

Main, P., Fiske, S. J., Germain, G., Hull, S. E., Declercq, J.-P., Lessinger, L. & Woolfson, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univ. of York, England and Louvain, Belgium.

Mallinson, P. & Muir, K. (1985). *J. Appl. Cryst.* **18**, 51–53.

Crystallographers

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 Editorial 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).

J. Appl. Cryst. (1990). **23**, 144

The 1989 Pauling Prize of the American Crystallographic Association for student work in crystallography was presented to **D. A. Adsmund** of the University of Minnesota and to **G. Zhou** of Oregon State University. Mr Adsmund received the award for work on predicting and analysing hydrogen-bond preferences of 2-aminopyrimidines. Mr Zhou's award-winning work involved studying the effect of the C5 methyl group of thymine on the structure of Z-DNA.

In 1988 the ACA presented the Pauling Prize to Sharon Lobert of Vanderbilt University for her X-ray fibre diffraction studies of a virus called the cucumber green mottle mosaic virus, watermelon strain.

Dr **David Sayre**, Research Division, IBM, T. J. Watson Research Center, Yorktown Heights, New York, USA, received the Fankuchen Award of the American Crystallographic Association. The citation was for his 'outstanding contributions to the development of innovative methods for crystal structure determination and for his contributions to the teaching of crystallography'. Dr Sayre, a past president of the ACA, has been with IBM since 1955. He has recently been involved in efforts directed toward determining the structures of large non-repeating objects such as biological cells using long-wavelength X-rays to measure their diffraction patterns.

The Fankuchen Award is presented jointly by the ACA and the Polytechnic University every three years to 'an outstanding crystallographer or X-ray diffractionist who is active in the field and has made significant contributions to research and teaching of crystallography'.

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.

J. Appl. Cryst. (1990). **23**, 144

International Organization of Crystal Growth (IOCG)

The Officers of the International Organization of Crystal Growth (IOCG), elected at the General Assembly held in Sendai, Japan, in August 1989, are as follows:

President: Professor B. Cockayne (UK); Vice-Presidents: Professor R. F. Sekerka (USA) and Professor A. A. Chernov (USSR); Secretary: Professor M. Schieber (Israel); Treasurer: Professor E. Kaldis (Switzerland). Professor R. Kern (France) is the Past President.

The bonds of contact and the co-operation between the IOCG and the Commission on Crystal Growth and Characterization of Materials of the IUCr remain excellent.

Professor Kaldis, the new Treasurer of the IOCG, and two other members of the IOCG Executive Committee, Professor I. Komatsu (Japan) and Professor K. W. Benz (Federal Republic of Germany) are involved in the above Commission. In addition, Professor V. V. Osiko (USSR) is appointed by the IOCG as an *ex officio* member of the Commission.

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.

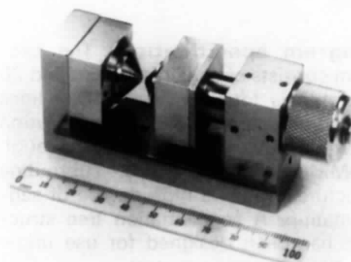
The International Union of Crystallography can assume no responsibility for the accuracy of the claims made. A copy of the version sent to the printer is sent to the company concerned.

J. Appl. Cryst. (1990). **23**, 144

Small Permanent Magnet Produces Uniform 2.5 Tesla

A new small permanent laboratory magnet that produces a uniform field of 2.5 Tesla to permit viewing with a light microscope or an X-ray beam is being introduced by Charles Supper Company, Inc. of Natick, Massachusetts.

The **Supper SPM-25 Mini-Magnet** produces a uniform magnetic field of 2.5 Tesla at a 1 mm gap and is continuously adjustable from 1 to 12 mm for varying the field. Designed to orient capillary tubes parallel or perpendicular to the field, a 1 mm hole runs through the entire magnet along the axis of the pole pieces.



The Supper SPM-25 mini-magnet

Measuring only 2.5 × 4.5 × 11 cm, the Supper SPM-25 Mini-Magnet is constructed with steel and iron parts that are nickel plated for corrosion protection. It is suitable for direct mounting on the stage of a microscope; an optional glass tube is available for light microscopy.

The Supper SPM-25 Mini-Magnet sells for US\$ 1495. Literature is available on request.

Charles Supper Company, Inc., Lee Supper, Marketing, 15 Tech Circle, Natick, MA 01760, USA

J. Appl. Cryst. (1990). **23**, 144–145

INRAD Model 151-030 Low Voltage Modulator

INRAD expands its line of electro-optic devices with the **Model 151-030 Low Voltage Modulator**. This transverse field device, incorporating four AD*P crystals, offers design features which provide excellent temperature stability and contrast ratio without the use of index matching fluids. The 'dry' construction allows the modulator to be mounted in any position and provides distortion-free operation with high-power laser beams.

INRAD manufactures crystals, laser components, optical coatings, laser systems and instruments for scientific, defense, aerospace, and industrial markets. Its common stock is traded under

the symbol INRD through the NASDAQ National Market System.

INRAD, 181 Legrand Ave, Northvale, NJ 07647, USA

J. Appl. Cryst. (1990). **23**, 145

Chem-X Inorganic Modelling Facilities Enhanced

The inorganic modelling facilities of Chem-X have been enhanced to provide for **unit-cell optimization, application of DLS-like symmetry restraints, use of x , y , z dynamics** and the **generation of complex crystal surfaces**. These enhancements strengthen Chem-X's position as a leading system for studying the structure and properties of zeolite catalysts, high-temperature superconductors and other inorganic crystal lattices.

The introduction of unit-cell optimization and symmetry restraints enables users to build models of zeolites or inorganic crystals from the minimum amount of information (*e.g.* chemical composition and coordination data). All cell parameters may be varied during optimization, as well as all atom positions. The use of new DLS-like restraints governing the separation of symmetry-related atoms in a lattice allows the symmetry of a structure to be preserved during both energy minimization and geometry optimization.

The Chem-X molecular dynamics facilities have been extended to simulate the motion of a structure with respect to atom positions (x , y , z dynamics) as well as bond or fragment rotations (torsional dynamics). This is particularly important in zeolite catalyst systems, as it enables researchers to study how the pores or channels in a structure relax as small molecules pass through the lattice.

Chem-X already allows crystal structures to be built up according to specified symmetry operators or space groups, and 'slices' taken through the structure. These facilities have been enhanced so that it is now possible to produce complex crystal surfaces formed by the intersection of multiple crystallographic planes. These planes are specified using standard Miller indices. Applications include catalyst studies, investigations of the epitaxial growth of superconducting films on various substrates, and other surface phenomena.

Chem-X runs on DEC VAX computers under VMS.

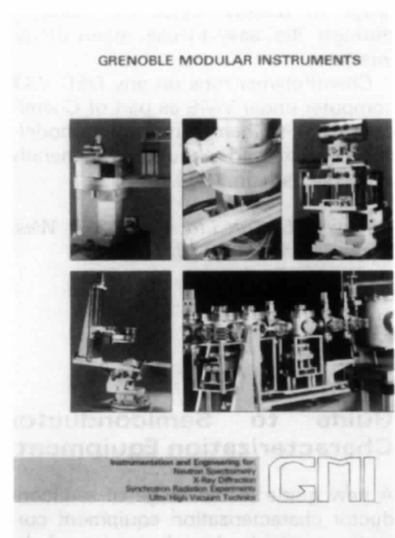
Chemical Design Ltd, Unit 12, 7 West Way, Oxford OX2 0JB, England

J. Appl. Cryst. (1990). **23**, 145

Brochure features UHV Instruments, Optical Components and Positioning Devices

A new brochure featuring a broad line of instrumentation for neutron spectrometry, X-ray diffraction, synchrotron radiation experiments, ultra high vacuum, and optics applications is being offered by Charles Supper Company of Natick, Massachusetts.

The **Grenoble Modular Instruments Brochure** features a broad line of modular spectrometers, X-ray scattering instruments, Weissenberg cameras, neutron diffractometers and spectrometers, optical components, collimators, monochromators, and rotational and translational stages. Charles Supper Company, Inc. is the exclusive North American distributor of these instruments.



Grenoble modular instruments brochure

Complete with full-color product photographs and diagrams, the six-page Grenoble Modular Instruments Brochure includes general information describing their modular concept which allows instrument designers to select and assemble the components and connecting or adjusting devices to suit their requirements.

The Grenoble Modular Instruments Brochure is available free from: Charles Supper Company, Inc., 15 Tech Circle, Natick, MA 01760, USA.

Charles Supper Company, Inc., Lee R. Supper, Marketing, 15 Tech Circle, Natick, MA 01760, USA

J. Appl. Cryst. (1990). **23**, 145

New-Look Chem-X

The performance and ease of use of Chemical Design's **Chem-X molecular modelling software** have been increased through major enhancements to the user interface and display facilities.

A faster new-look interface featuring pop-down menus, toggles and status boxes has been introduced, allowing modelling work to be carried out more quickly and efficiently. The menu tree has been completely redesigned to enable users to perform common modelling operations with the minimum of menu 'picks', while still providing easy access to more-complex facilities. Commonly used modelling setups (parameter values *etc.*) can be readily defined and retained for future use.

This development has been carried out hand-in-hand with enhancements to Chem-X's display and structure manipulation facilities.

A major rewrite of the graphics software has minimized the number of times a picture is redrawn, thus saving considerable time when working with large molecular structures. It is also possible to switch separate portions of the picture on and off independently, providing a wider variety of display options.

As part of the overall changes to Chem-X, a new manipulation menu has been introduced and is permanently available throughout the modelling session. Up to four molecular fragments and up to four bonds can now be selected for interactive manipulation using a dial box; alternatively, values can be picked from a 'scale bar' on the screen. Chem-X is the only molecular modelling system that provides for interactive rotation of several bonds on a range of high- and low-performance graphics systems.

Chem-X runs on VAX computers under VMS.

Chemical Design Ltd, Unit 12, West Way, Oxford OX2 0JB, England

J. Appl. Cryst. (1990). **23**, 145-146

A New Ion Milling Device for TEM

The Research Institute for Technical Physics of the Hungarian Academy of Sciences announces the new version of the successful **ion milling units IV1 and IV2**, which, besides high thinning

rate (Si: $>100 \mu\text{m h}^{-1}$ for steep incidence and $\sim 10 \mu\text{m h}^{-1}$ for an incidence at $2\text{--}3^\circ$ measured from the surface) and long-life sources, offers a unique possibility for all users working with extremely inhomogeneous specimens like multilayer structures, composite materials, alloys, ceramics etc.

Experimental and theoretical studies have shown that both the usual surface roughening and the radiation damage as well as the effect of great differences in sputtering rates can be well suppressed using grazing incidence. In this case, however, the current density becomes extremely low, as well as other unfavourable effects.

The sample holder of the new device **IV3** is electrically insulated and an adjustable retarding potential is applied to the sample. In this way it is possible to realize grazing incidence at the sample without a considerable decrease either in the ion current density or in the ion energy.

As a further advantage of the method, separation of the neutral atoms and ions is possible, and thinning can be performed either by neutral atoms only or by ions. The neutral content of the beam leaving the sources is variable by changing the exit apertures.

This new possibility, together with the eventual sample rocking (instead of rotation) and optical termination makes it possible to prepare specimens with a large transparent area and high surface quality.

The device can be mounted on most common pump stations.

The price is approximately US\$ 15000, depending on the accessories.

A. Barna, Research Institute for Technical Physics, Budapest, POB 76, H-1325 Hungary

J. Appl. Cryst. (1990). 23, 146

ChemPolymer - New Software for Polymer Modelling

Chemical Design, developers of the widely used Chem-X molecular modelling software, are pleased to announce a new Chem-X module aimed at polymer research. Exploiting Chem-X's open architecture, the **ChemPolymer tool-kit** integrates specialist polymer building and property calculation functionality with Chem-X's powerful interactive analysis and display facilities.

The latest member of the Chem-X family enables researchers to study the

properties of potential new polymers before they have been produced in the laboratory. ChemPolymer can be used to evaluate a wide range of physical or bulk characteristics, including free volume, stiffness, elasticity and geometrical parameters. The temperature dependence of properties such as entropies and free energies may also be calculated, using techniques based on statistical thermodynamics.

Correlations between modelling parameters and observed properties may be studied using existing Chem-X facilities which are fully integrated with ChemPolymer.

ChemPolymer is designed for quick and easy polymer modelling. Using advanced building techniques, ChemPolymer can not only generate regular, blocked and random copolymers from monomers, but also handle branching to form network and star polymers. ChemPolymer packs polymer chains to form crystalline domains, and also provides innovative functionality for modelling amorphous polymers. A wide range of display styles are available through the easy-to-use menu-driven interface.

ChemPolymer runs on any DEC VAX computer under VMS as part of Chemical Design's Chem-X molecular modelling system and should be generally available early in 1990.

Chemical Design Ltd, Unit 12, 7 West Way, Oxford OX2 0JB, England

J. Appl. Cryst. (1990). 23, 146

Guide to Semiconductor Characterization Equipment

A new guide to the range of semiconductor characterization equipment currently available has been issued by Bio-Rad Microscience. The guide includes equipment which enables carrier concentration and mobility to be obtained reliably and routinely both at the semiconductor surface and as a function of depth. A variety of measurement techniques are available including both electrical and optical based methods for the determination of impurities, crystal defects and dopants.

For a free copy of this guide, please contact *Dr B. C. Beadle, Bio-Rad Microscience Ltd, Bio-Rad House, Maylands Avenue, Hemel Hempstead, Hertfordshire HP2 7TD, England*

J. Appl. Cryst. (1990). 23, 146

Crystal Growth Chamber Speeds Vapor Diffusion Experiments

A new 24-chamber vapor diffusion plate that can be totally sealed with a mylar sheet and permits easy access to individual chambers without disturbing the others is being introduced by Charles Supper Company, Inc. of Natick, Massachusetts.

The **MVD/24 crystal growth chamber** is a vapor diffusion plate featuring 24 individual chambers that each have a plastic post in the center of the well to hold a protein drop. Ideally suited for performing a wide array of experiments, all chambers can be sealed simultaneously and accessed individually without disturbing the remaining wells.



The MVD/24 crystal growth chamber

Each cup in the MVD/24 crystal growth chamber has been designed to provide the maximum surface area for free diffusion during equilibration and the reservoir solution is held within the narrow moat surrounding the support post. Compatible with robotic crystallization systems, this design is very stable and prevents splashing whenever the chamber is transported.

The MVD/24 crystal growth chamber is supplied 50 per carton priced at US\$ 162.50 complete with mylar cover material. Literature is available on request.

Charles Supper Company, Inc., Lee R. Supper, Marketing, 15 Tech Circle, Natick, MA 01760, USA