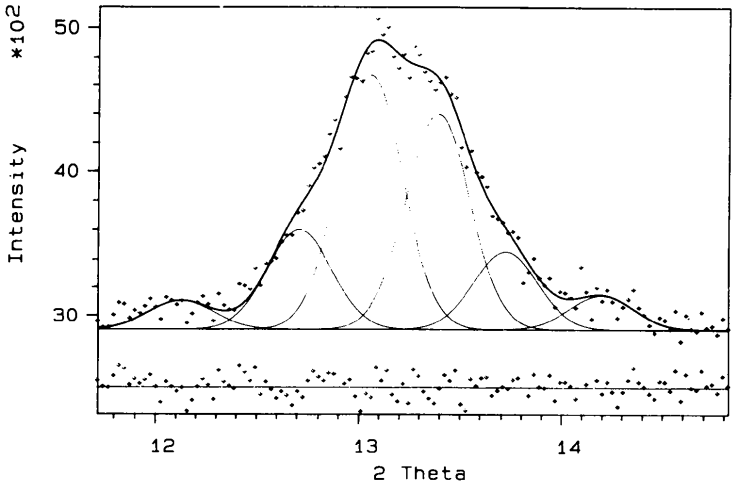

Fig. 2. Profile analysis of the $TbAsO_4$ magnetic 111 neutron diffraction peak measured at 0·4 K (data points). The analysis was performed by constraining the halfwidths of Gaussian functions according to the calibrated halfwidth characteristic of the diffractometer. The best fit (bold curve) ends with $R_{PF} = 2·3\%$ ($R_{PF}^{stat} = 1·6\%$) under the assumption of six curves (thin lines) representing three plus and minus satellite reflections each; a profile fit with only one Gaussian function results in $R_{PF} = 13·1\%$ (Kockelmann, 1989).

adapter. The program has been tested using a memory configuration of 640 kbyte and the operating system DOS 3.3. All necessary interface routines are implemented: driver for graphic display, mouse driver (Microsoft-compatible mouse) and plotter driver (HP-compatible plotter). The only input needed is the observed counting rates to be analysed. The appropriate angular scaling has to be defined by START, STEP, STOP information at the beginning of the data set. The refined parameter results are stored in a file PROFPRM, which additionally may contain *U, V, W* parameters to replace the program defaults.

Program specification: *PROFAN-PC* is dimensioned to handle data sets of up to 3275 data points. The data set has to be segmented into sections of up to 350 data points for performing the profile fitting. At maximum, 13 peak profiles containing three parameters each, *i.e.* 39 parameters, may be refined simultaneously.

A further version called *XPROFAN-PC* is provided to handle Pearson VII and pseudo-Voigt functions with four parameters each for an additional variation of Gaussian and Lorentzian profile contributions. *XPROFAN-PC* is limited to a maximum of 10 peak profiles and 40 parameters to be refined simultaneously.

Documentation and availability: The source code of *PROFAN-PC* is available on a PC diskette. The program is delivered including a diffraction data file for an immediate handling and performance test. A detailed description of all handling facilities is provided. To apply for a copy of the program one of the authors should be contacted at the above address.

Keywords: Personal computer program, profile analysis, peak decomposition.

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Crystallographers

J. Appl. Cryst. (1990). **23**, 445

This section is intended 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 Editoral Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

Professor **Frank C. Hawthorne**, Professor of Crystallography and Mineralogy at the University of Manitoba, has been elected a Fellow of the Royal Society of Canada. His work focuses on topological/graphical aspects of oxysalt minerals and their role in explaining mineral chemistry and behaviour in geological processes, and spectroscopic methods applied to mineral chemistry and characterization.

Professor **Arne Magnéli**, University of Stockholm, 1975–1978 IUCr President, has been awarded the Georges Chaudron Gold Medal by the French Society for High Temperatures and Refractories (Societé des Hautes Températures et des Réfractaires).

Professor **A. McL. Mathieson**, Honorary Professor in the Department of Chemistry, La Trobe University, Bundoora, Victoria, Australia, received an honorary degree of DSc from the University of St Andrews, Scotland, on 6 July 1989.

New officers have been elected for the Society of Crystallographers in Australia. Professor **J. W. White**, Research School of Chemistry, Australian National University, Canberra, ACT, is the new President. Dr **A. H. White**, School of Chemistry, University of Western Australia, Nedlands, Western Australia, is Vice-President. Dr **G. A. Williams**, Australian Radiation Laboratory, Yallambie, Victoria, is Secretary and Dr **C. H. L. Kennard**, Department of Chemistry, University of Queensland, St Lucia, Queensland, is Treasurer.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

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The Dorothy Hodgkin Prize of the British Crystallographic Association

In celebration of Professor Dorothy Hodgkin's 80th birthday, the British

Crystallographic Association (BCA) is pleased to announce the creation of the Dorothy Hodgkin Prize, in recognition of her great contribution to crystallography and to science in general.

Nominations for this prize are welcomed from any part of the crystallographic community and the award will be made at the time of the BCA Spring Meeting. Periodically the award will recognize specifically the achievements of young crystallographers.

The BCA is counting on the generosity of Dorothy's many friends and colleagues to make the prize financially worthwhile as well as prestigious. All donors will be named within the prize scroll and it is hoped that you will wish to be associated with this splendid and permanent tribute to Dorothy's scientific achievements. In order that the first award may be closely associated with Dorothy's 80th birthday, we wish to make the first presentation of the prize at the Sheffield Meeting of the BCA in March 1991. It is expected that Dorothy herself will be there to present the award at this time.

Please forward your contributions as early as possible to the Treasurer, Dr Ian Langford, Department of Physics, The University, Birmingham B15 2TT, England. (Cheques payable to The Dorothy Hodgkin Prize/BCA.) Further details concerning the nominations for the award will appear in future BCA Newsletters this year, or can be obtained from the BCA Secretary, Dr Judith Howard.

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 company concerned.

J. Appl. Cryst. (1990). **23**, 446

3D Chemical Structure Builder for Chem-X

Chemical Design announces the development of a **3D chemical structure builder** which allows fast and fully automatic conversion of 2D database connection tables into 3D molecular models. This enables pharmaceutical companies to build corporate 3D structure databases quickly and easily from existing 2D databases such as MACCS-II, DARC or OSAC. Using these new capabilities, 3D structures can typically be built at a rate of 1 per CPU s on a MicroVAX 3100.

The new 3D builder has been incorporated into the heart of the Chem-X molecular modelling system. It is based on proven Chem-X algorithms for interactive 3D model building using techniques such as sketching atoms and fusing commonly used molecular fragments. The method involves use of a fragment database of carbocyclic and heterocyclic rings and is similar to the approach described by Professor T. Wipke in *Tetrahedron Comp. Meth.* (1988). **1**, 141.

3D structure databases are important because it is the 3D arrangement of atoms in a molecule which determines its properties. Once a 3D database has been established, 3D search systems such as ChemDBS-3D can be used to identify those molecules which contain particular 3D patterns of atoms or groups. If such a 3D arrangement of atoms is believed to be associated with biological activity, for example, the search results in a set of potentially active drug molecules.

The 3D builder is just one of the many enhancements that Chemical Design make to the Chem-X software as part of on-going product development. It will be released with the July update of Chem-X to customers with support and consultancy contracts.

Chemical Design Ltd, Unit 12, *West Way, Oxford OX*2 0*JB, England*

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Millionths of Millimetres and Billions of Light Years – Carl Zeiss Mirror Systems for ROSAT

The German X-ray satellite ROSAT, the largest European research satellite to date, is carrying the most powerful X-ray telescope yet.

The heart of the **X-ray telescope** with a maximum aperture of 83 cm is the **mirror system developed and manufactured by Carl Zeiss,** West Germany. Its shape and surface structure cannot be compared with any telescope optics produced for other spectral ranges. X-ray mirrors are tube-shaped structures whose gold-coated internal surfaces reflect the X-rays with grazing incidence. According to an idea of the German physicist Hans Wolter, a perfect image is obtained if the X-rays are first reflected by a parabolic and then by a hyperbolic mirror. ROSAT features four concentrically nested Wolter telescopes of this type. The mirrors are made of Zerodur glass ceramic from Schott Glassworks, Mainz, and have been machined at Carl Zeiss with newly developed methods and tested with measuring equipment specially designed for this project.

The mirror surfaces deviate from the computed form by no more than 0·00002 millimetres. The smoothness even exceeds this value by a factor of 100. This means that Zeiss has created the largest, smoothest and most accurate X-ray mirror ever produced.

The resolving power of the instrument is twice as high as specified and permits two stars which are merely 2·5 angular seconds apart to be observed separately.

Carl Zeiss Oberkochen, Postfach 1369/1380, *D*-7082 *Oberkochen, Federal Republic of Germany*

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.

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Biomineralisation: chemical and biochemical perspectives. Edited by *S. Mann, J. Webb* and *R. J. P. Williams.* Pp. xiv + 541. Weinheim and New York: VGH Verlag mbH. Price DM 274.00. A review of this book, by S. K. Chapman, has been published in the August 1990 issue of *Acta Crystallographica,* Section B, pages 575–576.

A revolution in biotechnology. Edited by *Jean L. Marx.* Pp. 227. Cambridge University Press, 1989. Price £ 25.00, US$ 44.50. A review of this book, by J. R. Helliwell, has been published in the August 1990 issue of *Acta Crystallographica,* Section B, page 576.