CRYSTALS version 12: software for guided crystal structure analysis

Paul W. Betteridge, J. Robert Carruthers, Richard I. Cooper,* Keith Prout and David J. Watkin

University of Oxford, Chemical Crystallography Laboratory, Chemistry Research Building, Mansfield Road, Oxford OX1 3TA, UK. Correspondence e-mail: richard.cooper@chemical-crystallography.oxford.ac.uk

Received 11 September 2003
Accepted 1 October 2003

Keywords: refinement and analysis; single crystal; small molecule

1. The crystallographic problem

The determination of small-molecule structures from single-crystal X-ray data is being carried out by researchers with little or no crystallographic training. At the same time, completely automatic crystal structure analysis can still only be achieved under very favourable conditions. Many of the problems that cause automatic systems to fail could be resolved with suitable chemical insight, and until this is built-in, programs continue to need human guidance. *CRYSTALS* version 12 contains a modern crystallographic human-interface design, and novel strategies incorporating chemical knowledge and sensible crystallographic guidance into crystal structure analysis software.

2. Method of solution

CRYSTALS provides access to advanced crystallographic routines *via* a modern graphical user interface that new users will find familiar and easy to work with. The ease of use is enhanced by the inclusion of validation criteria similar to those currently used by the IUCr journals, and crystallographic guidance compiled with the help of many leading crystallographers.

Enabling synthetic chemists to carry out their own analytical crystallography will release an increased proportion of the time of professional crystallographers to handle the more challenging structures.

2.1. The graphical user interface

The GUI for Windows platforms provides access to underlying crystallographic commands *via* menus, buttons and dialogs, which will be intuitive to users of existing Windows software. Considerable programming effort has been expended to design a plain-text macro language which is used both to build the GUI and encode crystallographic decision making. This ensures that the contents and layout of the GUI are fully customizable by users; thus individual installations can be customized to suit local working practice or even language.

2.2. Guidance using *SCRIPTS*

The latest release features a complete set of macros (scripts) known as 'The Guide', which will guide a new user through a complete structure solution and refinement. As it proceeds, the program assesses the structure and performs simple validation checks in order to recommend an appropriate next action.

This approach has enabled users with a chemical training, but no crystallographic background, to bring reasonable quality diffraction data through to a publication-quality structure. Crucially, when the analysis runs into difficulties, the guide simply refuses to continue and advises the user to seek further expert assistance.

2.3. Program interfaces

CRYSTALS interfaces directly to other first-class software, including *PLATON* (Spek, 1998), the *SHELX* suite (Sheldrick, 1998), *SIRWARE* (Altomare *et al.*, 1999) and *WinGX* (Farrugia, 1999). Output includes CIF (Hall *et al.*, 1991), PDB, *SHELX* and PostScript diagrams.

3. Software environment and hardware

The current release of *CRYSTALS* runs on PCs under Microsoft Windows 95/98/Me/NT/XP. Recommended minimum specifications are: 200 MHz Pentium processor, 32 Mb of RAM and 18 Mb spare disk space. The program makes use of OpenGL routines in order to display the molecular diagram.

4. Program specification

The crystallographic routines are written in Fortran 77 (*ca* 800000 lines), while the graphical interface is C++ (*ca* 100000 lines). Over 400 *SCRIPT* macros are distributed with the program for automating or guiding various tasks.

5. Documentation and availability

CRYSTALS and accompanying manuals can be downloaded from http://www.xtl.ox.ac.uk/crystals.html. The program is free for academic and not-for-profit use. New releases are generally provided every one or two months. We would like to encourage users to submit bug reports, other feedback or feature requests. *CRYSTALS* has been demonstrated in workshops at the latest BCA and ACA annual meetings.

We gratefully acknowledge financial support from the CCDC and EPSRC grant number N06830/01.

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hall, S. R., Allen, F. H. & Brown, I. D. (1991). *Acta Cryst.* A**47**, 655–685.
Sheldrick, G. M. (1998). *SHELX97-2 Programs for Crystal Structure Analysis*, Institut für Anorganische Chemie der Universität, Tammannstrasse 4, D-37007 Göttingen, Germany.
Spek, A. L. (1998). *PLATON, a Multipurpose Crystallographic Tool*, Utrecht University, Utrecht, The Netherlands.

