Computer Program Abstracts

*The category Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Following normal submission, a Computer Program Abstract will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should follow the standard format given on page 189 of the June 1985 issue of the Journal [J. Appl. Cryst. (1985). **18**, 189–190] and on the World Wide Web at http://www.iucr.org/journals/jac/software/.*

Lists of software presented and/or reviewed in the Journal of Applied Crystallography are available on the World Wide Web at the above address, together with information about the availability of the software where this is known.

J. Appl. Cryst. (1999). **32**, 837–838

WinGX suite for small-molecule single-crystal crystallography

LOUIS J. FARRUGIA

Department of Chemistry, University of Glasgow, G12 8QQ, Scotland

(*Received 22 April 1999; accepted 28 April 1999*)

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 *SIR*92 (Altomare *et al.*, 1993) and refinement programs such as *SHELXL*93 (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), *SIR*92 (Altomare *et al.*, 1993), *SHELXL*93 (Sheldrick, 1993) and *ORTEP*III (Johnson & Burnett, 1996; Farrugia, 1997). Diffractometer file processing for CAD-4 and Siemens *P*4 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 *THMA*11 (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 *SHELX*97 (Sheldrick, 1997) and *SIR*97 (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 3.1*x*, 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™.

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.

Beurskens, P. T., Beurskens, G., Bosman, W. P., de Gelder, R., Garcia-Granda, S., Gould, R. O., Israel, R. & Smits, J. M. M. (1996). *The DIRDIF*96 *Program System.* Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Hall, S. R., Allen, F. H. & Brown, I. D. (1991). *Acta Cryst.* A**47**, 655–685.

Johnson, C. K. & Burnett, M. N. (1996). *ORTEP*III. Report ORNL-6895, Oak Ridge National Laboratory, Tennessee, USA.

Keller, E. (1989). *J. Appl. Cryst.* **22**, 12–22.

Mallinson, P. R. & Muir, K. W. (1985). *J. Appl. Cryst.* **18**, 51–53.

Merritt, E. A. & Bacon, D. J. (1997). *Methods Enzymol.* **277**, 505–524.

Molecular Structure Corporation (1995). *TEXSAN. Single Crystal Structure Analysis Software.* MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.

Sayle, R. & Milner-White, E. J. (1995). *Trends Biochem. Sci.* **20**, 374.
Sheldrick, G. M. (1986). *SHELXS*86. *Program for the Solution of Crystal Structures.* Institüt für Anorganische Chemie der Universität, Tammanstrasse 4, D-3400 Göttingen, Germany.
Sheldrick, G. M. (1993). *SHELXL*93. *Program for the Refinement of Crystal Structures.* Institüt für Anorganische Chemie der Universität, Tammanstrasse 4, D-3400 Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELX*97. *Programs for Crystal Structure Analysis.* Release 97–2. Institüt für Anorganische Chemie der Universität, Tammanstrasse 4, D-3400 Göttingen, Germany.
Siemens (1995). *SHELXTL. Structure Determination Software.* Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (1999). *PLATON. A Multipurpose Crystallographic Tool.* Utrecht University, Utrecht, The Netherlands.
Trueblood, K. N. (1978). *Acta Cryst.* A**34**, 950–954.
Walker, N. & Stuart, D. (1983). *Acta Cryst.* A**39**, 158–166.

J. Appl. Cryst. (1999). **32**, 838

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

CHENG DONG

Institute of Physics, Chinese Academy of Sciences, PO Box 603, Beijing 100080, People's Republic of China

(*Received 15 February 1999; accepted 18 February 1999*)

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 Sonnerveld 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 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 *TREOR*90 (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 (chengdon@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.

References

Dong, C., Chen, H. & Wu, F. (1999). *J. Appl. Cryst.* **32**, 168–173.
Dong, C., Wu, F. & Chen, H. (1999). *J. Appl. Cryst.* Submitted.
Ladell, J., Zagofsky, A. & Pearlman, S. (1975). *J. Appl. Cryst.* **8**, 499–506.
Rachinger, W. A. (1948). *J. Sci. Instrum.* **25**, 254–255.
Savitsky, A. & Golay, J. E. (1964). *Anal. Chem.* **36**, 1627–1639.
Sonneveld, E. J. & Visser, J. W. (1975). *J. Appl. Cryst.* **8**, 1–7.
Werner, P.-E., Eriksson, L. & Westdahl, M. (1985). *J. Appl. Cryst.* **18**, 367–370.

J. Appl. Cryst. (1999). **32**, 838–839

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

TH. PROFFEN[a]* AND R. B. NEDER[b]

[a]*Department of Physics and Astronomy and Center for Fundamental Materials Research, Michigan State University, East Lansing, Michigan 48824-1116, USA, and* [b]*Insitut für Mineralogie, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany*

(*Received 29 March 1999; accepted 31 March 1999*)

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 $\langle F \rangle$. The scat-