinite lattice structures.

5.2.5 Box of Enclosure

All atoms within a Cartesian box of user defined dimensions, about a user defined atom, are included in the illustration. This option does NOT expand all fragments, and hence allows the drawing of polymeric or infinite lattice structures. If the user wishes to have an enclosure box based on the unit cell vectors for such structures, then the **Unit Cell Contents** item **Auto Mode** should be selected, *and the Expand all fragments option must be switched off*.

5.2.6 ADR Add/Subtract/Reset

This item allows the user to specifically include or exclude or remove an atom designator run (ADR) so that a specified part of the unit cell, for example, may be drawn. The user is referred to the ORTEP-III manual for a detailed explanation of the term ADR.

5.2.7 Include H Atoms

This item and the next one form a toggle. If active (this is the default condition), H atoms will be drawn with the appropriate graphic representation (see the Thermal-H menu item, page 20).

5.2.8 Include Q Peaks

If this control is active, no H atoms will be drawn. The view orientation might change slightly if the default view option (**Best View** see 5.5.1) is active.

5.2.9 Exclude Options

This menu item allows the user to exclude atoms from the illustration by a variety of ways.

| | |
|--------------------------|---|
| 1. Element Type | Exclude all atoms of specified elemental type(s). |
| 2. Named Atoms | Exclude all atoms with specified name, including all its symmetry equivalents |
| 3. Selected Atoms | Exclude all atoms selected by mouse clicks. The symmetry equivalents are NOT excluded by this option. |
| 4. Atoms+SYMM | Identical to 5.2.9.3, except that symmetry equivalents WILL be excluded. |

5.2.10 Restore Options

This menu item allows the user to restore atoms that have been excluded by any of the above operations

| | |
|--------------------------|---|
| 1. Element Type | Restores all atoms of specified elemental type(s), except those selected by item 5.2.9.3 above. |
| 2. Named Atoms | Restores all atoms with specified name, including all symmetry equivalents. |
| 3. Selected Atoms | Restores all atoms selected by mouse clicks (i.e. items 5.2.9.3 and 5.2.9.4 above.) |
| 4. Atoms+SYMM | Restore all atoms. |

5.2.11 Select by Part No.

This menu item allows a user to select part of the structure using the SHELXL PART instructions. It is only available if the loaded file is a SHELX file and if that file contains PART instructions (otherwise this control is greyed). This is most useful when the structure contains extensive disordered sections where it is desired to show only one component of the disorder.

5.2.12 Add Centroid

This menu item initiates the mouse driven selection of atoms for a centroid calculation. The resultant centroid is included in the atoms list with a label Ct* (* is a unique number) and a covalent radius of 0.77Å (the same as a C-atom). There is no arbitrary limit to the number of centroids added in this way, but the total number of atoms in the ASU and centroids cannot exceed 996. Centroids generated in this way will not be drawn, but all bonds from these pseudo-atoms to all others which are longer than the parameter **CentroidBondMin** will be drawn as dashed lines. The value of the parameter **CentroidBondMin** may be modified using the **Change Ortep Parameters** menu item. This routine is particularly useful for drawing bonds from transition metals to π -bonded ring systems.

5.2.13 Invert Structure

The chirality of the entire crystal structure is inverted. Normally this is achieved by inversion through the origin. If the space group is one of the 11 pairs of enantiomeric space groups, then the space group is also switched to its corresponding enantiomorph. If it is one of the following *Fdd2*, *I4₁*, *I4₁22*, *I4₁md*, *I4₁cd*, *I-42d* or *F4₁32*, then the correct translational components are applied (see Bernardinelli & Flack, *Acta Cryt* (1985) A41, 500-511). NOTE : this is different from Version 1 of *Ortep-3 for Windows*, where only the asymmetric unit was inverted.

5.2.14 Display Crystal Data

Crystallographic information stored by ORTEP is displayed in a message box.

5.3. STYLE MENU

This menu controls the stylistic features of ORTEP, *i.e.* the exact graphical representation of the atomic thermal ellipsoids and interatomic bonds.

5.3.1 Select New Style

Five stylistic templates are available in *Ortep3 for Windows*, called **Default**, **OctantShaded**, **Highlighted**, **Plain** and **PLUTO**. These provide the basis for the graphical representations of ORTEP. The **PLUTO** style draws each atomic type as a sphere, with a radius proportional to the covalent radius. The other styles draw each atom as a thermal ellipsoid (save for hydrogen atoms) in various forms. The **Stick** mode is useful to get a suitable view quickly, as it is drawn much more rapidly. In this mode, bonds are drawn as simple lines, and atoms are represented by an asterix.

Thermal-H is not a style but an option. For all the styles mentioned above, hydrogen atoms will be drawn as spheres (by default 0.1 Å), with thin bonds. If the user wishes to draw hydrogen atoms with their refined thermal parameters (usually isotropic, but possibly anisotropic for neutron-diffraction structural analyses), then the **Thermal-H** option should be selected. All bonds to H-atoms will then be of the “standard” type (see 4.2 and 5.3.7). If anisotropic H-atoms are present in the input parameter file, then the **Thermal-H** option is set automatically.

5.3.2 Change ORTEP Parameters

As mentioned above, many of the parameters controlling the GUI and the operation of ORTEP may be modified dynamically through this menu item. A parameter box will be displayed when this menu item is selected, and any number of parameters may be modified. The program will not accept unsuitable values. The most common parameters which the user may wish to modify **EllipsoidProbability**, **ScreenLine-Width** and **StereoDisplacement** may also be modified using the popup menu obtained by a *right mouse-button click* anywhere on the graphics screen. A number of preset values are obtainable. The meaning of all the parameters is given in Table 6.1 below. In contrast to version 1 of *Ortep for Windows*, all parameters are now stored in the *ortep.ini* file.

5.3.3 Reset to Default Style

This menu item resets the style to the default for the currently selected style. This will only have an effect if the graphical representation of elements, atoms or bonds has been changed using **Set Element Style**, **Selected Atom Style**, **Set Bond Style**, **Selected Bond Style**. This option will also restore any deselected bonds.

5.3.4 Set Element Style

This item allows the user to change globally both the *graphical representation* of a particular element, and the value of the stored *covalent radius*. In practise, adjustment of the NPLANE, NDOT, NLINE and NDASH parameters for the Custom

Ellipsoid Style allows an element to be represented by any of the ellipsoid components available in *ORTEP-III* (see Fig 5). A self-explanatory dialog box is presented for modifying the ellipsoid representation. The default colours for all atomic types (the CPK colour scheme) are defined in the file *atomcols.def*. The user may ascribe any colour to any atom.

5.3.5 Selected Atom Style

It is also possible to draw any *individual* atom or sets of atoms in a selected style different from the standard element style set by **Set Element Style**. A self-explanatory dialog box is presented for modifying the ellipsoid representation.

5.3.6 Draw No Atoms

If active this menu item bypasses the drawing of all atoms, but leaves all the bonds in place. It may be useful in certain circumstances.

5.3.7 Set Bond Style

This item allows the user to modify globally the appearance of the standard bond. All the possible bond styles available in ORTEP-III are also available in *Ortep3 for Windows*. Both the number of fill-lines, bond width and bond colour may be modified, and dashed bonds may also be drawn.

5.3.8 Selected Bond Style

This menu item allows the user to select bonds or sets of bonds to be drawn in a selected fashion, different from the standard bond style. This option is useful for drawing weak interactions, hydrogen bonds etc.

5.3.9 Draw No Bonds

If active this menu item bypasses the drawing of all bonds, but leaves all the atoms in place. It may be useful in certain circumstances, for instance packing diagrams of ionic crystals.

5.3.10 Delete Selected Bond

This menu item initiates a mouse-driven routine allowing the user to select any number of individual bonds to be removed from the illustration. All symmetry equivalent sets of bonds will be removed by this option.

5.3.11 Restore Selected Bond

This menu item initiates a mouse-driven routine allowing the user to restore any number of individual bonds which have been removed by the above option. All symmetry equivalent sets of bonds will be restored by this option. All such restored bonds will be of the “standard” type.

| | <u>Without back or reverse axes</u> | <u>Full line back</u> | <u>Dotted back</u> |
|--|--|---|--|
| Principal ellipses | | | |
| | 705 NPLANE= 3 NDOT= 0 NLINEx= 0 NDASH= 0 | 705 NPLANE= 3 NDOT= -1 NLINEx= 0 NDASH= 0 | 705 NPLANE= 3 NDOT= 5 NLINEx= 0 NDASH= 0 |
| Principal and boundary ellipses | | | |
| | 702 | 705 NPLANE= 4 NDOT= -1 NLINEx= 0 NDASH= 0 | 705 NPLANE= 4 NDOT= 5 NLINEx= 0 NDASH= 0 |
| Principal ellipses and axes | | | |
| | 705 NPLANE= 3 NDOT= 0 NLINEx= 1 NDASH= 0 | 703 | 705 NPLANE= 3 NDOT= 5 NLINEx= 1 NDASH= 3 |
| Principal ellipses and axes with boundary | | | |
| | 706 | 705 NPLANE= 4 NDOT= -1 NLINEx= 1 NDASH= 3 | 705 NPLANE= 4 NDOT= 5 NLINEx= 1 NDASH= 3 |
| Principal ellipses and axes with boundary and octant shading | | | |
| | 701 | 705 NPLANE= 4 NDOT= -1 NLINEx= 5 NDASH= 3 | 705 NPLANE= 4 NDOT= 5 NLINEx= 5 NDASH= 3 |

Fig 5. Various combinations of ellipsoid components showing ORTEP instruction number and parameter values to produce each.

5.3.12 Restore All Bonds

This menu item will restore ALL bonds deleted with the items 5.3.10 or 5.3.12. All such restored bonds will be of the “standard” type.

5.3.13 Retrace

If this menu item is active, certain lines will be made heavier than others by retracing over the path several times with a slight displacement. The displacement is set by the ORTEP Parameter **RetraceDisplacement**, that is given a suitable default value. NOTE that this option results in considerably longer drawing times.

5.3.14 Stereo

If this item is active then a stereo pair of illustrations is drawn. These are rotated relative to each other by the ORTEP parameter **StereoRotationAngle** and the pair of drawings is separated by a distance given by **StereoDisplacementDistance**. The defaults supplied in *Ortep3 for Windows* may not be suitable in all cases, and the user should use her/his discretion. The view distance is automatically set to 30 in for stereo plots to give a realistic depth for stereopsis, though the user may modify this value through the ORTEP parameter **StereoViewDistance**. Certain other options are not possible if this mode is active, e.g. mouse labelling (since it is very important that the labels have the correct displacement for both drawings). If stereo plots with mouse labels are required, then the mono view should be previously mouse labelled, and the ORTEP font will be automatically selected.

5.3.15 Title

If active, this option will draw a title string. The title string is taken from a TITL or TITLE card, but a dialog box is presented so that the user may modify the string as desired. The title will be placed in the top left corner of the illustration, and may be moved by mouse dragging. Select Set Mouse Labels menu item and place the pointer near the left edge of the title string. The entire string may be dragged to any position, in the same way as a mouse label.

5.4. LABELS MENU

See Section 4.1 concerning the recommendations about atom labelling for *Ortep-3 for Windows*.

5.4.1 Labelling Mode

Five labelling modes are provided, and these are all ganged so that only one can be active at any time. The automatic placement of labels is implemented through ORTEP-III, but since this option uses the same x-y displacement of atom labels from all atomic centres, it is usually unsatisfactory for final output. It may be useful however in recognising atoms in the initial stages of drawing. The x-y displacement of atom labels is set by the ORTEP parameters **LabelTextXOffset** and **LabelTextYOffset**.

The recommended method of labelling is the **Mouse Labelling** mode. It is only sensible to use this mode once a final satisfactory view has been obtained (subsequent rotations and translations are applied to these mouse labels, but will normally only be appropriate for small rotations). The positions of, and the character strings for the labels are set and stored by the menu item **Set Mouse Labels**. If **Mouse Labelling** is selected, and there are no currently stored labels, then the **Set Mouse Labels** routine is automatically called. If stored labels are present, then the illustration will be drawn with these labels. Two types of font, GUI and ORTEP are available (see 4.6)

5.4.2 Set Mouse Labels

Once this menu item is selected, the screen display shifts to *interactive/select mode*, and all other menu items are disabled. The user should select an atom for labelling using the left mouse button, upon which a red dot will appear at the atomic centre, and the cursor changes to a cross-hair. The label position may then be changed by dragging the label across the screen. The left-bottom corner of the label will be placed near the cross-hair position. A right mouse-button click will confirm the label position, then the cursor changes back to the standard arrow pointer and the red spot marking the labelled atom changes to yellow. As many atoms as required may be labelled in this fashion. When placing labels using the mouse pointer, remember that as the font-size is increased, the label will “grow” from the left-bottom corner both upwards and in the right direction. If the **Print Graphics Screen** (see 5.6.6) option is used, true WYSIWYG output is obtained. Unit cells may be labelled in the same way as atoms (the corners of the unit cells are pseudo-atoms).

If two or more symmetry equivalent atoms are present in the illustration, the labels for these atoms are automatically adjusted to indicate the symmetry designator code. An extra trailing underscore ‘_’ (see 5.4.4) followed by up to twelve characters for the symmetry designator code is added (outside any brackets if present) to the label, for all symmetry positions except the primary position (equivalent position #1) of the asymmetric unit. By default, Roman numerals are used for the symmetry designator code, though this may be changed to Arabic numerals using General Preference #8.

5.4.3 Edit Mouse Labels

This option allow the user to delete all mouse labels or modify the character strings for individual labels, including the symmetry designator codes. Note that changing the mouse labels DOES NOT affect the atom name.

5.4.4 Underscore on Labels

If this option is active, an underscore will be placed between the label and the symmetry designator code. For atoms in equivalent position #1, no symmetry designator code is added. If this control is NOT active (default) and the **Mouse Labels (GUI Font)** is selected, then the symmetry designator codes for the mouse labels will be drawn as *superscripts*, thereby complying with *Acta Cryst* requirements for labels.

5.4.5 Brackets on Labels

If this option is active, brackets will be drawn around the numerical part of the atom label.

5.5. VIEW MENU

This menu consists of several viewing-modes that are all ganged, so that only one may be active at any time. The default, and usually the most satisfactory starting view is **Best View**. When any of these modes are selected, all stored rotations and translations are set to zero.

5.5.1 Best View

This option calculates the mean plane, and sets the highest axis of inertia of the molecule normal to the screen. This will usually give the view with the least overlap, *i.e.* the ‘best view’. Occasionally (*e.g.* if the molecule comprising the illustration has perfect spherical symmetry such as a tetrahedron or octahedron, or if less than three non-colinear atoms are present) it is not possible to calculate a ‘best view’. The program then issues a warning message in the ConsoleWindow, and automatically switches to standard view.

5.5.2 Standard View

This option places the centroid of the molecule in the centre of the screen, with the crystallographic *a* axis vertical, and the *c** axis normal to the screen.

5.5.3 Select Normal Plane

This option allows the user to select three atoms by mouse clicks, which form a plane. The three atoms should be non-colinear, but the algorithm is quite robust, and virtually colinear atoms may be chosen without a program error. The view direction is then set normal to this plane, with the screen X-direction set along the vector atom1-atom2 and with the vector atom1-atom3 lying in the screen XY-plane in the +ve Y direction (upwards).

5.5.4 Select Edge Plane

This option is identical to the above, except that the view direction is set to be along the chosen plane, so that the viewer sees this plane edge-on.

5.5.5 View Normal To (100) { (010), (110) }

These options provide views where the crystallographic *bc*, *ac*, *ab* planes respectively are placed in the plane of the illustration. The first axis of the pair lies along the screen x-direction (horizontal), with the second axis lying in the xy-plane (*i.e.* plane of the screen). The *a** axis etc is normal to the screen, and for crystal systems with orthogonal axes (orthorhombic, tetragonal, cubic), these views correspond to views down the crystallographic *a*, *b* and *c* axes respectively.

5.5.6 Continuous Rotation

This option allows continuous rotation of the illustration through the current rotation angle. The default direction is +X, but this direction may be changed by hitting the following keys:

Arrow up -X

Arrow down +X

Arrow left -Y

Arrow right +Y

Page up +Z

Page down -Z

The rotation may be halted by hitting any other key (apart from some control keys) or by depressing the mouse button in the graphics area for several seconds.

5.6. GRAPHICS MENU

This set of menu options control how the illustration appears on the graphics screen, and also the production of hardcopy and metafile output from the screen graphics

5.6.1 Select Colour

The colours assigned to all graphical objects - atoms types , bonds, text (labels and title), unit cell outline, foreground (used only for monochrome illustrations) and background may be modified from this menu item. Any loaded colour may be chosen without restriction for each graphical object.

5.6.2 Background Style [Plain/Graduated/Patterned]

The background may be drawn as a plain colour, graduated from black at the top of the screen to the selected colour at the bottom or patterned. Note that the graduated or patterned backgrounds use many colours and are only effective for colour depths of 16-bit or greater. They look distinctly odd on a 256-colour display and quite ridiculous on a 16-colour display. The **Patterned** option uses a 2-dimensional Fourier series to produce variations in the colour intensity (similar to that used in SCHAKAL). The ORTEP Parameter **PatternNumber** controls the number of terms used in the Fourier summation (and hence changes the pattern). The patterned background takes some time to calculate, but is stored and only recalculated if the background colour or **PatternNumber** are changed.

5.6.3 Colour Plot/Monochrome Plot

The user may select either a monochrome, or a colour illustration. The latter is the default, but the former is recommended if the **Print Graphics Screen** option is to be used with an attached printer which does not support colour. The monochrome mode uses the foreground colour (default White) selected in 5.6.1 above.

5.6.4 Clear Graphics Screen

This option clears any illustration from the graphics screen.

5.6.5 Select Graphics Font

The Graphics Font (point size, colour, effects and font style) used for the labels and title-text may be selected from a dialog box. Any loaded Windows font may be chosen, though clearly some are much more suitable than others. Only those labels set by the mouse labelling routine will use this font. These labels may also be used for the metafile outputs (see 5.1.4) The HPGL format has only one font-type (pseudo Courier) but there are more fonts available in PostScript output. The program will choose the closest PostScript font to the current Graphics Font.

5.6.6 Print Graphics Screen

With this option, the current illustration is copied directly to an attached printer. This facility uses the Microsoft printer drivers, so the actual result will depend on local conditions. It has not been tested on a large number of printers, but the copy obtained from HP laser printers is of excellent quality. There are two choices for the print size - landscape A4 or direct journal size (DJS). Many primary journals e.g. ACS journals now ask for illustrations at the correct size for direct reproduction. The sizes of the A4 plot is handled automatically - the height will be the maximum resolution of your printer and the width chosen to retain the horizontal/vertical aspect ratio of 4:3. The size of the DJS plot is now handled by the ORTEP parameter **DJS_ScalingFactor** which is the proportion relative to the landscape A4 plot (default 0.25). The linewidths for each format are chosen automatically and will depend on the **PlotLineWidth** used for the screen display (normally 1). It is possible to tweak the plotted linewidth using the ORTEP Parameters **PlotA4_LWScale** and **PlotDJS_LWScale** which are normally set to 1.0. The user may need to experiment to get suitable settings of these parameters. Instead of printing the illustration directly, is also possible to save the plot as a plot-file (from the Printer Dialog Box). The format of this plot-file will depend on the local printer, e.g. for a LaserJet 4ML, it is in PostScript (Microsoft dialect).

5.6.7 Copy To Clipboard

This menu item copies the current illustration *exactly as is* to the clipboard. This may subsequently be inserted into another Windows program e.g. a word-processor or graphics processor program.

5.6.8 Export as Bitmap file

The screen illustration may also be saved as a raster metafile in a number of sizes and bitmap formats, and relies on the plugin program *IrfanView*. If this program is not available, then the only file format which can be saved is the (very inefficiently stored) Windows Bitmap format (.BMP files). The Portable Network Graphics format (.PNG files) is a most efficient bitmap format and is selected by default.

5.6.9 Draw Frame

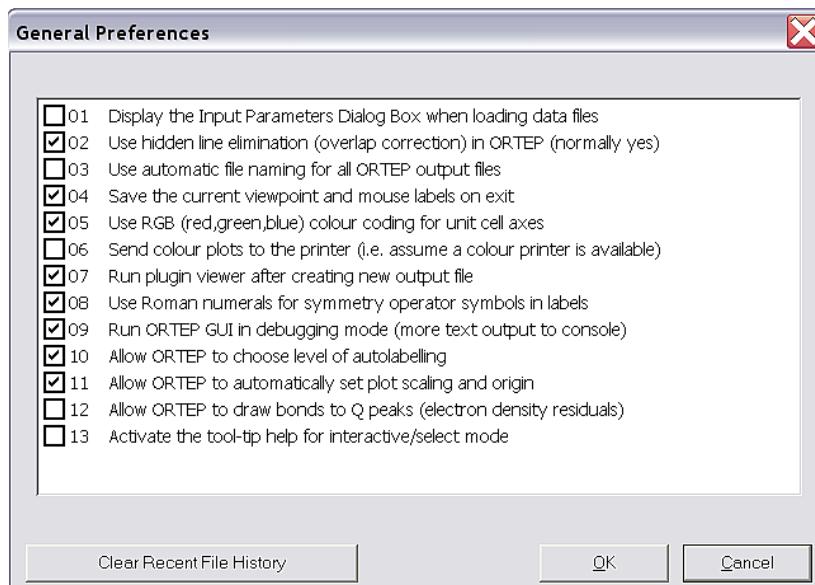
By default, no frame is drawn around each illustration. Selecting this item will add a frame.

5.7. OPTIONS MENU

These menu items allow the user to make rarely required changes to the standard settings.

5.7.1 General Preferences

This option brings up the General Preferences Dialog Box, which allows the user to set a number of program options. These options are detailed in the Appendix, Table 6.2. The settings are stored in the INI file, which is written whenever the program is closed or a new file is read in. This dialog box also allows the user to delete the recently opened file history.



5.7.2 Configure Plugins

This option brings up the Configure External Plugin Dialog Box, show in Appendix 6.1. The setting are stored in the INI file, which is rewritten whenever the program is closed or a new file is read in.

5.7.3 Run ORTEP Direct

If this option is selected, the GUI is bypassed and an ORTEP illustration is created directly from the file *OrtepInstruction*. This is a feature for the expert user, who knows how to manually edit the file to achieve desired results.

5.7.4 Run POV-Ray/PostScript Viewer/HPGL Viewer/Raster3D

This option allows the user to launch the external plugins from within *Ortep-3 for Windows* using the last created relevant file as input.

5.8. CALCULATE MENU

These menu items show the results of geometrical calculations, RMS analysis of the anisotropic thermal parameters, or display some current parameters.

5.8.1 List Bonds, List Angles, List RMS

Either all bonds, all angles or all RMS displacements of the adp's are calculated by ORTEP-III, and the raw list output is shown in a scrollable box.

5.8.2 List Atoms

All atoms in the illustration are listed with their names, symmop numbers and unit cell translations.

5.8.3 List Symmops

The current ORTEP symmetry operators are shown with their number, so that symmops may be related to the graphic symbols used for the labels (see 5.4.2 and **Symmop Symbols 5.4.6**).

5.8.4 Interactive GEOM

With this menu item, either 2, 3 or 4 atoms may be mouse-selected for bond distance, bond angle or torsion angle calculations. If two atoms A,B are selected, the A-B distance in Å is displayed. If three atoms A,B,C are selected, the angle A-B-C is displayed, together with the A-B and B-C distances in parentheses. If four atoms A,B,C,D are selected, the torsion angle A-B-C-D is displayed, together with the A-B, B-C, C-D distances and the A-B-C and B-C-D angles in parentheses. If more than 4 atoms are selected, or if the OK button (or right mouse-button) is clicked, the selection array is cleared for another calculation.

6. APPENDICES

Table 6.1 ORTEP Parameters [¶]

| ORTEP Parameter | Meaning | Default value |
|---------------------------|---|---------------|
| BondSearchDistanceMax | Maximum allowable bond distance (Å) | 4.0 |
| BondSearchDistanceMin | Minimum allowable bond distance (Å) | 0.65 |
| BondToleranceFactor | The maximum searchable bond distance between two atoms A and B is the sum of their covalent radii plus this parameter (Å) | 0.2 |
| CentroidBondMin | Minimum bond distance (Å) for added centroids | 1.65 |
| DJS_ScalingFactor | Proportion of direct journal size (DJS) plot relative to Landscape A4 plot. | 0.25 |
| EllipseSmoothingParameter | Smaller values produce a smoother ellipsoid. Allowed values in the range 0.0 - 3.0 | 1.0 |
| EllipseProbability | Percentage probability for thermal ellipsoids; range 10-99 | 50 |
| InitialDrawingStyle | Drawing style (default/OctantShaded/Highlighted/Plain) adopted when program starts | default |
| InitialPlotStyle | Plot style (colour/monochrome) style adopted when program starts | colour |
| LabelTextXOffset | Horizontal offset for label placement (in) | 0.45 |
| LabelTextYOffset | Vertical offset for label placement (in) | 0.45 |
| MaximumAtomsAutoLabel | Autolabelling is switched off if more than this number of atoms are drawn | 70 |
| MouseSensitivity | Ratio of mouse drag to rotation angle (arbitrary units) | 100 |
| OverlapMargin | Margin around overlapped bonds and atoms | 0.04 |
| PatternNumber | Number of terms in Fourier summation for patterned background (1-20) | 20 |
| PenWidthHPGL | Pen width for HPGL file output (arbitrary units) | 1.5 |
| PenWidthPostScript | Pen width for PostScript file output (arbitrary units) | 20 |
| PerspectiveViewDistance | Perspective view distance for standard plots | 30.0 |
| PlotA4_LWScale | Linewidth scaling factor for Print Graphic Screen hardcopy output (A4) | 1.0 |
| PlotDJS_LWScale | Linewidth scaling factor for Print Graphic Screen hardcopy output (DJS) | 1.0 |
| PlotLineWidth | Linewidth factor for all plots (arbitrary unit) | 1 |
| PlotMargin | Blank margin around drawing (in) | 0.1 |
| PlotScaleFactor | Scale factor for non-automatic scaling | 0.9 |
| RetraceDisplacement | Displacement for retracing lines (in) | 0.005 |
| RotationAngle | Rotation increment for buttons on the tool bar | 10 |
| StereoDisplacement | Distance between the two images in a stereo plot (in) | 4.0 |
| StereoRotationAngle | Rotation angle (+ and -) for stereo plots (deg) | 2.7 |
| StereoViewDistance | Perspective view distance for stereo plots | 30.0 |
| StereoViewScaleFactor | Scale factor used for stereo plots | 0.32 |
| SuperscriptDisplacement | Vertical displacement of superscript text in proportion of font size | 0.5 |
| SuperscriptSize | Size of superscript text in proportion of font size | 0.8 |
| UnitCellAxisLabel_A(B/C) | Label for the A (B/C) unit cell corner | A (B/C) |
| UnitCellOriginLabel | Label for the unit cell origin | ORGN |

[¶] These parameters may be modified using the Ortep Parameters Dialog Box, and are all stored in the INI file.

Table 6.2 General Preferences¹

| # | Description | default status |
|----|---|----------------|
| 1 | If on, display the Input Parameters Dialog Box when loading a new file | off |
| 2 | If on, use the hidden line elimination (overlap correction) facility in ORTEP | on |
| 3 | If on, use automatic file naming for output files (graphics & coordinate files) so that all new files are written to the working directory with a unique name (no overwriting). If off, files are written to the home directory, always with the same name. | off |
| 4 | If on, the current viewpoint and mouse labels are saved in a file called OrtViewMatrix in the working directory. It only makes sense to have this facility switched on if there is only one data file per directory | on |
| 5 | If on, unit cell axes are drawn with RGB colour coding (a=red, b=green c=blue) | on |
| 6 | If on, assume that a colour printer is attached to computer, and send plots in colour to the printer. If printer is a monochrome printer, then the colours will be dithered in shades of grey. Generally if the printer is monochrome, it is best to switch this option off | off |
| 7 | If on, automatically run the associated plugin program when a new graphic output file is created (e.g. if a POV-Ray instruction file is created, then POV-Ray will be run immediately after to render that file to a raster image file) | on |
| 8 | If on, use Roman numerals for symmetry designator codes. This is mandatory for Acta Cryst journals. Otherwise normal arabic numerals are used for the codes | on |
| 9 | If on, run the GUI in debugging mode, which will produce more output in the OrtepConsole Window. Occasionally useful if things go wrong. | off |
| 10 | If on, allows ORTEP to choose automatically the level of labelling. If more than MaximumAtomsAutoLabel number of atoms are drawn, then labelling is switched off | on |
| 11 | If on, allows ORTEP to set automatically the plot scaling and origin. If this is switched off, then it will probably be necessary to adjust the plot scaling using the zoom button | on |
| 12 | If on, then bonds will be drawn to Q-peaks, assuming a C-atom radius, otherwise they are just drawn a pseudo-atoms | off |
| 13 | If on, activates the tool-tip help facility for the interactive/select windows | on |

¹ These parameters may be modified using the General Preferences Dialog Box, and are all stored in the INI file.

Table 6.3 Other parameters stored in INI file

| Name | Meaning | Default value |
|----------------------|---|---------------|
| POVRayExecutable | Fullpath name of POV-Ray executable | no default |
| PostScriptExecutable | Fullpath name of PostScript interpreter (eg GSview) | no default |
| GraphicsExecutable | Fullpath name of Graphics file view(eg IrfanView) | no default |
| HPGLExecutable | Fullpath name of HPGL interpreter (eg PRINTGL) | no default |
| EditorExecutable | Fullpath name of text editor (eg c:\ortep_2\editor.exe) | no default |
| BackGroundColor | Default colour of background | Black |
| BackGroundStyle | Default style of background(plain/graduated/patterned) | plain |
| ForeGroundColor | Default colour of foreground (monochrome plots) | White |
| UnitCellOutline | Default colour of unit cell edges | Yellow |
| BondColor | Colour of standard bonds | White |
| TextColor | Default colour of title font | White |
| POVRayFloorColor | Default floor colour for POV-Ray | DkGreenCopper |
| POVRayCutoutColor | Default cutout colour for POV-Ray ellipsoids | RichBlue |
| POVRayEquatorColor | Default equator colour for POV-Ray ellipsoids | Black |
| GraphicsFontName | Font to be used for labels/text | Arial |
| GraphicsFontSize | Font style to be used for labels/text | Arial |
| GraphicsFontColour | Font colour to be used for labels/text | Arial |
| GraphicsFontSize | Point size of labels/text font | 14 |

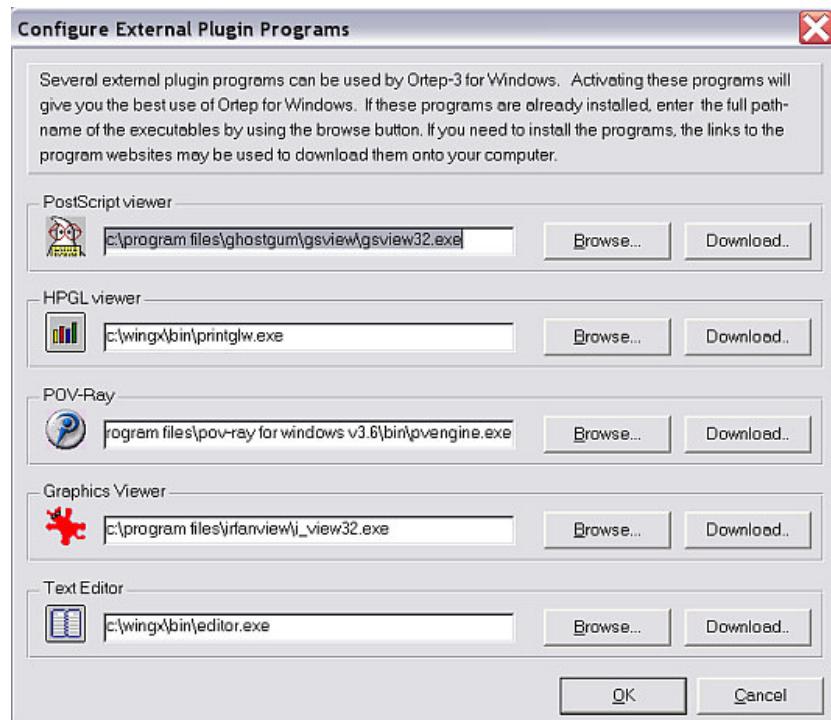
¹ These parameters may be modified using various program options, and are all stored in the INI file.

Table 6.4. Colour names and RGB values defined in Ortep-3 for Windows

| Colourname | R | G | B | Colourname | R | G | B |
|----------------|----------|----------|----------|-------------------|----------|----------|----------|
| Aquamarine | 0.439216 | 0.858824 | 0.576471 | IndianRed | 0.309804 | 0.184314 | 0.184314 |
| BakersChoc | 0.36 | 0.2 | 0.09 | Khaki | 0.623529 | 0.623529 | 0.372549 |
| Black | 0 | 0 | 0 | LightBlue | 0.74902 | 0.847059 | 0.847059 |
| Blue | 0 | 0 | 1 | LightGray | 0.658824 | 0.658824 | 0.658824 |
| BlueViolet | 0.62352 | 0.372549 | 0.623529 | LightGrey | 0.658824 | 0.658824 | 0.658824 |
| Brass | 0.71 | 0.65 | 0.26 | LightSteelBlue | 0.560784 | 0.560784 | 0.737255 |
| BrightGold | 0.85 | 0.85 | 0.1 | LightWood | 0.91 | 0.76 | 0.65 |
| Bronze | 0.55 | 0.47 | 0.14 | LimeGreen | 0.196078 | 0.8 | 0.196078 |
| Bronze2 | 0.65 | 0.49 | 0.24 | Magenta | 1 | 0 | 1 |
| Brown | 0.647059 | 0.164706 | 0.164706 | MandarinOrange | 0.89 | 0.47 | 0.2 |
| CadetBlue | 0.372549 | 0.623529 | 0.623529 | Maroon | 0.556863 | 0.137255 | 0.419608 |
| Clear | 1 | 1 | 1 | MediumAquamarine | 0.196078 | 0.8 | 0.6 |
| CoolCopper | 0.85 | 0.53 | 0.1 | MediumBlue | 0.196078 | 0.196078 | 0.8 |
| Copper | 0.72 | 0.45 | 0.2 | MediumForestGreen | 0.419608 | 0.556863 | 0.137255 |
| Coral | 1 | 0.498039 | 0 | MediumGoldenrod | 0.917647 | 0.917647 | 0.678431 |
| CornflowerBlue | 0.258824 | 0.258824 | 0.435294 | MediumOrchid | 0.576471 | 0.439216 | 0.858824 |
| Cyan | 0 | 1 | 1 | MediumSeaGreen | 0.258824 | 0.435294 | 0.258824 |
| DarkBrown | 0.36 | 0.25 | 0.2 | MediumSlateBlue | 0.498039 | 1 | |
| DarkGreen | 0.184314 | 0.309804 | 0.184314 | MediumSpringGreen | 0.498039 | 1 | |
| DarkOliveGreen | 0.309804 | 0.309804 | 0.184314 | MediumTurquoise | 0.439216 | 0.858824 | 0.858824 |
| DarkOrchid | 0.6 | 0.196078 | 0.8 | MediumVioletRed | 0.858824 | 0.439216 | 0.576471 |
| DarkPurple | 0.53 | 0.12 | 0.47 | MediumWood | 0.65 | 0.5 | 0.39 |
| DarkSlateBlue | 0.419608 | 0.137255 | 0.556863 | Mica | 0 | 0 | 0 |
| DarkSlateGray | 0.184314 | 0.309804 | 0.309804 | MidnightBlue | 0.184314 | 0.184314 | 0.309804 |
| DarkSlateGrey | 0.184314 | 0.309804 | 0.309804 | Navy | 0.137255 | 0.137255 | 0.556863 |
| DarkTan | 0.59 | 0.41 | 0.31 | NavyBlue | 0.137255 | 0.137255 | 0.556863 |
| DarkTurquoise | 0.439216 | 0.576471 | 0.858824 | NeonBlue | 0.3 | 0.3 | 1 |
| DarkWood | 0.52 | 0.37 | 0.26 | NeonPink | 1 | 0.43 | 0.78 |
| DimGray | 0.329412 | 0.329412 | 0.329412 | NewMidnightBlue | 0 | 0 | 0.61 |
| DimGrey | 0.329412 | 0.329412 | 0.329412 | NewTan | 0.92 | 0.78 | 0.62 |
| DkGreenCopper | 0.29 | 0.46 | 0.43 | OldGold | 0.81 | 0.71 | 0.23 |
| DustyRose | 0.52 | 0.39 | 0.39 | Orange | 1 | 0.5 | 0 |
| Feldspar | 0.82 | 0.57 | 0.46 | OrangeRed | 1 | 0.498039 | 0 |
| Firebrick | 0.556863 | 0.137255 | 0.137255 | Orchid | 0.858824 | 0.439216 | 0.858824 |
| Flesh | 0.96 | 0.8 | 0.69 | PaleGreen | 0.560784 | 0.737255 | 0.560784 |
| ForestGreen | 0.137255 | 0.556863 | 0.137255 | Pink | 0.737255 | 0.560784 | 0.560784 |
| Gold | 0.8 | 0.498039 | 0.196078 | Plum | 0.917647 | 0.678431 | 0.917647 |
| Goldenrod | 0.858824 | 0.858824 | 0.439216 | Quartz | 0.85 | 0.85 | 0.95 |
| Gray | 0.752941 | 0.752941 | 0.752941 | Red | 1 | 0 | 0 |
| Gray05 | 0.05 | 0.05 | 0.05 | RichBlue | 0.35 | 0.35 | 0.67 |
| Gray10 | 0.1 | 0.1 | 0.1 | Salmon | 0.435294 | 0.258824 | 0.258824 |
| Gray15 | 0.15 | 0.15 | 0.15 | Scarlet | 0.55 | 0.09 | 0.09 |
| Gray20 | 0.2 | 0.2 | 0.2 | SeaGreen | 0.137255 | 0.556863 | 0.419608 |
| Gray25 | 0.25 | 0.25 | 0.25 | SemiSweetChoc | 0.42 | 0.26 | 0.15 |
| Gray30 | 0.3 | 0.3 | 0.3 | Sienna | 0.556863 | 0.419608 | 0.137255 |
| Gray35 | 0.35 | 0.35 | 0.35 | Silver | 0.9 | 0.91 | 0.98 |
| Gray40 | 0.4 | 0.4 | 0.4 | SkyBlue | 0.196078 | 0.6 | 0.8 |
| Gray45 | 0.45 | 0.45 | 0.45 | SlateBlue | 0 | 0.498039 | 1 |
| Gray50 | 0.5 | 0.5 | 0.5 | SpicyPink | 1 | 0.11 | 0.68 |
| Gray55 | 0.55 | 0.55 | 0.55 | SpringGreen | 0 | 1 | 0.498039 |
| Gray60 | 0.6 | 0.6 | 0.6 | SteelBlue | 0.137255 | 0.419608 | 0.556863 |
| Gray65 | 0.65 | 0.65 | 0.65 | SummerSky | 0.22 | 0.69 | 0.87 |
| Gray70 | 0.7 | 0.7 | 0.7 | Tan | 0.858824 | 0.576471 | 0.439216 |
| Gray75 | 0.75 | 0.75 | 0.75 | Thistle | 0.847059 | 0.74902 | 0.847059 |
| Gray80 | 0.8 | 0.8 | 0.8 | Turquoise | 0.678431 | 0.917647 | 0.917647 |
| Gray85 | 0.85 | 0.85 | 0.85 | VeryDarkBrown | 0.35 | 0.16 | 0.14 |
| Gray90 | 0.9 | 0.9 | 0.9 | Violet | 0.309804 | 0.184314 | 0.309804 |
| Gray95 | 0.95 | 0.95 | 0.95 | VioletRed | 0.8 | 0.196078 | 0.6 |
| Green | 0 | 1 | 0 | VLightGrey | 0.8 | 0.8 | 0.8 |
| GreenCopper | 0.32 | 0.49 | 0.46 | Wheat | 0.847059 | 0.847059 | 0.74902 |
| GreenYellow | 0.576471 | 0.858824 | 0.439216 | White | 1 | 1 | 1 |
| Grey | 0.752941 | 0.752941 | 0.752941 | Yellow | 1 | 1 | 0 |
| HuntersGreen | 0.13 | 0.37 | 0.31 | YellowGreen | 0.6 | 0.8 | 0.196078 |

APPENDIX 6.1 External Plugin Programs:

Ortep3 for Windows is designed to work in concert with *WinGX*. It also makes use of a few external plugin programs which are not included in the distribution, but are freely available on the web. The dialog box shown below allows the user to configure *Ortep3 for Windows* to work with these programs. It is strongly recommended to use these plugin programs to enhance the capabilities of *Ortep3 for Windows*. A basic text editor is supplied with the release, but you may wish to replace this with your favourite editor.



APPENDIX 6.2 Installing Ortep3 for Windows:

The program is provided as a standard Windows self-installation, which should serve most purposes. However, you may wish to customise your installation, and the following information may be useful. There are three directories used by *Ortep-3 for Windows*, the **program directory**, the **home directory** and the **working directory**. Please read Section 4.11, which describes these directories and the files they should contain in detail. Usually the **program directory** and **home directory** are the same directory, but if you wish to set up a networked version, then it is very useful to keep these two directories separate.

APPENDIX 6.3 References

1. L. J. Farrugia (1997) *J. Appl. Cryst.* **30**, 565.
2. M. N. Burnett & C. K. Johnson (1996) ORTEP-III: Oak Ridge Thermal Ellipsoid Plot Program for Crystal Structure Illustrations, Oak Ridge National Laboratory Report ORNL-6895.
3. Ortep-III manual : <http://www.ornl.gov/ortep/ortep.html>
4. The Raster3D suite of programs for UNIX systems may be obtained from :
<http://www.bmsc.washington.edu/raster3d/html/raster3d.html>

A Windows version of these programs has been implemented in the WinGX suite of programs available from :

<http://www.chem.gla.ac.uk/~louis/software/wingx/>

5. The program *POV-Ray* is obtainable as an executable for a number of different platforms from the web-site

<http://www.povray.org/>