Documentation: Documentation is written in HTML and can be browsed over the Internet or installed locally.*

Availability: *RSREF* is distributed under license over the Internet from http://www.sb.fsu.edu/~rsref. It is distributed without charge to academic users. Users will also need a license for *TNT* (Tronrud *et al.*, 1987), and *O* (Jones *et al.*, 1991).

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* Documentation for *RSREF* has been deposited with the IUCr (Reference: LI5011). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Chapman, M. S. (1995). *Acta Cryst.* **A51**, 69–80.

Chapman, M. S. & Blanc, E. (1997). *Acta Cryst.* **D53**, 203–206.

Chapman, M. S. & Rossmann, M. G. (1996). *Acta Cryst.* **D52**, 129–142.

Diamond, R. (1971). *Acta Cryst.* **A27**, 436–452.

Graham, I. S. (1996). *HTML Sourcebook.* 2nd ed. New York: Wiley.

Jones, T. A. & Liljas, L. (1984). *Acta Cryst.* **A40**, 50–57.

Jones, T. A., Zou, J.-Y., Cowan, S. W. & Kjeldgaard, M. (1991). *Acta Cryst.* **A47**, 110–119.

Tronrud, D. E., Ten Eyck, L. F. & Matthews, B. W. (1987). *Acta Cryst.* **A43**, 489–501.

Wall, L. & Schwartz, R. L. (1991). *Programming Perl.* Sebastapol, CA: O'Reilly.

FOURDEM: a demonstration program for Fourier synthesis and other crystallographic concepts

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The crystallographic problem: In the experience of the authors, students frequently face problems understanding the abstract concepts of Fourier transformation and reciprocal space. The use of computers allows the demonstration of those concepts using multimedia presentations and computer simulations (Proffen & Neder, 1996). The program

FOURDEM demonstrates specifically the Fourier synthesis technique. A version of the program running only on Macintosh computers was published by Welberry & Owen (1992). Among the frequent responses to this paper were various requests for a version of the program to run on IBM-PC compatible computers. As a result, a Microsoft Windows and a DOS version of the program *FOURDEM* have been developed and are now made available in addition to the Macintosh version.

Method of solution: The input data (h, k, $|F|$ and the phase φ) can either be entered interactively or be read from a file. On the Macintosh platform, two different programs are used, whereas the DOS and Windows versions allow one to use both modes in the same program. Further details of the applications of the program are given in Welberry & Owen (1992).

Software environment: The Macintosh and DOS version of the program is written in standard Fortran77 with additional assembler and/or toolbox routines for the graphical interface. The Windows version is written in Turbo C++. All versions of *FOURDEM* are distributed as executables.

Hardware environment: The program has been successfully used on various Macintosh and PowerMac platforms as well as on different DOS computers. The Macintosh version requires at least an 8-bit grey scale and a 640 × 480 display. The DOS version uses a VESA graphics driver (one such driver is included in the distribution) and uses a resolution of 800 × 600 pixels and a depth of 256 colours. The DOS version of the program needs about 550 kbytes of free memory. The Windows version will run using Windows 3.1 as well as Windows 95. There are no special hardware requirements for this version, although graphical output benefits from a colour depth of at least 256 colours. Disk space required for installation is below 1.4 Mbytes for all versions.

Program specification: The synthesis of 50 reflections takes about 2 to 7 min depending on the computer used and the number of display updates required.

Documentation: The program distribution for both platforms contains the program(s), example input files and a short manual describing the program and the required input and gives hints for the installation.

Availability: The program for both platforms is available *via* the World Wide Web at http://rschp2.anu.edu.au:8080/proffen/fourdem/fourdem.html. The program can be used free of charge and authors having difficulties accessing the

Internet can obtain a copy from the authors by sending a 3.5 in floppy disk.

Keywords: Fourier synthesis, teaching.

References

Neder, R. B. & Proffen, Th. (1996). *J. Appl. Cryst.* **29**, 727–735.

Welberry, T. R. & Owen, K. (1992). *J. Appl. Cryst.* **25**, 443–447.

Crystallographers

Peter Wheatley 1921–1997

Peter Jaffrey Wheatley, who died on 12 May 1997, had an influential and varied career in physical chemistry, crystallography and structural chemistry. His publications (more than 100 papers and five books), his editorial work for *Acta Crystallographica*, his teaching, and his classic text *Molecular Structure*, first published in 1959 and translated into 15 languages, make him a key figure in the development of crystallography from the 1950s.

Peter was nearly a Yorkshireman, born in Cheshire but moving counties as an infant! He was educated in Sheffield before going to Oxford around the start of the war. He had scarcely begun his degree course when, as Bombardier Wheatley, he was sent to the Far Eastern theatre, was captured during the fall of Singapore and survived four terrible years as a prisoner of war. After recovering his health, he returned to Oxford, gained a first in Chemistry in two years, a DPhil in Physical Chemistry within a further two years, and was married to Jo (also from Sheffield). His Thesis had sections on (*a*) flame propagation and (*b*) molecular structure, and his second research year was carried out as a Commonwealth Fellow at the University of Minnesota. His distinguished crystallographic career developed at the University of Leeds, where he moved in 1951 and where he wrote the first drafts of *Molecular Structure*. In 1957, Peter and Jo, now blessed with three daughters, moved to Switzerland, where he worked for nine years in the Laboratories of Monsanto Research S.A. in Zurich.

Following a year as Visiting Professor in Tucson, Arizona, Peter returned to academic life in the UK in 1967, to the Department of Physical Chemistry at Cambridge. Here he ran an active

research group, the graduates of which now hold positions all over the world, became a Fellow of Queens' College, and was renowned at both Departmental and College level for his teaching and lecturing. He also served as British Co-editor of *Acta Crystallographica* from 1969 to 1980, processing a phenomenal number of papers with care, knowledge and not a little tact! Peter was very active in College life being, at various times, Junior Bursar, Senior Bursar and Director of Studies in Natural Sciences at Queens'. He was made a Life Fellow when he retired in 1988. On his retirement Peter joined the Crystallographic Data Centre part-time as the Senior Database Editor who 'sorted out' the more complex problems that arose during the CCDC's checking process, leaving only a couple of years ago due to failing health. His contribution at the CCDC was immense, due to his infectious enthusiasm and deep knowledge of his subject.

As a person, Peter was both a very private man, who delighted in his family and the progress of his grandchildren, and also an engaging and humorous companion with an endless capacity to surprise. He always detected and laughed at the absurdities of life, and debunked anything pompous or pretentious. He had a lifelong interest in many sports and played cricket enthusiastically (and extremely capably – as this bowler rapidly came to know!) well into his fifties. Peter was a wonderful colleague and friend and many areas of life are the poorer for his passing.

FRANK ALLEN

Software Reviews

Software for review in this section should be submitted directly to the Software-Review Editor (P. S. White, Department of Chemistry, CB#3290 Venable Hall, University of North Carolina, Chapel Hill, NC 27599-3290, USA).

Lists of software presented and/or reviewed in the Journal of Applied Crystallography are available on the World Wide Web at http://www.iucr.ac.uk/journals/jac/software/, together with information about the availability of the software where this is known.

J. Appl. Cryst. (1997). **30**, 568

ORTEP-3 for Windows – a version of *ORTEP*-III with a Graphical User Interface (GUI)

LOUIS J. FARRUGIA. Available from the author (e-mail: louis@chem.gla.ac.uk; WWW: http://www.chem.gla.ac.uk/~louis/ortep3). Version 1.0 Beta, 1997. Free.

ORTEP-3 [L. J. Farrugia (1997). *J. Appl. Cryst.* **30**, 565] is a useful GUI for the latest version of the venerable *ORTEP*

program, the standard program for the preparation of thermal ellipsoid drawings of crystal structures. Mastering the preparation of the input to *ORTEP* has always been something of a challenge for students, especially as familiarity with programming and data input has decreased as a result of the spread of 'user friendly' crystallographic software. *ORTEP*-3 provides a Windows interface, with reasonably intuitive point-and-click commands to generate *ORTEP* drawings, and facilitates labeling, rotation, and the preparation of stereo and packing drawings as well as all the other features available in *ORTEP*-III. One of the best features is the preparation of a standard *ORTEP*-III input file, which can be edited to achieve effects that might be difficult to produce directly with the *ORTEP*-3 program, such as final tweaking of packing drawings. As the authors admit in the instruction manual, *ORTEP*-3 can be slow, and it certainly is on the lower end of the spectrum of PCs on which it runs. However, on a 90 MHz Pentium, the speed of execution is quite acceptable, and even for *ORTEP* users who are familiar with the preparation of input files, *ORTEP*-3 can be a significant time saver.

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Books Received

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.

J. Appl. Cryst. (1997). **30**, 568

Synchrotron radiation techniques in industrial, chemical and materials science. Edited by K. L. D'AMICO, L. J. TERMINELLO and D. K. SHUH. Pp. viii + 259. New York: Plenum Publishing Corporation, 1996. Price US $89.50. ISBN 0-306-45389-4. This contains proceedings of two American Chemical Society symposia (Washington, DC, August 1994 and Chicago, IL, August 1995) devoted to the title topic. Their intent was 'to present a broad overview of several current topics in industrial, chemical and materials-based SR research to a chemically inclined audience'.

X-ray and neutron dynamical diffraction, theory and applications. Edited by A. AUTHIER, S. LAGOMARSINO and B. K. TANNER. Pp. ix + 419. New York: Plenum Publishing Corporation, 1996. Price

US $125.00. ISBN 0-306-45501-3. This volume collects the proceedings of the eponymous 23rd International Course of Crystallography, a NATO Advanced Study Institute, held in Erice, Sicily in April 1996. The first part reviews the basic principles of dynamical diffraction by perfect and nearly perfect crystals, the second deals with diffraction topography, the third with X-ray standing waves, the fourth with the theory and applications of high-resolution diffractometry, the fifth with multiple-beam diffraction and the sixth with X-ray and neutron interferometry

Quasicrystals. A primer. (Second edition.) By C. JANOT. Pp. xvi + 409. Oxford: Clarendon Press, 1995. Price £49.50. ISBN 0-19-851778-5. A review of this book, by W. Steurer, has been published in the July 1997 issue of *Acta Crystallographica Section A*, page 526.

Industrial crystallization – Process simulation, analysis and design. By N. S. TAVARE. Pp. xxviii + 527. New York: Plenum Publishing Corporation, 1995. Price US $95.00. ISBN 0-306-44861-0. A review of this book, by J. Nývlt, has been published in the July 1997 issue of *Acta Crystallographica Section A*, pages 527–528.

Atomic and ion collisions in solids and at surfaces. Edited by ROGER SMITH. Pp. ix + 309. Cambridge University Press, 1997. Price £45.00 (US $69.95). ISBN 0-521-44022-X. A review of this book, by D. Jacobs, has been published in the July 1997 issue of *Acta Crystallographica Section A*, page 528.

Collected works of Dorothy Crowfoot Hodgkin. Vol. I. Insulin. Vol. II. Cholesterol, penicillin and other antibiotics. Vol. III. General crystallography and essays. Edited by G. G. DODSON, J. P. GLUSKER, S. RAMASESHAN and K. VENKATESAN. Pp. cxliii + 2230. Bangalore: Indian Academy of Sciences, 1996. Price US $120 (individual vols. US $40). ISBN 81-7296-029-4. A review of this book, by E. Baker, has been published in the July 1997 issue of *Acta Crystallographica Section A*, pages 528–530. Copies of these books can be ordered from: The Indian Academy of Sciences, C. V. Raman Avenue, Post Box No. 8005, Sadashivanagar P. O., Bangalore 560 080, India; The British Crystallographic Association, Professor J. A. K. Howard, Department of Chemistry, University of Durham, South Road, Durham DH1 3LE, England; or Polycrystal Book Service, 425 Dayton Towers Drive, No. 12F, Dayton, OH 45410, USA.