in the *SHELX* file for all space groups and generates the required symmetry instructions for *ORTEX*. *ORIN* generates instructions for 'long' bonds, can translate the asymmetric unit and can append unit-cell corners to the atom list. A 'fast' colour-coded stick rotator is provided to allow rapid view selection. *ORTEX* will generate drawings of this view with many options. Some of the options are: bonds only, bonds and atom outlines, bonds and thermal ellipsoids and bonds with atom outlines and atom-centred numbering in two print sizes. Any view may be rotated on any of *x*, *y* and *z* in any order. Any drawing may be written to a plot file.

Standard VGA is the default screen mode and three SVGA modes up to 1280 × 1028 are available. The 800 × 600 mode works on most machines and the higher modes work best on VESA machines. All screen modes use a black background and two options that include a title are suitable for making slides.

If the unit cell is appended by *ORIN*, the cell outline can be drawn. This is colour coded to allow easy identification of the origin and the *a*, *b* and *c* directions. Two lattice-packing modes are provided. Simple application of the space-group operations to asymmetric units in one or more cells can be used to examine the crystal lattice; a cell-fill mode is also provided. In cell-fill mode, the program attempts to fill one or more unit cells with asymmetric units.

Colour or black-and-white files may be written in HPGL or for the DeskJet series of plotters. The HPGL files may be printed on LaserJet III or 4 or inserted into a drawing package.

Hardware environment: The program requires at least a 386/387, DOS 5, 4 Mbytes of RAM, a VGA screen and about 3 Mbytes of disk space.

Documentation and availability: The program, together with manual and test files is available on 1.44 Mbyte floppy disks or *via* ftp from the author, IN%P.McArdle@UCG.IE.

Keywords: Crystallography; *ORTEP*; *SHELX*; PC; protein; PDB; unit cell; plot file.

References

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

Sheldrick, G. (1993). *SHELXL*-93. *Program for the Refinement of Crystal Structures*. Univ of Göttingen, Germany.

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

Crystallographers

This section is intendeed to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to The Executive Sectretary, 2 Abbey Square, Chester CH1 2HU, England.

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Professor **Anthony Kevin Cheetham**, Director of the Materials Research Laboratory at the University of California at Santa Barbara, USA, and Professor of Solid State Chemistry in the Royal Institution, London, was elected a Fellow of the Royal Society on 10 March 1994. He was distinguished for his work on determining the chemical structure of materials, especially inorganic materials. He has developed and exploited neutron beams and synchrotron radiation, especially powder profile methods to analyse the structure of solid-state materials not amenable to single-crystal X-ray and spectroscopic techniques. This has enabled him to interpret the behaviour of microporous catalysts and adsorbers, of great potential industrial value.

Professor **George Guy Dodson**, Professor of Biochemistry in the University of York and Head of the Division of Protein Structures at the National Institute for Medical Research, was elected a Fellow of the Royal Society on 10 March 1994. He is renowned for performing X-ray analyses of numerous biological substances in order to determine their structure and form. He has undertaken a major study on insulin in different forms, both naturally occurring and man made. He has also undertaken extensive investigations into bacterial genetic material and into haemoglobin. His laboratory solves the structures of crystalline proteins from all over the world.

Professor **James Fraser Stoddart**, Professor of Organic Chemistry in the University of Birmingham, was elected a Fellow of the Royal Society on 10 March 1994. He was distinguished for the design and discovery of new approaches to the synthesis of novel organic substances using the techniques of molecular recognition and supramolecular chemistry. He combined a number of techniques from synthetic chemistry to establish the principles of self-assembly and template direction in organic synthesis. His work opens up the possibility of novel chemical sensors. It has created completely new areas of experimental inquiry in organic chemistry and the investigation of new organic materials.

Notes and News

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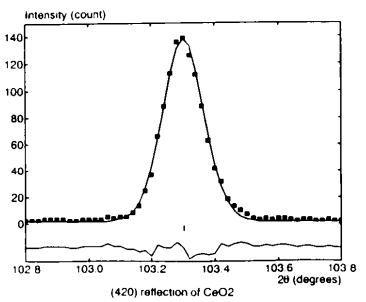
The new high-resolution neutron powder diffractometer (HRNPD) is now available at the Brookhaven high-flux beam reactor (HFBR). This new user facility offers resolution in neutron powder diffraction patterns exceeding that of many 'home laboratory' X-ray diffractometers in the high-angle region where the highest peak densities usually occur. First operated on 1 July 1993, the HRNPD has an instrumental profile that is smooth and nearly symmetric as well as narrow. To combine high resolution with high intensity, the unit features a 25-element 'Venetian-blind' monochromator design and 64 ^{3}He detectors.

As is shown by the 420 reflection of CeO_2 below, the FWHM of the instrumental profile is no more than 0.15° at 103°(2θ) with 11′–11′–5′ collimators in place. This corresponds to $(\Delta d)/d$ in the 10^{-4} range. With this unusually high resolution and an excellent flux on specimen (*e.g.* 3×10^5 neutrons cm^{-2} s^{-1} with the HFBR operating at half power), the HRNPD takes a leading place among the neutron powder diffractometers of the world. Many studies dependent on details of the reflection profiles (*e.g.* slight splitting from subtle phase changes, correct separation of the contributions from different phases, microstructure studies *via* details of 'line' broadening) are now made possible.



420 reflection of CeO_2

The HRNPD is being operated as a national/international facility by a PRT (participating research team) to which is allocated 50% of the instrument's time. The other 50% is now available to general users on a competing proposal basis. There is no charge for using it for research work that is neither proprietary nor for commercial gain. One may gain access to the instrument either as a general user or, on occasion, through collaboration with a PRT member. For a General User Proposal Form, write to Ms Rae Greenberg, HFBR User Program

Administrator, Physics Department, Brookhaven National Laboratory, Upton, NY 11973, USA. For a list of PRT members and their addresses, contact Professor R. A. Young, PRT Chairman for the HRPND, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332, USA.

New Commercial Products

Announcements of new commercial products are published by the Journal of Applied Crystallography *free of charge. The descriptions, up to 300 words or the equivalent if a figure is included, should give the price and the manufacturer's full address. Full or partial inclusion is subject to the Editor's approval and to the space available. All correspondence should be sent to the Editor, Dr A. M. Glazer, Editor* Journal of Applied Crystallography, *Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX*1 3*PU, England.*
The International Union of Crystallography can assume no responsibility for the accuracy of the claims made. A copy of the version sent to the printer is sent to the compny concerned.

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Mirror Optics

The Molecular Structure Corporation (MSC) has introduced a **high-performance focusing mirror system** that produces a three- to fourfold improvement in flux relative to a standard graphite monochromator. The system is completely integrated with the Rigaku R-AXIS imaging-plate system and rotating-anode source. It is easily coupled with the R-AXIS 2θ stage developed by MSC. It is also sold as a stand-alone unit. Diffraction experiments requiring a high-flux fine-focus X-ray source will benefit from this device.

The double-focusing mirror optics assembly is enclosed in an He-filled chamber with leaded glass front for safe viewing during alignment. The optics consist of a Pt-plated 160 mm focusing mirror. Both mirrors have a remote control for translation, bending and slit insertion. A fluorescent screen and attenuators are also enclosed in the He-filled chamber, which can be changed by a remote selection switch. The collimator is attached to a high-precision *xy* assembly.

The system was designed to be easy to align, generally taking less than 30 min. The alignment is unique in that it starts with the mirror nearest the X-ray source and proceeds component by component all the way to the alignment of the φ axis.

Molecular Structure Corporation, 3200 Research Forest Drive, The Woodlands, TX 77381, *USA.*

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Efficient SHG/THG Generation of Ultrafast Lasers

An **all-reflective second- and third-harmonic-generation system** is now available from INRAD for use with ultrafast Ti:sapphire lasers. Model 5-050 features a compact reflective design to minimize pulse distortion due to chromatic aberration and group-velocity dispersion that typically are found in lens-based systems. A precision optical delay, polarization-altering optics and crystals are all contained in one compact package. A selection of crystals and optics is available to maintain either fs or ps pulse durations with efficient SHG from 350 to 450 nm and THG from 233 to 300 nm. Typically, 100 mW of average THG power can be obtained while maintaining a THG pulse duration of 200 fs, as shown by cross-correlation measurements of the third harmonic and fundamental with an INRAD model 5-14BX computerized autocorrelator.

INRAD, 181 *Legrand Avenue, Northvale, NJ* 07647, *USA.*

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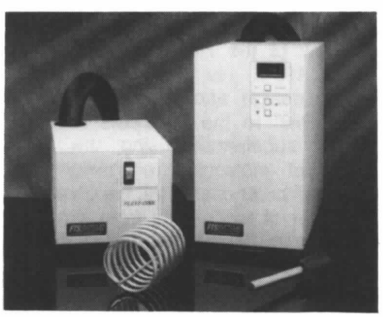
Cold Probe

The new **FC55 immersion cooler** generates temperatures down to $-55°C$ using non-CFC refrigerant gas in a reliable mechanical refrigeration system. The FC55 can be used in place of dry ice or liquid nitrogen as a cooling source for liquid baths or as a cold trapping surface to trap solvents or other condensates from vapor streams. The FC55 generates cooling power of more than 230 BTU h^{-1} at $-40°C$ and has a footprint of only 10.5 in wide $\times$ 16.5 in deep.



The FC55 cold probe

FTS Systems, Inc., PO Box 158, *Rt* 209, *Stone Ridge, NY* 12484, *USA.*

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, *USA). As far as practicable, books will be reviewed in a country different from that of publication.*

J. Appl. Cryst. (1994). **27**, 440–441

The Rietveld method. (IUCr Monograph on Crystallography, No. 5.) Edited by *R. A. Young.* Pp. x + 298. Oxford: International Union of Crystallography/Oxford University Press, 1993. Price £45.00. ISBN 0-19-855577-6.

In 1969, H. M. Rietveld published his seminal paper on structure refinement based on the complete powder diffraction profile rather than a limited amount of low-angle integrated intensity data. This paper laid the foundation for a dramatic renaissance of powder diffraction, widely regarded at the time as a valuable tool for phase identification and qualitative analysis but of little use for quantitative structure determination. The coming-of-age of Rietveld refinement, as it is now known, was celebrated in June 1989 at an International Workshop on the Rietveld Method, hosted by the Netherlands Energy Research Foundation at Rietveld's home institution in Petten and organized by the Commission on Powder Diffraction of the International Union of Crystallography.

The Rietveld method is an outcome of the Petten meeting but is certainly not a Proceedings in the accepted sense. The contributing authors, all of them leaders in the field, were requested to write articles suitable for a book aimed primarily at those with some experience of the technique but also providing some introductory material for beginners. The first drafts of these chapters underwent considerable revision under the guidance and encouragement of the editor and the end result is not only an authoritative and coherent text but also an excellent reference work covering the literature up to the start of 1991 or thereabouts.

The first chapter (R. A. Young) provides an excellent introduction to the Rietveld method. It contains an account of the basic mathematical procedures used in the fitting to the diffraction pattern, the types of parameters to be refined, a list of the peak-shape functions commonly used, corrections for preferred orientation (one of the more troublesome systematic errors afflicting X-ray powder data), some of the popular computer programs currently available, criteria of fit and precision and accuracy,