structural chemistry at the Faculty of Pharmaceutical Sciences. He retired from Osaka University in 1967 and moved to Kwansei-Gakuin University, where he was Professor of Chemistry. He continued research work with his students until he reached almost 80 years of age.

Known as Toku Watanabé, he maintained good relationships with his overseas as well as domestic friends. He presided over Alliance Française d'Osaka for some time and was given an Ordre National du Mérite for his activity in helping cultural exchange between the two nations. He was well aware of the unfavourable living conditions of foreign students in Japan, especially those from developing countries, and made efforts to improve them.

His life was indeed dedicated to the study of science and to the love of mankind.

K. OSAKI

Dr **M. A. Carpenter**, Department of Earth Sciences, University of Cambridge, has been awarded the 1989 Mineralogical Society of America Award for his outstanding work on the elucidation of order/disorder and exsolution behaviour in minerals using various experimental and theoretical approaches combined with transmission electron microscope observations on microstructures.

Professor **M. N. G. James**, Professor of Biochemistry at the University of Edmonton, Alberta, Canada, has been elected a Fellow of the Royal Society, in recognition of his X-ray crystallographic analyses on proteins, which have been characterized by the application of techniques giving precision of structural results. His studies on serine and acid proteases and of troponin C have led him to make substantial contributions to the understanding of the mechanisms in which these proteins are involved.

Professor **Arne Magnéli**, University of Stockholm, has been awarded the 1989 Gregori Aminoff Gold Medal and Prize for his epoch-making studies of the crystallographic building principles of complicated oxide compounds which have revolutionized our view of the relation between structure and stoichiometry within the field of inorganic chemistry. This, the tenth such award, will be presented to Professor Magnéli at the Royal Swedish Academy of Sciences meeting on 7 June 1989.

Previous recipients of the award are P. P. Ewald (1979), Sir Charles Frank (1981), G. Hägg (1982), J. M. Robertson (1983), D. Harker (1984), A. Guinier (1985), E. F. Bertaut (1986), O. Kratky (1987) and I. Karle (1988).

Dr **Helen D. Megaw** has been awarded the Roebling Medal, the highest award of the Mineralogical Society of America for eminence in outstanding original research, for her numerous contributions to feldspar crystallography and crystal chemistry and her research on barium titanate and perovskite ferroelectric materials.

Dr **David Sayre**, Research Scientist at the IBM Thomas J. Watson Research Center, Yorktown Heights, New York, USA, will be presented with the seventh Fankuchen Award at the July 1989 meeting of the American Crystallographic Association in Seattle. The award is made triennially. Dr Sayre's many achievements include pioneering work on direct methods of structure determination, the refinement and extrapolation of low-resolution phases to higher resolution in macromolecules, and work on imaging large non-repeating objects with soft X-rays.

Professor **K. Wade**, Professor and Chairman of the Department of Chemistry at the University of Durham, has been elected a Fellow of the Royal Society, in recognition of his contributions to inorganic and organometallic chemistry, especially for his formulation of rules (known as Wade's rules) governing the structures of clusters of metal or metalloid atoms.

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, Professor M. Schlenker, Editor* Journal of Applied Crystallography, *Laboratoire Louis Néel du CNRS, BP*166, *F*-38042 *Grenoble CEDEX, France.*

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. (1989). **22**, 297

Huber X-ray Guinier Diffractometer System 600

The **Guinier Diffractometer System 600** delivers digital diffractogram data of powdered, liquid or solid samples. All goniometers are driven by a Stepper Motor Control 9005 with a reproducible step-scan increment of 0·001° θ minimum. There is an adjustable slit screen whose center moves exactly on the focusing circle of 114·6 mm diameter. With an NaI(Tl) scintillation detector under computer control, a full θ range of 50° is scanned within some 25 min, if necessary. The diffractogram data are stored and handled by an HP Series 300 workstation running the program *G*600. The software is written in unsecured and freely accessible HP Basic and includes: data acquisition *via* IEEE 488, automatic θ calibrations using internal or external standards, data noise reduction by smoothing and fitting procedures. Peak search and data refinement to an accuracy better than 0·001° (θ). Graphics output to CRT, matrix printer or 6-color plotter. Data transfer to any host computer *via* RS 232 C is possible.

Flat powdered specimens at room temperature are measured on **Model 642**. Depending on crystallite dimensions of the powder a resolution of less than 0·035° (FWHM θ) is affordable.

On **Model 644**, only one single capillary of some 20 mm length can be investigated. Together with the **Temperature Control 9633** it allows for measurements of structural phase changes between room temperature and 900 °C maximum. Resolution is 0·1° (FWHM θ).

Model 645 is designed for the study of phase changes in the region from 10 to 350 K. Specimens have to be powdered as in model 642. A closed-cycle He cryostat is supported by an extra compression unit and controlled by a temperature device *via* IEEE 488. θ ranges from 0 to 50°, the resolution is similar to model 642.

Model 653 is for solid specimens which may be coated with a thin film of material different from the substrate. The primary beam strikes the sample surface at grazing incidence up to 10°. The resolution may reach 0·2° minimum.

As an option, one may use a **Heater 655** together with the **Controller 9633** to reach 600 °C approximately. For the evaluation of some preferred orientation, one may use an optional **Texture Device 656**.

Prices depend on options and range from DM 120 000 to DM 300 000.

*Huber Diffraktionstechnik GmbH, D-*8219 *Rimsting, Federal Republic of Germany*

J. Appl. Cryst. (1989). **22**, 297–298

Chem-X Molecular Modelling Software Enhanced

The January 1989 release of Chemical Design's **Chem-X molecular modelling software** contains a range of new features, some of which are summarized below.

The Chem-X molecular fitting capabilities have been enhanced to allow

chemical structures to be fitted together by matching vectors as well as by superimposing atoms. Vectors that can be matched in this way include vectors normal to planes, dipoles, and vectors representing other properties set up using the ChemLib module of Chem-X. This allows structures to be fitted according to their vector properties rather than simply by aligning atoms, and can be used, for example, to fit together five- and six-membered rings, or two structurally dissimilar molecules. No other commercially available software package provides this facility. (Fitting is important because it allows the modeller to study the similarities and differences between molecules and their properties by superimposing them graphically.)

Another important new feature is the automatic identification of the local maxima and minima of any function plotted out as a contour map, including wavefunction, electrostatic potential and electron density maps. Dummy atoms are automatically placed at the maxima and minima of the mapped function and may be used to fit two or more maps together. Information on the volume inside each map contour, the surface area at each contour, and the position and value of the maxima and minima is then available to the modeller, and can be written directly to a database. This is valuable when comparing maps to derive structure–activity relationships or to develop pharmacophores.

The January release of the **ChemQM module** of Chem-X now provides a transparent interface to Version 4.0 of the quantum mechanical program *MOPAC*, which has also been implemented on Chemical Design's transputer-based MITIE superworkstation. Other programs already implemented on the MITIE include the molecular dynamics program *AMBER* and the *ab initio* program *GAMESS*, as well as the powerful rule-based Chem-X conformational analysis routines.

Chem-X runs on DEC VAX computers under VMS.

Helen Gasking, Chemical Design Ltd, Unit 12, 7 *West Way, Oxford OX*2 0*JB, England*

J. Appl. Cryst. (1989). **22**, 298

Low-Cost Workstations for Molecular Modelling

Very competitively priced molecular modelling workstations based on Digital Equipment Corporation's recently announced VAXstation 3100 (the 'desktop VAX') are now available from Chemical Design. The new **P-GRAF 2 workstations** run Chemical Design's powerful Chem-X software and are available in a variety of configurations.

Prices range from only £8000 for a diskless system configured for addition to an existing Chem-X system, to £36 000 for a stand-alone P-GRAF 2 system with 8 Mbyte memory, 19″ colour monitor, 912 Mbyte disk, tape drive, tailored VMS environment and Chem-X software. Discounts are available to academic institutions.

For this price, P-GRAF 2 systems offer outstanding computational performance combined with 1024×864 colour graphics running DECwindows. Systems may also be configured to include a high-performance 3D graphics terminal.

Tests have shown that the new P-GRAF 2 workstations run on average three times faster than MicroVAX II-based systems for a range of typical modelling applications. For tasks which involve considerable disk access (*e.g.* searching databases) the performance of the P-GRAF 2 is even more impressive.

Chemical Design believes that there is considerable demand for a cost-effective modelling workstation that can also be closely coupled with existing chemical information management systems and databases. The VAX/VMS environment supplied with P-GRAF systems is uniquely well suited to this type of integration.

The P-GRAF 2 systems are the newest members of Chemical Design's growing family of molecular modelling workstations. Others include MicroGRAF systems (based on the MicroVAX 3000) and the top-of-the-range MITIE superworkstation, a transputer-based parallel processing system running at up to 360 MIPS.

All Chemical Design workstations are supplied as integrated packages with their own built-in system management procedures and are fully supported by Chemical Design. They are easy to use and are designed to be operated by chemists, not computer specialists.

Helen Gasking, Chemical Design Ltd, Unit 12, 7 *West Way, Oxford OX*2 0*JB, England*

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. (1989). **22**, 298

Thermotropic liquid crystals. (Critical reports on applied chemistry, Vol. 22.) Edited by *G. W. Gray*. Pp. xii+178. Chichester, England and New York, USA: John Wiley and Sons, 1987. Price £38.

Thermotropic liquid crystals, fundamentals. (Springer Series in Chemical Physics, Vol. 45.) By *G. W. Vertogen* and *W. H. de Jeu*. Pp. xi+324. Berlin: Springer-Verlag, 1987. Price DM 134.

A review of these books, by Patrick G. Barber, has been published in the May 1989 issue of *Acta Crystallographica*, Section A, pages 347–348.