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 Commision on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 of the June 1985 issue of the Journal [J. Appl. Cryst. (1985). **18**, 189–190].*

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ORTEX–an interactive version of *ORTEP* for use on a PC.

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The crystallographic problem: *ORTEP* (Johnson, 1971) can be tedious to use, often requiring extensive file editing to obtain the desired result. This fast PC version gives the user access to colour thermal-ellipsoid pictures that can be manipulated in a 'what you see is what you get' fashion. Plot files can be generated in a form in which they may be easily annotated on the PC. This version of *ORTEX* is an enhanced version of that previously described for use on a VAX (McArdle, 1991).

Method of solution: For *SHELX*76 or *SHELXL*93 users, a program *ORIN* generates a default file for input to *ORTEX*. H atoms may be excluded and any atom chosen as the origin. There is an option that may generate longer bonds from second-row and heavier atoms. All input files are in free format. *ORTEX* input files (without thermal ellipsoids) may also be generated from CSSR files. *ORTEX* generates a stick drawing with tapered bonds and displays the current axial rotations. Three rotations are permitted on any of *x*, *y* or *z* and in any order. The user may then select from the following: (0) end program; (1) rotate stick drawing; (2) draw bonds and atom thermal ellipsoids (with anisotropic atoms as cross-hatched open footballs, isotropic atoms with boundary ellipses, equators and meridians and H atoms as boundary ellipses); (3) draw bonds and atom-boundary ellipses with atom-centred labelling; (7) generate a HPGL plot file; (9) help, which lists all options; and (12) as (2) with no shaded footballs to reduce the plot file size of large drawings.

Software and hardware environment: The program requires a VGA screen, DOS 5 and a 386/387 with 4 Mbytes of RAM or better. Plot files may be printed directly on LaserJets III or 4 or on DeskJet printers. The HPGL files may also be inserted into *DRAW-PEREFECT*, *WORD* for WINDOWS or similar software where they may be modified or annotated.

Program specification: The program functions (0)–(12) are obtained by typing the function number. The current rotational position is always displayed on screen but is only included in labelled plots. The program automatically adjusts the plot size and the ratio of the border to plot size to prevent ellipsoid edges falling outside the plot range. All features work with up to approximately 250 atoms and with some restrictions the limit is 499 atoms.

Documentation and availability: The programs are available on a 1.44 Mbyte 3.5 in floppy disk. A test file of input data and an instruction manual are provided. The manual describes the installation and use of *ORTEX* and some of the important features described include the production of stereoviews and a lattice search for H bonding.

Keywords: crystallography, *ORTEP*, *ORTEX*, PC.

References

Johnson, C. K. (1971). *ORTEP*. Report ORNL-3794, revised. Oak Ridge National Laboratory, Tennessee, USA.

McArdle, P. (1991). *J. Appl. Cryst.* **24**, 972.

Notes and News

J. Appl. Cryst. (1993). **26**, 752

The International Centre for Diffraction Data (ICDD) has established a Crystallography Scholarship Fund to encourage promising graduate students to pursue crystallographically oriented research. Applications for these awards must be received by the ICDD no later than 31 October 1993. For details, contact the Secretary, International Centre for Diffraction Data, Newtown Square Corporate Campus, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA.

Books Received

J. Appl. Cryst. (1993). **26**, 752

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

Mathematical crystallography – an introduction to the mathematical foundations of crystallography. Reviews in mineralogy, Vol. 15 (revised). By *M. B. Boisen* and *G. V. Gibbs*. Pp. xii + 460. Washington, DC: The Mineralogical Society of America, 1992. Price (paper) US $20.00. ISBN 0-939950-26-X. A review of this book, by Edward Prince, has been published in the September 1993 issue of *Acta Crystallographica* Section A, page 791.

Solids far from equilibrium. Edited by *C. Godrèche*. Pp. xvi + 588. Cambridge: Cambridge University Press, 1992. Price £60.00. ISBN 0-521-41170-X. A review of this book, by D. T. J. Hurle, has been published in the September 1993 issue of *Acta Crystallographica* Section A, pages 791–792.

Quantitative Data File for ore minerals. Third edition. Edited by *A. J. Criddle* and *C. J. Stanley*. Pp. lxiv + 635. London: Chapman and Hall, 1993. Price £75.00. ISBN 0-412-46750-X. This work is produced by the Commission on Ore Mineralogy of the International Mineralogical Association and is intended for use in mineral identification. A lengthy introduction describes the use of the Data File. It provides chemical compositions, graphs of reflectance spectra in air and, where available, reflectance data under oil immersion at selected wavelengths for 510 mineral species and 125 compositional or structural variants. The crystal system is noted in each case and cross references are provided to available X-ray data in the Powder Diffraction File of the ICDD.