WinGX - Crystallographic Programs for Windows
Release and Installation Notes for Version 1.80.00

WinGX is a MS-Windows™ system of programs for solving, refining and analysing single crystal X-ray or neutron diffraction data. The system has been designed to provide a consistent, user-friendly interface to the best publicly available crystallographic programs. Many well-known programs are included, as well as interfaces to popular programs such as SHELX, SIRWare (97/2002/2004). This program has taken a great deal of effort, over several years, to produce. It is licensed *free of charge* to academic, scientific and educational users, but due to licensing restrictions is *unavailable for commercial users*. If you use the system please acknowledge this by quoting the following reference:

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

Release 1.80.00 is suitable for all flavours of Windows (95/98/ME/NT/2000/XP/VISTA). In a program of this size, it is difficult to ensure that all bugs have been removed, and the author will be pleased to hear of any problems. Please see Section 1.5.

1.1 System requirements

The program is supplied as a 32-bit executable.
The *minimum* requirements are

- IBM-PC compatible machine with a Pentium (or equivalent) processor
- 256 Mb RAM memory
- Colour display with > 8 bits per pixel (i.e. 16K colours or more)

1.2 Enhancements over *WinGX* version 1.70.01

A large number of enhancements, many small changes and bug-fixes have been introduced to WinGX since version 1.70.01, the previous official release - see
http://www.chem.gla.ac.uk/~louis/software/wingx/modif.html
on the WinGX website for full details .

1.3 System installation

The program is supplied as an archive ZIP file (WGX_180.ZIP) which contains the file SETUP.EXE. To install the program, run SETUP and follow the instructions. The program and associated system files can be installed on any drive, and should also work across networks - *WinGX* is installed in Glasgow on a UNIX based network and no networking problems have been experienced. The default home directory is c:\wingx. The terms *folder* and *directory* are used interchangeably in this document.

- Before starting an installation, it is best to delete old versions of *WinGX*. In particular, old versions of WINGX.INI should be deleted to ensure a pain-free installation. Remember to save your old license file in another location !!

The installation will create the following subdirectories of {app}

```
{app}\bin        (for all system executables and dll's)
{app}\files      (for system files - you may wish to make this
                  directory read-only)
{app}\manuals    (for PDF documents)
```

where {app} is the directory chosen for installation. In the examples below, it is assumed that the default directory "c:\wingx" is used. After the program files have been installed you will also need to follow the instructions in Sections 1.3.1 - 1.3.3 below (also consider Sections 1.3.4 - 1.3.5) to complete the installation.

1.3.1 Setting system environment variables

WinGX uses two *environment variables* to locate essential system files. The examples below assume the default installation folder "c:\wingx" but you will need to change this if the installation folder is different. The procedure for setting environment variables depends on the version of Windows. If you do not know how to set environment variables on your computer see http://www.chem.gla.ac.uk/~louis/software/faq.html

If WinGX is installed over a network, these variables must be set on every machine from which WinGX is run.

WINGXDIR (this points to the location of the file WINGX.INI)
SET WINGXDIR=c:\wingx
This environment variable MUST point to a folder with write-access. If WinGX is installed over a network, it is often the case that the installation folder has read-only access. It is *not necessary* that the file WINGX.INI is in the same folder as all the other system files. Indeed if *WinGX* is installed over a network, it is useful for individual users to have their own private versions of WINGX.INI. The license file "WinGX-license" should be placed in this same directory.

PGFONT (this points to full path-name of the PGPLOT system file GRFONT.DAT)
SET PGFONT=c:\wingx\files\grfont.dat
This environment variable is required for the PGPLOT graphics library (compiled in WGXLIB02.DLL) which is used by several programs in the *WinGX* suite

1.3.2. Getting the *WinGX* license

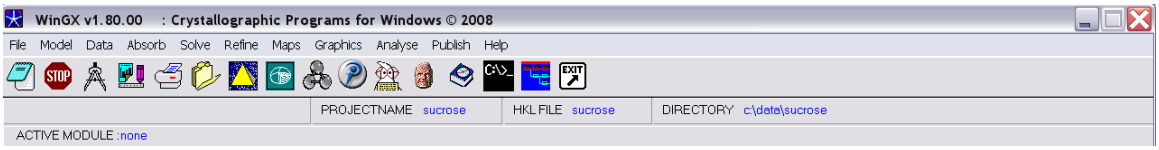
WinGX requires a license to run. You can get a license by return email by filling in the form at :

http://www.chem.gla.ac.uk/~louis/software/licenseform.html

Follow the instructions given in the returned email message. The license form allows me to keep a record of who uses the program, so I can inform when updates or bug fixes are available.

1.3.3 Setting up *WinGX*

If the above instructions have been followed correctly, then the *WinGX* program starts with the Main menubar of the program shown below . You may wish to place an icon for the program on your desk-top.



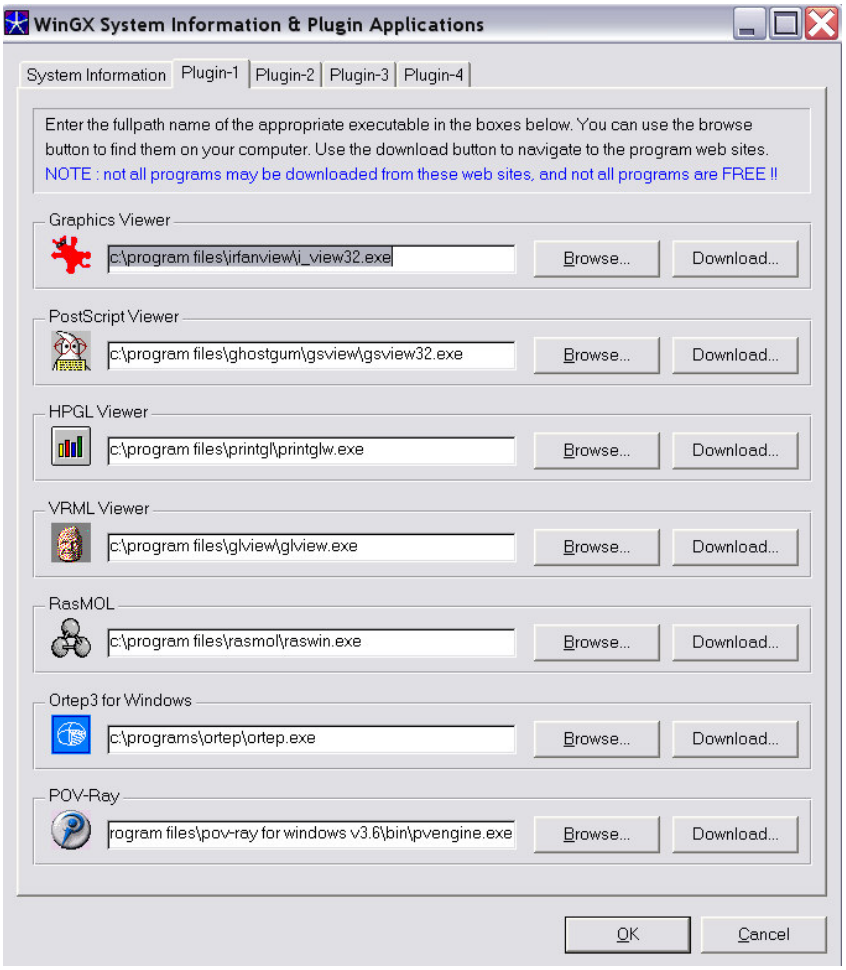
WinGX uses a number of plug-ins. If a previous version of the file WINGX.INI is *not* found during the installation process, then an automatic routine will build a new version by attempting to find as many of the plug-ins as possible. The current version will only search the same drive as the program has been installed, and it may well fail if WinGX has been installed on a network with read-only access. It may be necessary to modify this file by hand. The following three programs are stand-alone programs, but are also designed to work well in the WinGX environment. They can be obtained from the Glasgow Chemical Crystallography web-site.

- Ortep-3 for Windows from http://www.chem.gla.ac.uk/~louis/software/ortep3/
- STRUPLO for Windows from http://www.chem.gla.ac.uk/~louis/software/struplo/

The following programs are strongly recommended. They are free of charge to academic users and available from their respective web-sites:

- The excellent free graphics viewer IRFANVIEW from http://www.irfanview.com/ Irfan Skiljan has kindly given permission for the latest release to be bundled with the WinGX release (see in applications directory of WinGX).
- GSView (PostScript viewer) from http://www.cs.wisc.edu/~ghost/index.htm
- POV-Ray (excellent ray-tracing program) from http://www.povray.org
- RasMol (structure viewer) most recent version which reads CIF's from http://www.iucr.ac.uk/iucr-top/cif/software/rasmol/
- SHELX programs from http://shelx.uni-ac.gwdg.de/SHELX/
- SIR97/SIR2004 from http://www.ic.cnr.it/
- GLView (VRML viewer) from http://www.snafu.de/~hg
- SCHAKAL99 (Egbert Keller's superb molecular/crystal structure display program) from http://www.krist.uni-freiburg.de/ki/Mitarbeiter/Keller/schakal.html

Once all these programs have been obtained and installed, it is necessary to inform WinGX of their location on your computer. This is most easily done by opening the **WinGX Applications Panel** accessible either from Files-SYSTEM-Setup menu item or by clicking the toolbar button (second from the right).



Enter the full pathname of each of these executables into the respective edit boxes (or use Browse facility). This utiliity writes these entries to the configuration file WINGX.INI. The program SCHAKAL99 will need a special set-up :

- In order to use SCHAKAL99 with *WinGX*, you will first need to obtain the program from the web site. Dr. Egbert Keller has recently made the program freely available on the web. SCHAKAL99 is executed from *WinGX* using the supplied utility program RSCHAKAL.EXE. This program assumes that you have used the default extension RES for SHELX data files and that data files are placed in the folder {app}\dat\, *i.e.* use the following entry in the SCHAKAL99 INI file

```
default prefix and suffix for SHELX file names:
U X  -1  "C:\sch99\dat\  .res"
```

- If you have NOT installed SCHAKAL99 in the default c:\sch99 directory then you will also need to edit the SCH99.INI file to reflect the location of the program and associated files.
- You will need to enter the fullpathname of the SCHAKAL99 executable using the System Setup and Information dialog box. The program will now run from the SCHAKAL menu item of the **Graphics** menu. If your structure name is *compid* then you need to type the following responses (**show in bold**) at the SCHAKAL prompts

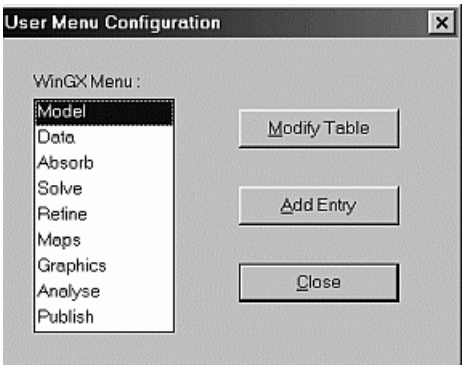
```
>>> U X
XtalDat File = ? >>> compid
```

```
InpData File = ? >>>  <return>
Continue ? >>> <return>
>>> X (to get initial view)
```

1.3.4 System Preferences

It is possible to set some preferences from the menu item File-SYSTEM-Preferences. but the default values in the program are usually suitable, at least for learning how to use the program. For PLATON and Ortep-3 it is possible to choose the file which is automatically read by the program. By default PLATON will read an SPF-format file which is automatically created each time PLATON is executed. The information for this file will be obtained from the SHELX.LST file (so that the least-squares errors on the coordinates may be obtained) if it exists, or the *name.RES* file or finally the *name.INS* file. The *name.CIF* file may also be used if coordinate errors are required.

1.3.5 User-defined Menu Items



In *WinGX* it is possible to implement user-defined menu items, so that favourite programs may be run from the *WinGX* Main menubar. While the WINGX.INI file can be manually edited, it is much easier now to use the GUI from File-SYSTEM-User Menu Items. The startup GUI is shown above. Up to ten items may be appended to each of the menu items MODEL to PUBLISH (i.e. a total of 90 extra user-defined programs may be added to the WinGX Main menubar. From the GUI you can either edit the entire table for a particular menu, or add an individual item. Command line options are added in a separate entry. “Menu Tag” is a character string (12 characters maximum) which will appear in the menu. The only restriction is that all *user-defined* menu items MUST have different tag names (but they can have the same name as standard menu items). If the compound name is required on the command line (to define files *etc*) then use the alias %comp%. This will be replaced by the actual compound name at run time. The user program to be executed can either be a Windows executable, a DOS executable or a DOS BAT file.

1.4. Disclaimer

Users of the *WinGX* system MUST be registered users of SHELX programs and SIR92 (and also SIR97/SIR2004). See the following web-sites for registration details for these programs :

SHELX programs : http://shelx.uni-ac.gwdg.de/SHELX/

SirWare programs : http://www.ic.cnr.it/

The program is supplied on an “as is” basis. While every effort has been made to ensure these programs run without error, LJF accepts no responsibility for any damages arising from the use or misuse of this software. There is no obligation on the part of LJF to provide support for this software, though all reasonable enquiries will be answered.

1.5. Bug reports and queries

At present there are no known problems with version 1.80.00

Suspected bugs in any of the *WinGX* programs should be reported using the Bug Report Form available at :

http://www.chem.gla.ac.uk/~louis/software/bug.html

Please email any other queries regarding WinGX to the address below. I will make a serious attempt to answer all reasonable enquiries, but I cannot help with vague statements such as “I have tried your program and it does not work”.

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