

Computer Program Abstracts

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WinGX suite for small-molecule single-crystal crystallography

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The crystallographic problem: The processing of a small-molecule structure from single-crystal X-ray or neutron diffraction data through structure solution and refinement to preparation of publication material is a well established and usually a reasonably automated procedure. There are several excellent commercial software packages, such as *SHELXTL* (Siemens, 1995) and *TEXSAN* (Molecular Structure Corporation, 1995), which provide all the necessary programs to undertake this procedure, but these packages are often quite expensive and usually tied to the sale of specific diffractometer hardware. The *WinGX* suite provides an integrated and freely available set of Microsoft Windows[®] programs to accomplish this task.

Method of solution: Throughout the past three decades, a great deal of superb crystallographic software, which is in the public domain or which is at least freely available, has been written. Such programs include the structure-solution packages *SHELXS* (Sheldrick, 1986), *DIRDIF* (Beurskens *et al.*, 1996) and *SIR92* (Altomare *et al.*, 1993) and refinement programs such as *SHELXL93* (Sheldrick, 1993). In general, each program system uses a different file syntax for common crystallographic information. To ensure that the whole structural determination procedure is as automated and simple as possible, it is desirable to spend little

time and effort in the data transfer between different programs. The *WinGX* suite is a coherent collection of programs running under Microsoft Windows[®], in which the best available public domain software has been included. It contains some of the programs from the *GX* suite (Mallinson & Muir, 1985), hence its name. The transfer of information between different programs is handled automatically, and manual editing of files is kept to a minimum, commensurate with the need to maintain transparency of use. Most programs have graphical user interfaces (GUIs) for selection of options.

The *WinGX* suite includes well established programs, such as *SHELXS* (Sheldrick, 1986), *DIRDIF* (Beurskens *et al.*, 1996), *SIR92* (Altomare *et al.*, 1993), *SHELXL93* (Sheldrick, 1993) and *ORTEPIII* (Johnson & Burnett, 1996; Farrugia, 1997). Diffractometer file processing for CAD-4 and Siemens *P4* files is possible, with profile fitting. Several absorption correction methods are available, *e.g.* analytical, Gaussian grid, ψ scans, multiscan (Blessing, 1995), *DIFABS* (Walker & Stuart, 1983). Contoured electron-density Fourier maps may be drawn and examined in cases of disorder. A number of programs for the analysis of results are provided, including *PLATON/PLUTON* (Spek, 1999), *PARST* (Nardelli, 1995) and *THMA11* (Trueblood, 1978). A range of graphics programs are available for structure visualization, while publication- and presentation-quality graphical hard-copy may also be obtained using the ray-tracing programs *POV-Ray* (<http://www.povray.org>) and *Raster3D* (Merritt & Bacon, 1997). Publication output via the CIF format (Hall *et al.*, 1991) is fully supported and extensive checking of CIF syntax and IUCr data validation is possible. One feature of *WinGX* is the possibility to customize the program. A large number of user-definable menu items may be added, so that users may launch their own desired and favourite applications from the *WinGX* menu. There are inbuilt interfaces to external graphics programs, such as *RasMol* (Sayle & Milner-White, 1995) and *SCHAKAL* (Keller, 1989), and to newer programs like *SHELX97* (Sheldrick, 1997) and *SIR97* (Altomare *et al.*, 1999). A large number of utility routines have been written to automate transfer of data from other systems, edit model files, display data *etc.*

Software environment and program specification: The program uses the *SHELX* and CIF formats for the major file operations and archiving. Virtually all system files use ASCII format and so may be edited using standard text

editors. Most of the operations are *via* intuitive Windows GUIs.

Hardware environment: The program may be implemented on IBM PC or compatible computers running Microsoft Windows[®] versions 3.1x, Windows 95/98 or Windows NT. At least a 486 66 MHz machine is recommended with 16 Mbyte of RAM, and at least 20 Mbyte of free disk space.

Documentation and availability: The executable program, together with full documentation, is available free of charge to academic users *via* <http://www.chem.gla.ac.uk/~louis/wingx>.

Although the program is written in Fortran77, a large number of non-standard FTN77 calls are used to create the GUI. For this reason, the source code is not available. There is an extensive on-line hypertext manual with links to relevant internet sites.

Keywords: single crystal; program package; PC; Microsoft Windows[®].

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PowderX: Windows-95-based program for powder X-ray diffraction data processing

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The crystallographic problem: A Windows-95-based program (*PowderX*) has been written for powder X-ray data processing and analysis. It can be used for plotting X-ray patterns, data smoothing, background subtraction, α_2 elimination, peak search, indexing and zero-angle error correction. *PowderX* can also be used for data format conversions to prepare the input data for Rietveld refinement and structure determination programs such as *DBWS*, *FULLPROF*, *GSAS*, *SIMPRO* and *EXPO*.

Method of solution: *PowderX* takes full advantage of the graphical interfaces of Windows 95. Pull-down menus and a

mouse are used to control the program executions. *PowderX* provides convenient tools for processing powder X-ray diffraction data. The Savitsky–Golay (Savitsky & Golay, 1964) method or any of another three methods can be used for data smoothing and peak search. Background subtraction can be made either automatically by the Sonneveld method (Sonneveld & Visser, 1975) or manually by mouse clicking. The α_2 elimination can be performed either using the methods of Rachinger and Ladell (Rachinger, 1948; Ladell *et al.*, 1975), or using a new method developed by the author of the program.

Software environment and hardware environment: *PowderX* is written in Visual Basic and runs under Windows 95 or Windows 98. Minimum hardware specification: a 486 or above processor, a VGA colour monitor, a mouse, 8 Mbytes of RAM, 8 Mbytes of hard disk space.

Program specification: *PowderX* can read 13 data formats, produced by either angular-dispersive or energy-dispersive X-ray diffraction techniques on various diffractometers (manufactured by Mac Science, Philips, Siemens, Rigaku, *etc.*). It uses a new and accurate $\text{Cu } K\alpha_2$ elimination algorithm (Dong, Chen & Wu, 1999). With *PowderX*, zero-angle shift can be corrected automatically before indexing and no internal standard material is required (Dong, Wu & Chen, 1999). It can produce the input file for *TREOR90* (Werner *et al.*, 1985) after an automatic peak search, so only minor editing is needed.

Documentation: Online help describes the main features of the program and provides instructions for the user. A user's manual is also available as a Microsoft *Word* document in rich text format.

Availability: The files for standard windows installation of the program and the user's manual are freely available for academic and non-commercial use. The program may be obtained from the author by e-mail (chengdong@aphy.iphy.ac.cn). This program has more than 80 users in the world to date.

Keywords: powder X-ray diffraction; data processing; indexing; peak search; data format conversion.

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DISCUS, a program for diffuse scattering and defect structure simulations – update

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The crystallographic problem: In contrast to the determination of the average structure based on Bragg scattering, there is no general procedure to extract information about the disorder of a material from its diffuse scattering. Two years ago, we first published the program *DISCUS* (Proffen & Neder, 1997), which allows the creation of defect structures and the simulation of diffuse scattering. The program can also be successfully used to aid teaching of diffraction physics (Neder & Proffen, 1996). This abstract gives an overview of the changes and enhancements between the published version 2.01 and the current version 3.2.

Method of solution: The program *DISCUS* allows one to create structures from the contents of an asymmetric unit using the space-group symbol. Structures can be modified using the Fortran-style interpreter or built-in functions of the program. Disordered structures can be analyzed, *e.g.* by calculating bond-length distributions, and the Fourier transform can be calculated. *DISCUS* includes a module for reverse Monte Carlo (RMC) simulations. We will focus here on the new features of the program. The Fourier transformation is now calculated about six times faster and allows the subtraction of the average structure factor (*F*). The scat-