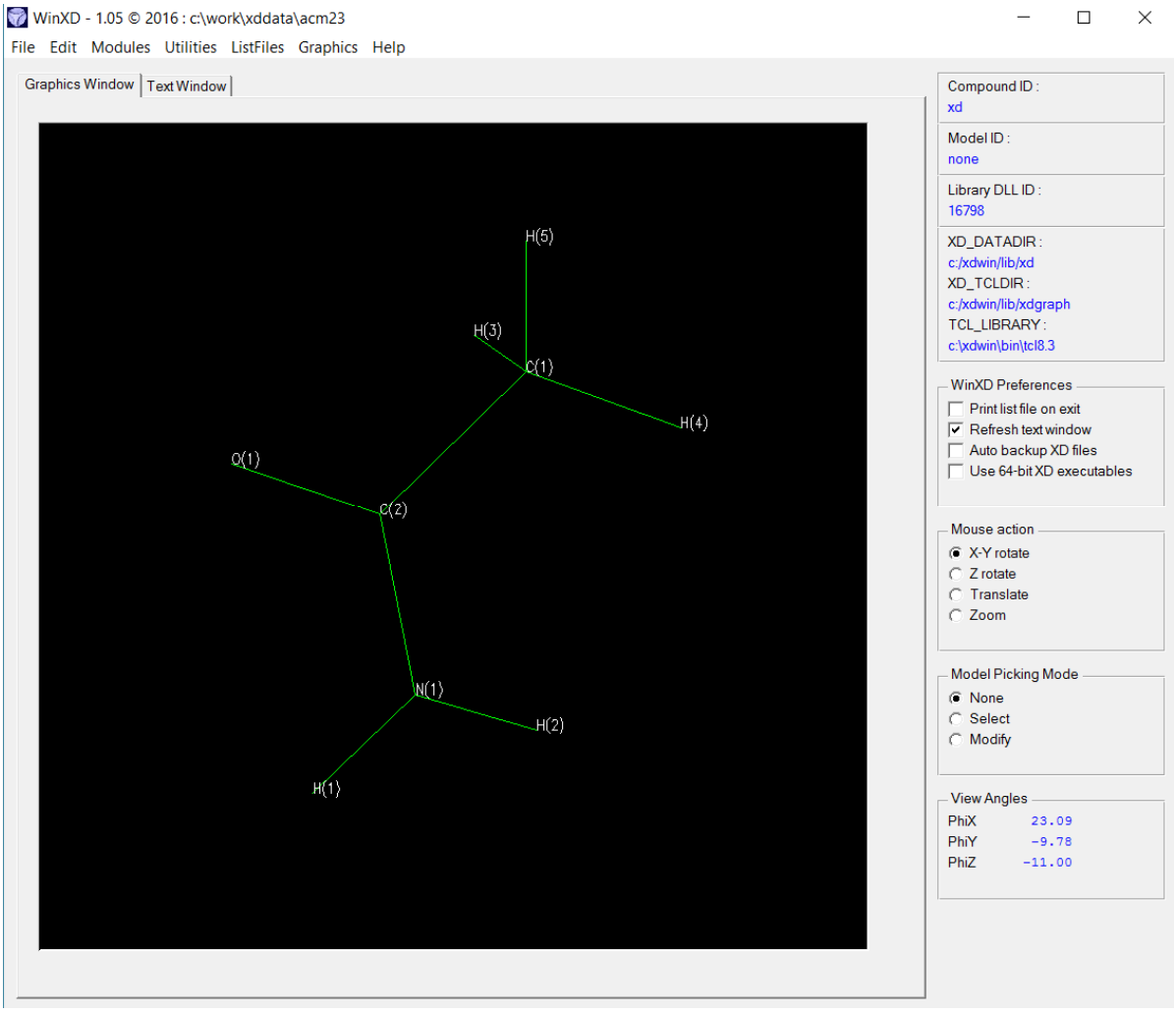
WinXD Manual

1.1 Introduction

WinXD is a shell program for the Windows version of **XD**. It allows the user to modify the main instruction file *XD.MAS* through a GUI interface, as well as execute all XD modules. Some graphical displays are also available in addition to the graphics in **XDGRAPH**.

The XDWIN main Window is as shown below. It has two panes, one allocated to graphical output, the other to text output. The program automatically switches between these panes according to the menu items selected. The status panel to the right displays the current compound and model ID's, the current working directory and various user preferences regarding the operation of these two panes.



The Track-ball Action and Model Picking Modes are only operative when the graphics display is in Model or Bond Path mode.
Starting in version 2016.01 of XD for Windows, it is **no longer necessary** to set any environment variables, though if they are set they will be used as

previously. The default values of XD_DATADIR, XD_TCLDIR and TCL_LIBRARY are determined from the location of the executable, so the directory structure should not be changed after the program has been installed. Their values are displayed on the front panel, in red if they are assigned by the program, or in blue if actually set by the user (see Chapter 12 of XD manual).

Also starting in XD version 2016.01 for Windows, if your computer is running a 64-bit operating system, it is possible to choose to run either the 32-bit or 64-bit XD system modules. In fact, apart from long jobs involving XDLSM or XDPROP, there is probably no advantage in using the 64-bit versions. Some of the XD module programs are currently not available as 64-bit executables.

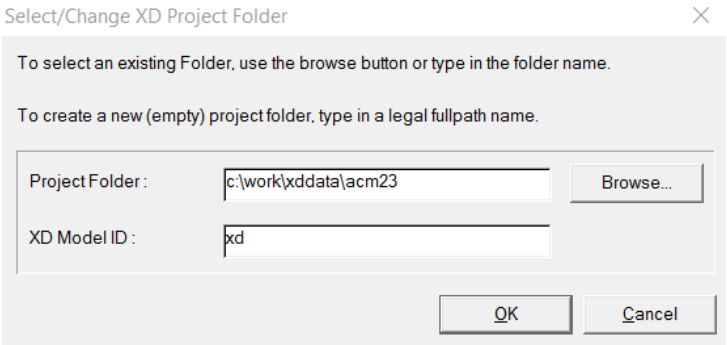
When the GUI is started, information about the location of some important files is displayed in the Text Window.

```
Main Program Binaries Directory : c:\xdwin\bin\
Directory of INI file           : C:\Users\louis\AppData\Roaming\xd2016\
Path of DPLOT executable        : C:\Program Files (x86)\DPlot\dplot.exe
Path of PostScript viewer       : c:\program files\ghostgum\gsview\gsview64.exe
Path of POV-Ray executable      : c:\program files\pov-ray\v3.7\bin\pvengine64.exe
Path of MoleCoolQT executable   : C:\Users\louis\AppData\Local\MoleCoolQt64\molecoolqt.exe
Path of PGPLOT binary FONT file : C:\Users\louis\AppData\Roaming\pgplot\grfont.dat
Path of PGPLOT RGB definitions  : C:\Users\louis\AppData\Roaming\pgplot\rgb.txt
Path of current work directory  : c:\work\xddata\acm23
Monitor Resolution (pixels)     :   1280  1024
WinXD Graphics Screen (pixels)  :    800   800
```

2 File menu

2.1 Select/Change Project Folder

This option allows the user to change the current working folder and the XD job names. When ***WinXD*** is closed, these values are saved, so that the program restarts in the previous folder. The following dialog box opens, allowing the user to type or browse to a new working folder. To select the folder, simply click on any file in that folder.



2.2 Explore Work Directory

This option opens up the Windows Explorer in the current working folder, allowing the user to delete/rename files *etc* in the normal Windows fashion.

2.3 Reload Data

This option reloads the XD.MAS, XD.INP & XD.RES files, so updating the system if these files have been edited manually

2.4 Recent Project Folders

This option allows users to change the current working directory to previous projects

2.5 Open XD Master File

This option loads XD.MAS into the system Editor, so that this file may be manually edited (often the quickest way!)

2.6 Open XD ParameterFile (INP)

This option loads XD.INP into the system Editor, so that this file may be manually edited.

2.7 Open XD ParameterFile (RES)

This option loads XD.RES into the system Editor, so that this file may be manually edited.

2.8 Open XD ReflectionFile

This option loads XD.HKL into the system Editor, so that this file may be manually edited.

2.9 Clear Text Window

This option refreshes the text window

2.10 Export to GAMESS-UK

This option takes the current structural data in the parameter file and creates a default input file for the quantum calculation package GAMESS-UK.

2.11 Export to GAUSSIAN

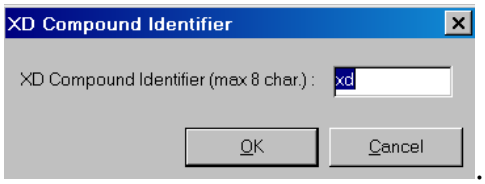
This option takes the current structural data in the parameter file and creates a default input file for the quantum calculation package GAUSSIAN03/09.

2.12 Export to SHELX

This option takes the current structural data in the XD parameter and reflection files and creates input files (SHELX.INS & SHELX.HKL) for the refinement package SHELX.

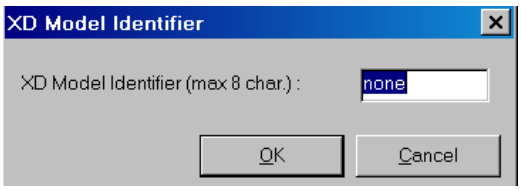
2.2.12 Set Compound Identifier

This option gives a dialog box which allows the user to change the XD compound ID string (cid). This is done automatically when each project is loaded, so should not be necessary to modify this.



1.2.7 Set Model Identifier

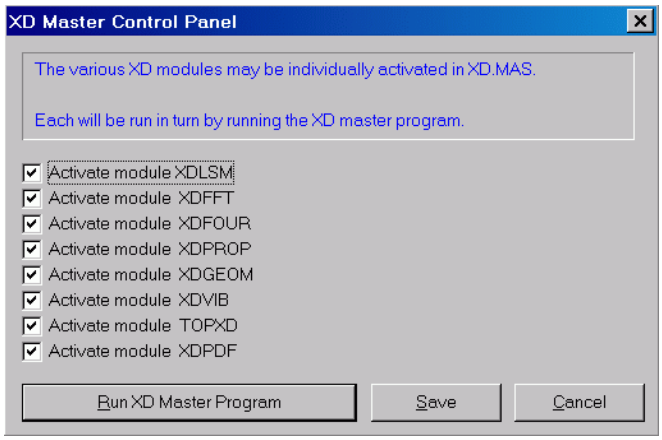
This option gives a dialog box which allows the user to change the XD model ID string (mid).



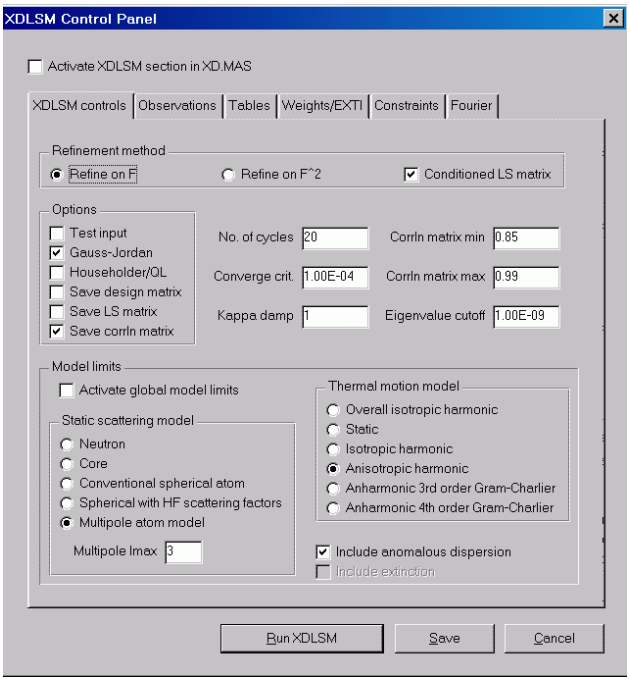
3. Edit menu

3.1 XD Master

This option gives a dialog box which allows the user to change active status of the main XD modules in the XD.MAS file, and execute all those modules using the Master XD program. All activated modules will be executed in the sequence indicated in the XD Master Control Panel. The Save button saves a new XD.MAS file, but does not run any programs. The corresponding sections are activated for those programs which have GUI editable commands (currently this excludes XDVIB, TOPXD and XDPDF).



3.2 Module Commands



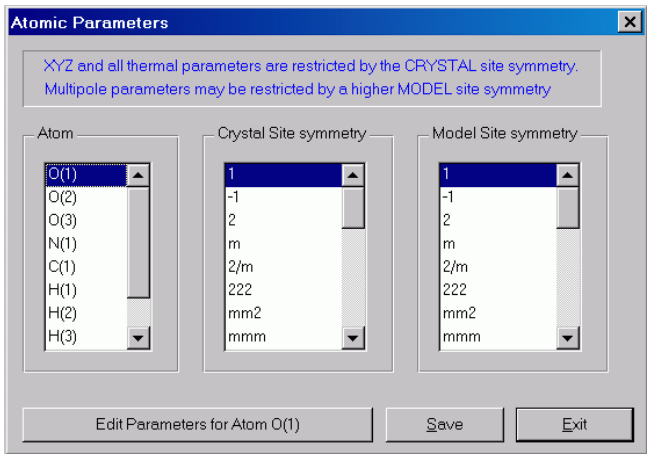
This option opens dialog boxes which allow the user to modify virtually all the parameters and commands for the XD modules XDLSM, XDFOUR, XDFFT, XDPROP & XDGEOM in the XD.MAS file. If the "Auto backup XD files" button in the main GUI is checked, then everytime WinXD writes new master or parameter files, it saves the current versions of XD.MAS/XD.INP/XD.RES as the files XD_MAS.BACKxxxx *etc* (where xxxx is a four digit number between 0001 and 9999, with the larger numbers representing the most recent versions). The Commands dialog boxes will overwrite the XD.MAS file. In the current version of ***WinXD***, the commands for XDVIB, TOPXD and XDPDF in the XD.MAS file are not editable by the GUI, but are copied verbatim to the new XD.MAS file.

An example of a command dialog box for XDLSM is shown above. In some cases, not all parameters may be edited. The layout of these dialog boxes closely follows that in the XD manual. The meaning of individual parameters is not discussed in this manual. It is essential that the user is familiar with the meaning of the parameters from reading the XD manual. Even experienced users of XD should note that the commands for XDPROP have changed significantly from previous versions, and there is no substitute for reading the manual. The command GUI for XDPROP in particular is complicated, reflecting the numerous capabilities of the program.

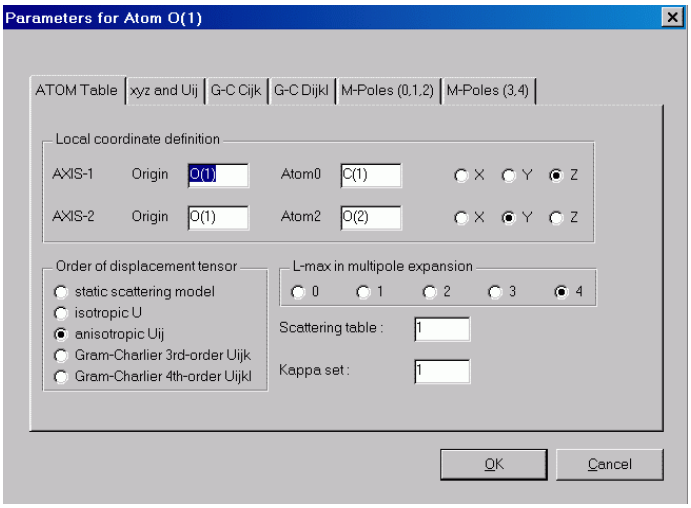
3.3 Parameters

This option opens dialog boxes which allow the user to modify almost all the atomic parameters in the same way as for the commands in XD.MAS. The results are written to a new parameter file. **IMPORTANT** - the file XD.RES is chosen in preference as the parameter file over XD.INP, if it is present in the working directory. All edits will be carried out on the chosen parameter file.

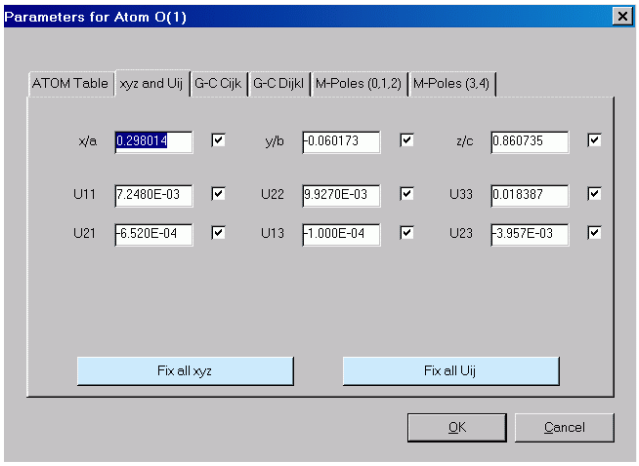
If you have edited XD.RES and wish to run an XD program, it is essential to copy the new version of XD.RES to XD.INP (Utilities menu item RES→INP). This is NOT done automatically !



Select an atom and press the "Edit Parameters" button. This gives you the EditAtom dialog box, an example is shown below



The global parameters set on the front pane limit those parameters which may be edited. For instance, if the level of the displacement tensor is set to anisotropic Uij, then the Gram-Charlier C^{ijk} and D^{ijkl} coefficients cannot be edited. Likewise, if the L-max level in the multipole expansion is set to 3, then the hexadecapole parameters cannot be modified for that atom in the GUI. Each parameter has an associated checkbox next to the actual value of



the parameter, which indicates whether this parameter should be refined. These may be changed globally by the blue buttons in the Window. NOTE that any changes to the parameters are not saved permanently, unless the SAVE button in the "Atomic Parameters" dialog box is pressed.

3.4 Customise Display

This option opens a dialog box which allows the user to modify the font used in the text window and the size of the graphics window to suit your screen resolution. The size of the graphics window can only be set to sensible values.

3.5 Plugin Programs

XD and the WinXD GUI writes a number of files (primarily graphical files) which require external, publically available programs to view. To access all the new features of XD, it is recommended that these programs are also installed. They are all available as *Windows™* executables.

MoleCoolQT - a program for visualising iso-surfaces and mapped iso-surfaces

http://www.molecoolqt.de/

An excellent program written by Christian B. Hübschle is now freely available for academic users. This produces iso-surface plots directly from the XD grid files or Gaussian format cube files output by XDPROP, and alleviates the deficiencies of the *Windows™* version of XDGRAPH.

Molekel version 5.4 - a program for visualising iso-surfaces and mapped iso-surfaces

http://molekel.software.informer.com/5.4/

This program reads the Gaussian style cube files written by XDPROP.

Ghostview - a program for visualising PostScript files

http://www.ghostscript.com/download/

This program reads the PostScript files written by XDPROP.

POV-Ray - a ray-tracing program for high quality graphical rendering

http://www.povray.org/

This program reads the scene description files written by the WinXD GUI and the utility program rays2pov.

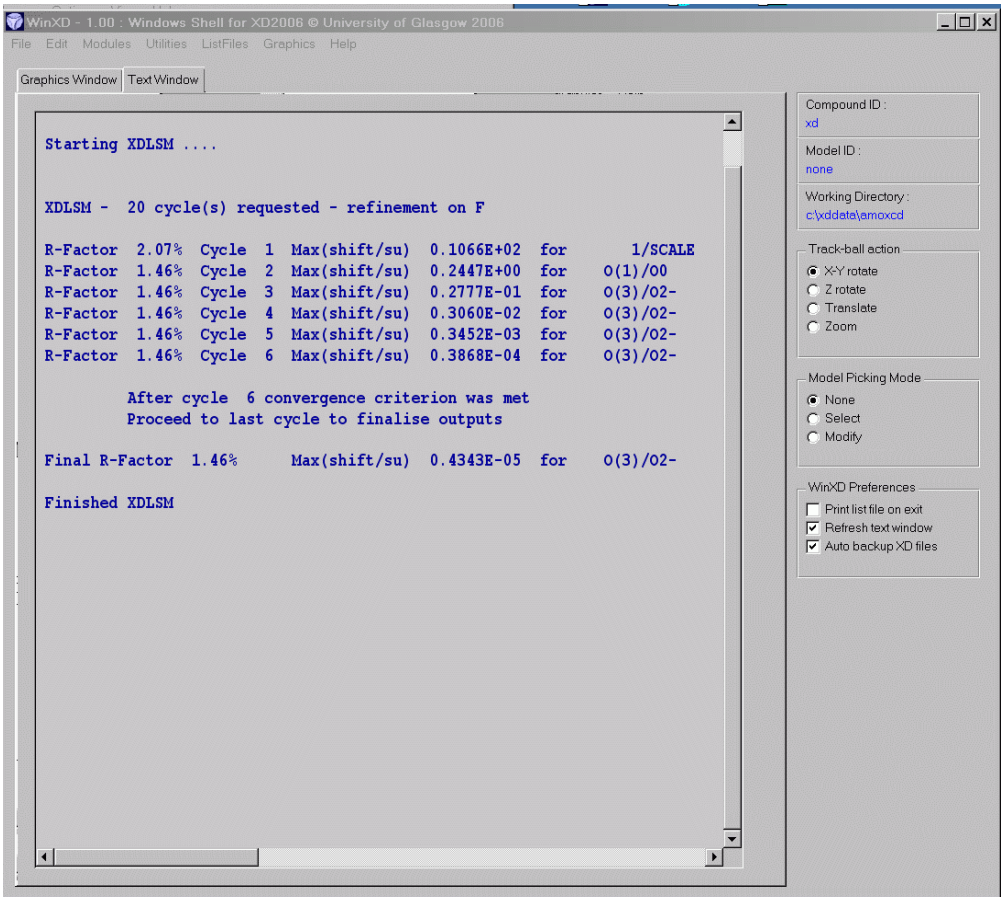
DPLOT - a program for visualising graphs

http://www.dplot.com/

This program is required for the Ellipticity Profile option. The full program has now become quite expensive, but a free simplified version DPLOTViewer is available free of charge from the same web site. It will not allow you to save graph plots though.

4. Modules menu

These menu items launch the individual programs in the XD suite. Input is always taken from XD.MAS, XD.INP & XD.HKL (if required). The text output that is normally directed to the console in the Windows console & Linux versions of XD is displayed in the TextWindow of the GUI



5. Utilities menu

These menu items launch a number of utility programs for the XD suite, to aid in the execution & interpretation of the charge density analysis. Some of these options require plug-in programs (see Section 3.5).

5.1 XDBLOCK

This option allows the user to undertake a blocked least-squares refinement, where in different cycles, separate sets of the parameters are refined. This is to help in the convergence of the model in cases where there are high correlations between parameters. This is in fact very common, particularly when kappa parameters are refined. A set of four versions of XD.MAS need to be prepared prior to execution of option XDBLOCK, namely xd.mas.1, xd.mas.2, xd.mas.4 and xd.mas.4. This will differ solely in the refinement keys of the parameters. The user is at liberty choose which sets of parameters to refine in each block, but one suggestion is :
(1) all positional and thermal parameters
(2) all multipole parameters
(3) the kappa parameters
(4) as many of the above which allow convergence of the model

5.2 XDLSPAR

This option prints to the text window a summary of the current refinement and parameter values.

5.3 Grid File Operations

This menu option allows the user to perform operations on an XD grid file or set of XD grid files.

5.3.1 ADDGRID

This option allows the user to combine two or more XD grid files to create a new grid file. **All grid files combined in this way must be of identical dimensions (i.e. have same number of grid points in all directions) and must have the same origin**. The allowed operations are add, subtract, multiply or divide and users can also change the scaling coefficient (default 1.0) or the exponent (default 1.0) of each grid file. This flexibility allows the user to build new properties grid files. As an example, a grid file of the reduced density gradient s(**r**)

$$s(\mathbf{r}) = |\nabla\rho(\mathbf{r})| \; / \; [2(3\pi^2)^{1/3}\,\rho(\mathbf{r})^{4/3}]$$

is produced by combining grid files containing the gradrho and rho properties. The exponent and coefficient for the first file gradrho are left at their default values, while the coefficient of the rho grid file is set to $6.187335 = 2(3\pi^2)^{1/3}$ and the exponent is set to 1.33333 and the operation

applied to the rho grid file is division. As an alternative, the grid files could be multiplied, with the exponent set to -1.33333. In fact this example is redundant, as the reduced density gradient s(**r**) is already calculated in XDPROP. Note also that in this example, there could be computation problems, e.g. if a rho value was less than or equal to zero.

5.3.2 SCALEGRID

This option allows the user to apply a scaling factor to a single grid file.

5.4 XD.FOU File Operations

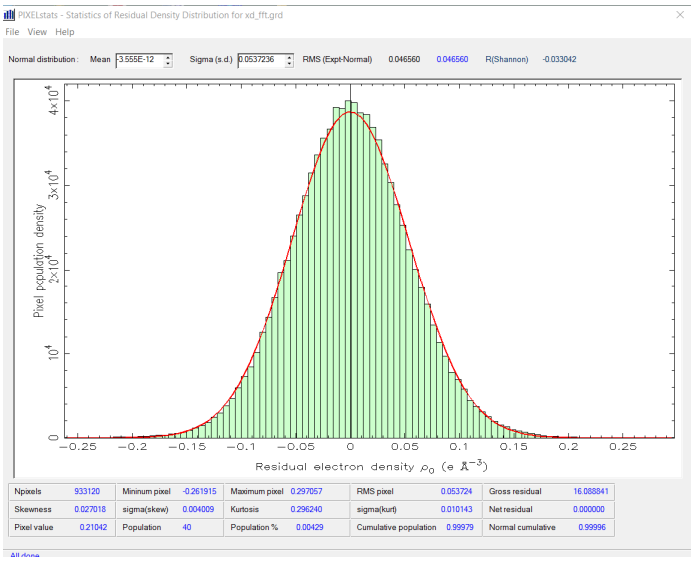
This menu option allows the user to convert the binary file xd.fou into a formatted ASCII form (RDFOU) or an unformatted ASCII form (FOU2ASC). The latter file retains the full accuracy of the binary file. The operation ASC2FOU converts this unformatted ASCII file into binary format. The main purpose of these utilities is to allow transfer of `xd.fou` between different platforms such as Linux, since the binary form of files is highly platform-specific

5.5 RES -> INP

This menu option renames the `xd.res` file to `xd.inp`. It is intended for use with the refinement program XDLSM, which users should note DOES NOT rename the updated parameter file automatically. When running the XDBLOCK utility, this renaming is done automatically.

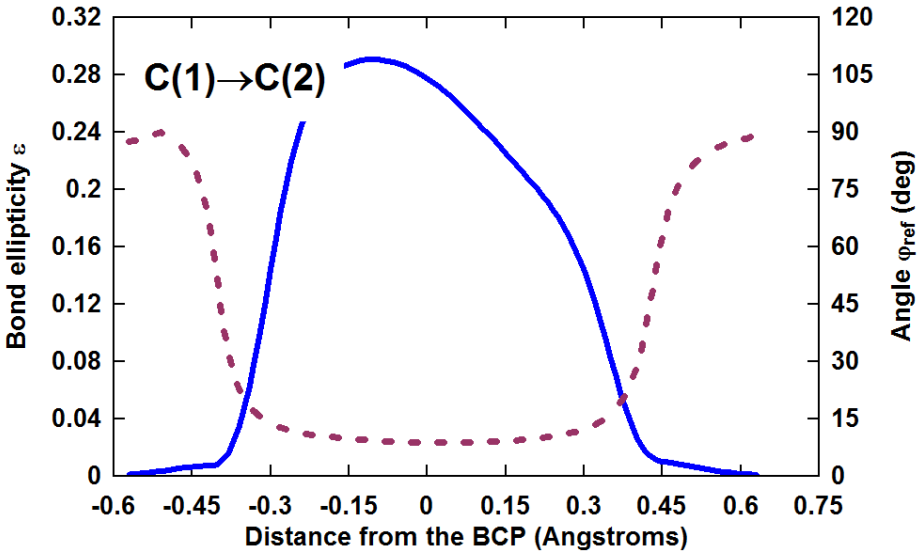
5.5 Residual Density Analysis

This utility runs the PIXELStats program which examines the residual density values in the grid file `xd_fft.grd` following the method described by Henn & Meindl. The program XD_FFT must be run previously, with the *gridf flag set. In the absence of un-modelled features, the distribution of residual values should be very close to a Gaussian distribution. Any deviation from this distribution indicates either that the model is insufficiently flexible, or that there are un-modellable errors in the reflection data.



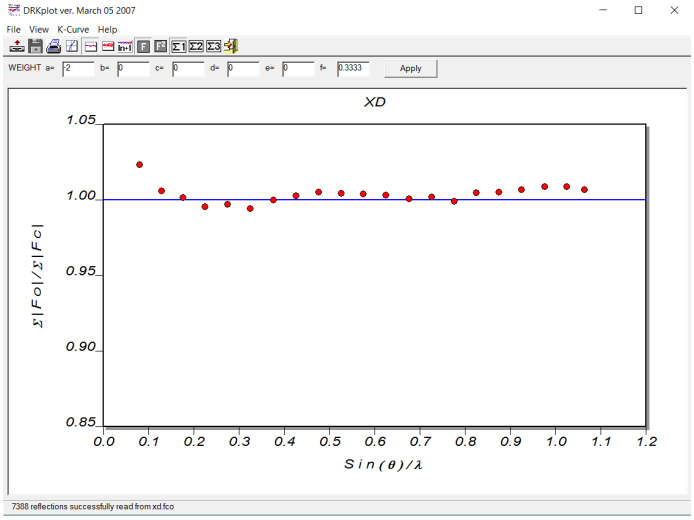
5.6 Ellipticity Profiles

This utility uses the DPLOT plug-in program and the menu item will not appear unless WinXD detects that DPLOT (or DPLOTViewer) is already installed on your computer. The module XDPROP must have been run immediately prior to using this utility (so that the output file `xd_pro.out` contains the required information). A bond path search using CPSEARCH/BPATH instruction with the *profile flag set on the BPATH instruction must be undertaken - see the XDPROP manual for further details. **In the current version of this utility, only a single bond path search can be visualised in each XDPROP run**. In addition, the **verbosity** flag for the XDPROP section in the `xd.mas` file must be set to a value greater than 1 (which is the default value) so that the detailed profile information is present in `xd_pro.out`. If more points along the profile are required, then decrease the value of the pstep parameter (**ds**) from its default value of 0.005 (see XPROP manual).



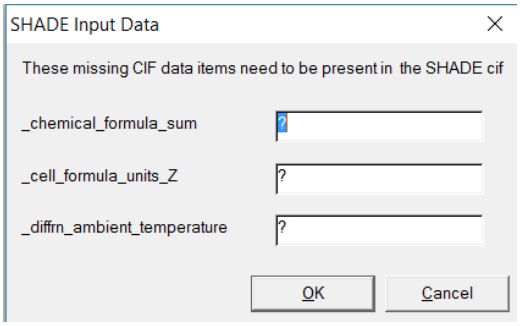
The user is also asked about defining a reference vector, so that the angle φ_{ref} between the principal axis of the ellipticity and this defined vector can be plotted. The above example is for one of the C-C bonds in a coordinated cyclopentadienyl ligand. The reference vector is the normal to the least squares plane of the five C atoms in the ring. The value for the angle φ_{ref} is close to zero in the region of the C-C bcp, which indicates in turn that the main direction of ellipticity is perpendicular the five-membered ring, as is expected for a π-bond.

5.7 DRK-Plot



This utility runs the DRK-Plot program which provides another visual indicator of the quality of fit. Perhaps the most important plot is that of the scale factor versus resolution, which in an ideal case should be completely flat throughout the resolution range. The plot shown below indicates a slight scaling error for the very lowest resolution data of a few percent. A bigger deviation here would be worrying as these low resolution data carry the most important information about the charge density effects.

5.8 SHADE Interface



This utility provides an interface to the SHADE server (current version is SHADE3 at http://shade.ki.ku.dk/docs/shade3/shade3.html), which calculates estimated values of the H atom anisotropic thermal motion from a databank. A special CIF file as input data for this server is required, which is created by the **SHADE Input** option. Most information is obtained

automatically from `xd_lsm.cif` and `xd_geo.cif` (which must both be present), but some essential data is not available, and the user is asked to provide this.

The resulting CIF (`shade_input.cif`) should then be submitted to the SHADE server, using the text string "shade" for both the Job Title and CIF data_block name. Once the SHADE job has run, the output CIF, called `shade_0000.total.cif` (where 0000 is a job number allocated by the SHADE server) should be downloaded and placed in the working directory. The option **SHADE Update** should then be run. This reads the SHADE output CIF and creates a new version of `xd.inp` called `xd.inp.new` which contains the computed adp's for the H atoms and their updated *jtf* flags. Further refinement with XDLSM can continue after this file has been renamed as `xd.inp` and the `xd.mas` file has been edited to account for the fact that the H atoms now have anisotropic thermal parameters. These adp's should now NOT be refined under normal circumstances.

6. Listfiles menu

These menu items will print to the text window the full output listing files of the main XD modules `xd_***.out`.

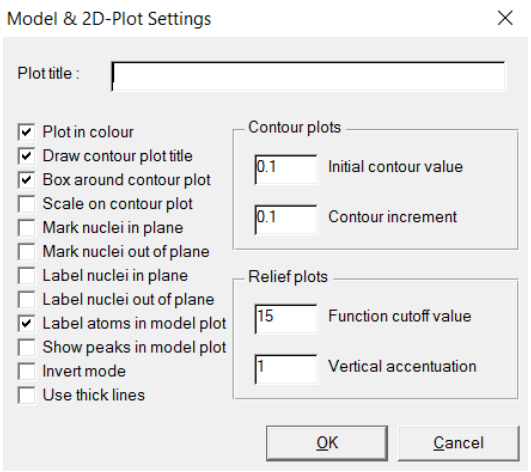
7. Graphics menu

7.1 Model

This option (the default plot) shows the current model in `xd.inp`. Note that only the crystallographic asymmetric unit is shown

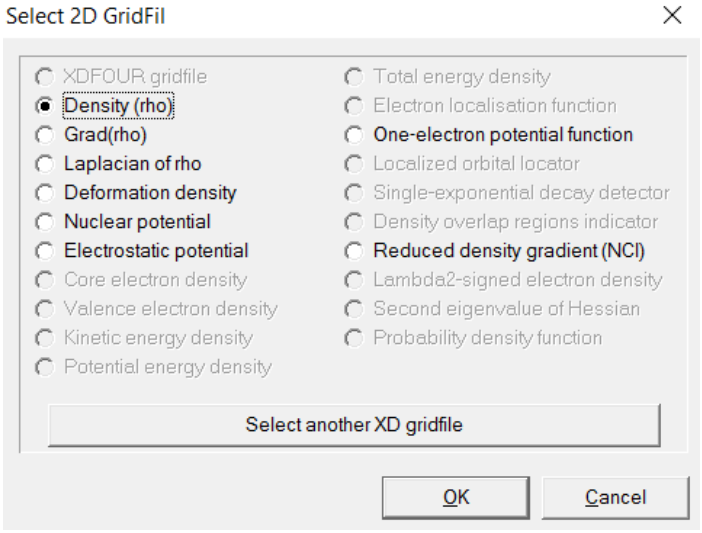
7.2 Model & 2D Settings

This option allows the user to configure the appearance of the model plot and the 2D plots in sections **7.3** and **7.4**.



7.3 2D Contour plot

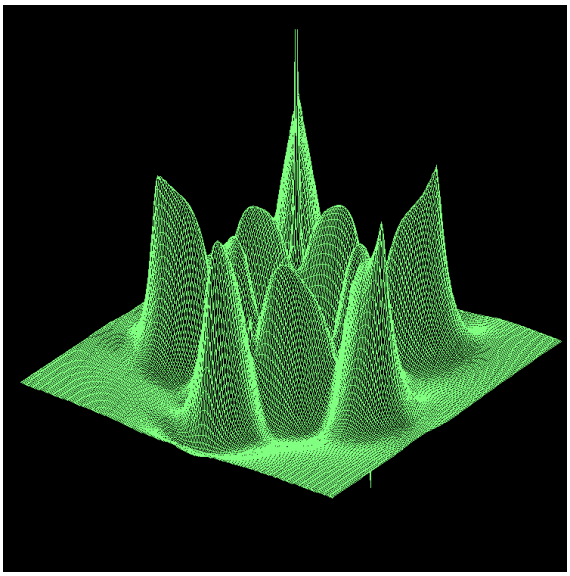
This option produces a contour plot of the selected 2D XD grid file



The dialog box shown above only activates those grid files in the current working directory which have been verified as 2D.

7.4 2D Relief plot

This option display a 2D grid file in the relief format. The vertical accentuation (see **7.2**) will probably need to be adjusted for an optimal view.

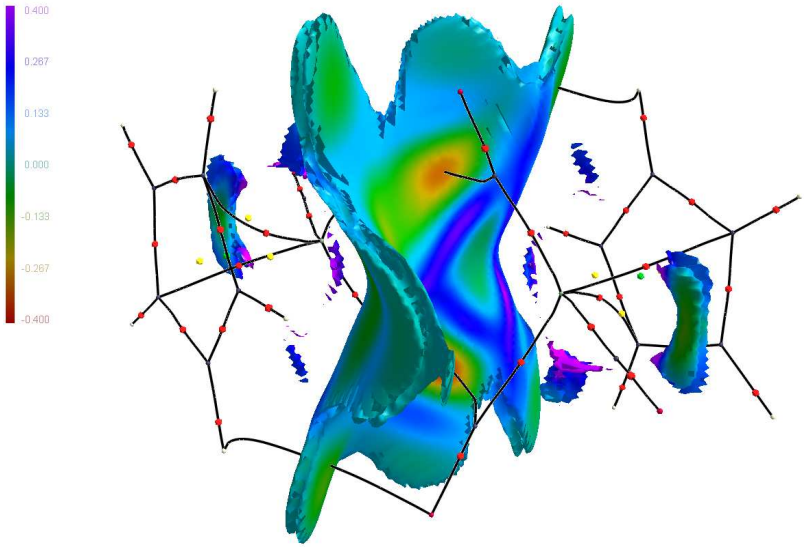


7.5 Mapview

This option launches the external Mapview program (included in the WinXD distribution) which provides a more sophisticated display of the 2D grid files. Sections of 3D grid files can also be displayed in Mapview.

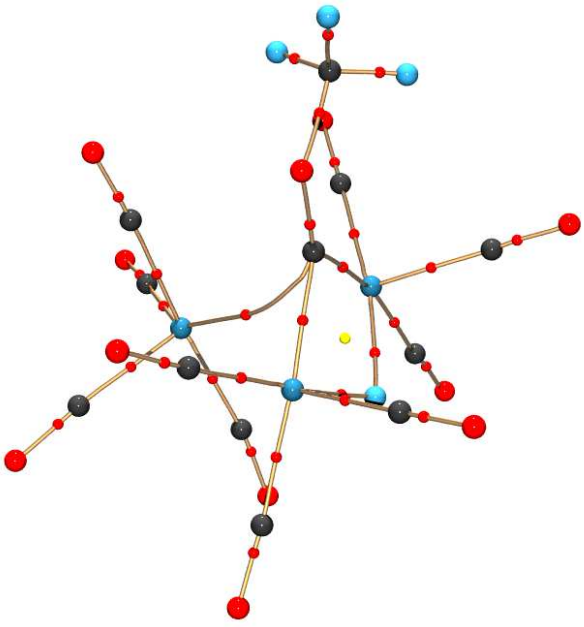
7.6 Isosurface (MoleCoolQT)

This option launches the plugin program MoleCoolQT, which can be used to produce sophisticated isosurface plots from properties in 3D grid, including the mapping of one property onto the isosurface of a second property.



7.7 Plot Molecular Graph

This option show the molecular graph, i.e. all bond paths with their associated (3,-1), (3,+1) and (3,+3) critical points, colour coded in red, yellow and green respectively. The molecular graph is most easily computed in XDPPROP using the MOLGR directive. The files `xd_rho.cps` and `xd.pth` must be present in the current working directory. The graph can be saved in POV-ray format for publication purposes.



7.8 Plot Atomic Graph

This option prepares a file called `atomgraph.dat` which is created from bubble type searches in the Laplacian around a single atomic centre. Output files from XDPROP & TOPXD in which these searches have been conducted is scanned for information about the critical points. The dialog box provides more detailed information. The graph can be saved in POV-ray format for publication purposes.

7.9 Plot Inter Atomic Surface

This option uses the `rays.dat` or `*.rays` files from XDPROP/TOPINT or TOPXD runs to visualise one or more interatomic surfaces. The graph can be saved in POV-ray format for publication purposes.

7.10 Plot Source Function

This utility parses the XDPROP output containing the source integrations and writes POV-Ray files to visualise the integrated SF. Spheres are drawn with a volume proportional to the percentage contribution from the basin, blue is positive, red is negative and the yellow sphere is the position of the reference point. The master POV-Ray file called "sf2pov.pov" includes a file e.g. "file.001" which contains the actual percentages for each reference point. This filename should be changed in the master file for drawing each reference point image. The master POV-Ray file may be manually edited to change the appearance of plots, e.g. change the colour scheme.

The following special conditions apply :

1. All SF integrations must be in the same XDPROP output and all atoms should be integrated.
2. All reference points must be in the `xd_rho.cps` file, as the rho(bcp) density is read from here.

7.11 Hirshfeld Surface Plots

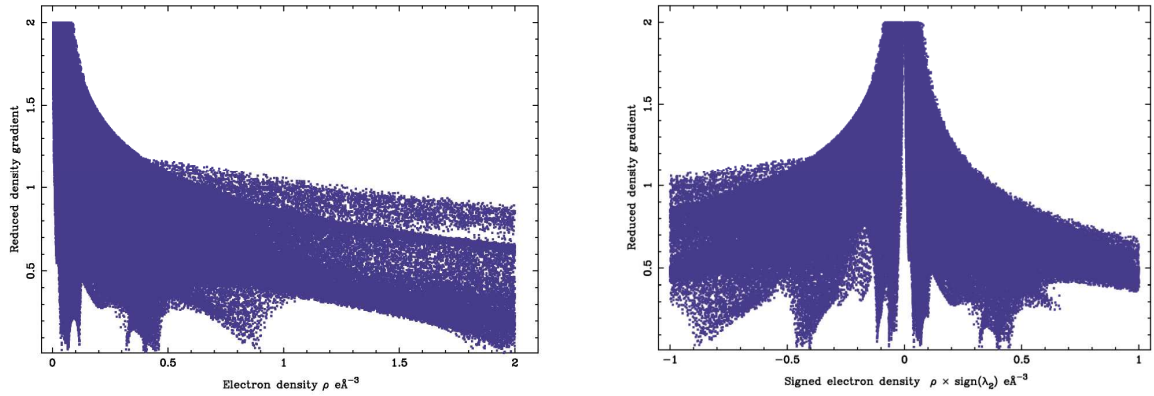
To map properties onto a Hirshfeld surface using XD MoleCoolQT, you first need to prepare two XD 3D grid files using the *IAM option in XDPROP. These two gridfiles must have the same number of grid points in all directions and also must have the same origin. The two gridfiles used to create the Hirshfeld gridfile are :

(i) a grid file with the IAM density of the isolated molecule, and
(ii) a grid file with the IAM density of the molecule in the crystal.

The resultant gridfile `xd_hrsh.grd` contains the Hirshfeld weights. This is used as the ISO_GRID in MoleCoolQT and for a Hirshfeld surface, the iso value should be set to 0.5. If you wish to map a property (such as esp) onto this isosurface, you will also need to prepare a third grid file of identical dimensions and origin, containing this property. This utility is also now fully incorporated into XDPROP with the "CUBE Hirsh" option. See the XDPROP manual for further details.

7.12 NCI Plots

The first option of NCI Plot produces 2D plots of the reduced density gradient (NCI) versus rho & signed(rho). You must create 3D XD grid files of all three properties, i.e `xd_nci.grd`, `xd_rho.grd` & `xd_srho.grd` before running this utility. These grid files must be of identical sizes and origins. If not, plots will not be produced. The plots are written as PostScript files and as DPLOT plot files, and are used to choose the values of the rho and srho cut-offs for writing visualization grid files, which is the second option of NCI Plot. This option reads the three grid files and writes a new NCI grid file `xd_nci_viz.grd` in which limits on rho and/or srho can be applied. All points in the visualization grid file which fall outside the selected ranges of rho and/or srho will be assigned an arbitrary large value of the NCI, so these regions will be invisible in isosurface plots. These grid files may be visualised using MoleCoolQT.



7.13 Slater Function Plots

This option provides plots of a single zeta Slater radial function using the chosen parameters *n(l)*, *ζ(l)*, κ and r_{max}.

7.14 Scattering Curve Plots

The scattering curves for all the elements in the current chemical structure are drawn

7.15 Save as Post-Script File/POV-Ray File

This current graphical image in the graphics window is saved in PostScript or (if possible) in POV-ray file format. Not all plots can be saved in the latter format.