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

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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.

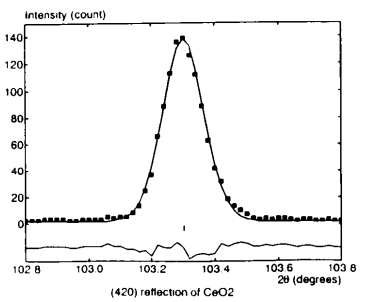
Professor **James Fraser Stoddart**, Professor of Organic Chemistry in the University of Birmingham, was elected a Fellow of the Royal Society on 10 March 1994. He was distinguished for the design and discovery of new approaches to the synthesis of novel organic substances using the techniques of molecular 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

J. Appl. Cryst. (1994). **27**, 439–440

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