

Downloads

WinGX is a MS-Windows system of programs for solving, refining and analysing single crystal X-ray diffraction data for small molecules. It provides a consistent and user-friendly GUI for some of the best publically available crystallographic programs, and has interfaces to other popular programs such as SHELX-97 and SirWare programs (SIR-97, SIR-2004).

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

Author: Louis J. Farrugia

Department of Chemistry, Joseph Black Building,

University Of Glasgow, Glasgow G12 8QQ

Telephone +44 (0)141 330 5137

FAX +44 (0)141 330 4888

*L. J. Farrugia, J. Appl. Cryst. (1999),***32**, 837-838.

WinGX Program Features

1. Utility programs to write initial model files, name.INS and STRUCT.CIF. Utility programs to operate on these files and import/export other file formats.
2. Programs for data reduction of Enraf Nonius CAD4 and Siemens P4 diffractometer files. Support for KappaCCD, Bruker SMART/APEX, Rigaku data and a GUI for SORTAV.
3. Graphical representation of the [reciprocal lattice](#) and [reflection profiles](#).
4. Numerous [absorption corrections](#), including analytical, gaussian quadrature, spherical-crystal, psi-scans, DIFABS, XABS2 and MULTISCAN (Blessings method for multiple equivalents).
5. Structure solution by DIRDIF-08, SUPERFLIP, SHELXS86, PATSEE and SIR-92, and interfaces to SIR-97/SIR-2004/SHELXS97.
6. Structure refinement with SHELXL-97 (externally available)
7. Fourier maps, [contouring](#), XHYDEX location of hydrogen atoms.
8. Several graphics programs, including CAMERON, [ORTEP-3](#), [STRUPLO](#), [PLUTON](#). Interfaces to SCHAKAL and RasMOL, and the ray-tracing programs [POV-Ray](#) and [Raster3D](#). See examples of POV-Ray rendered pictures [here](#).
9. Programs for analysis of crystallographic results, including PLATON, PARST, THMA11
10. Publication of CIF based files and tables, validation of CIF files using IUCr CIF checking algorithms & PLATON checking tools. Interfaces to word processing packages *e.g.* MS-Word.
11. User modifiable interfaces to other MS-DOS or MS-Windows programs.
12. A very useful set of introductory [TUTORIALS for WinGX](#) has been made available at the CCP14 site (thanks to Lachlan Cranswick). The DOOBRY test data set for these tutorials is available [here](#).
13. WinGX may be used across networks. All WinGX programs accept either DOS or UNIX style ASCII files.

Platon - Windows

PLATON is written by [Ton Spek](#), and is a versatile crystallographic tool implementing a large variety of standard geometrical calculations (i.e. bonds, angles, torsions, planes, rings, inter-molecular contacts (H-Bond analysis), Coordination etc), tests (i.e. for missing symmetry, voids in the lattice etc.), utilities (cell transformation, SHELXL input etc.), graphics (e.g automatic labelled 'ORTEP-lookalike plots and the molecular graphics program PLUTON) and several filters (e.g. the DIFABS technique for empirical absorption correction (Walker & Stuart), and the SQUEEZE option for handling disordered solvents, described by Sluis & Spek, *Acta Cryst.* **1990**,A46, 194). This latter option places great demands on the available memory.

PLATON for Windows

This is an MS-Windows implementation of the latest UNIX version of PLATON. It is identical to the UNIX version, except that System S is not included (it is too Unix specific). It is suitable for all versions of Windows (95 /98 /ME /NT /2000 /XP/VISTA).

A PC with a Pentium (or equivalent) processor and with at least 32 Mb of RAM memory is recommended. The program works with all screen resolutions, but is best suited for 800x600 or higher.

<http://www.chem.gla.ac.uk/~louis/software/platon/index.html>

DIRDIF –

DIRDIF-2008 is a program for solving crystal structures. Major features are the use of Patterson methods, and special direct methods for solving symmetry problems. Powerful procedures are provided for the use of chemical knowledge to solve difficult structures. Ab-initio direct methods and structure refinement are not included in **DIRDIF-2008**.

The **DIRDIF-2008** program is written by Paul T. Beurskens and coworkers of the University of Nijmegen, Netherlands and is available for a variety of other platforms from the [official DIRDIF website](http://www.chem.gla.ac.uk/~louis/software/dirdif/index.html).

<http://www.chem.gla.ac.uk/~louis/software/dirdif/index.html>