means of a mouse to perform one of the following:

MOVE: Interactive manipulation of atomic positions. An atom and the position to which it is to be moved are selected from the current section using the mouse. The map section and the modified position are then displayed. All the atomic positions of the section are held in a working array and may only be saved to the Brookhaven file by selecting the *SAVE* option from the menu.

INSW: Interactive insertion of water molecule positions. Any number of water molecules may be introduced into the working array until the option is cancelled. When *SAVE* is selected these positions are written to the end of the Brookhaven file. Atom names and dummy labels are assigned by the program.

INSA: Interactive insertion of atomic positions. An atom may be inserted into any residue of the protein. The atom type and its required position are specified by the user. The atom's location in the Brookhaven file must also be specified by the user.

DIST: Interactive determination of interatomic distances. Two positions are selected using the mouse and the distance between them is displayed in ångströms.

ZOOM: Any region of the displayed map section can be selected using the mouse and magnified. All options may be applied to this magnified region.

SECU: Display of map sections. The sections are displayed sequentially in the upwards direction.

SECD: Display of map sections. The sections are displayed sequentially in the downwards direction.

NAYB: Nearest neighbours. A position is selected using the mouse and all atoms within a contact distance of 3·5 Å are listed together with the contact distances and the sections on which each lies. The position of these atoms may be displayed as a projection onto the current section.

PLOT: Outputs a hard copy of the section displayed on the terminal.

SAVE: All current coordinates of the displayed section are saved and written to a Brookhaven file.

END: Exits without saving.

Software environment: *IMAP* operates under the VAX/VMS operating system and is written in Fortran 77. It requires GINOF and NAGF libraries.

Hardware environment: *IMAP* was developed using a Pericom terminal on a VAX (8200/750/780) at Liverpool Polytechnic. The current software allows the user to select Tektronix drivers t4014, t4010 or t4111. Hard copy is obtained on Calcomp plotters using the driver CC81 or CC1051. This interactive graphics program requires the use of a mouse.

Program specification: The present version of the program enables simple manipulation and distance measurements in proteins and other macromolecules. It is planned to introduce other useful features. Currently under development is an option to display the molecule as a 2D projection in a plane defined by any three atoms selected interactively.

The program listing contains approximately 3000 lines. *IMAP* has been tested using several proteins of different space groups and has also been independently tested at the Department of Chemistry at the University of York.

Documentation: A user manual is available including test examples. An overview of the program structure is also available.

Availability: A copy of the executable code can be obtained by sending a magnetic tape to the Structural Biophysics Unit at Liverpool Polytechnic. A copy of the source code may be provided at the discretion of the authors.

Keywords: Molecular graphics, electron density maps, proteins, inexpensive, water structure, Tektronix.

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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).

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Tokunosuké Watanabé 1904–1988

Tokunosuké Watanabé, Professor Emeritus of Osaka University and of Kwansei-Gakuin University, passed away suddenly on 7 October 1988 from a heart attack.

Tokunosuké Watanabé was one of the fore-runners of modern crystallography in Japan and helped Professor I. Nitta to create an active group for X-ray crystallography as part of his laboratory of crystal chemistry at Osaka University. He was one of the first members of the Japanese National Committee for Crystallography, established in 1949, and served as such until 1969.

In 1956 he attended an IUCr meeting in Madrid, held by the Commission on Crystallographic Teaching, and served as a member of the Commission until 1960, submitting a report on crystallographic teaching in Japan. Later he served as a member of the IUCr Commission on *Structure Reports*, succeeding Professor Nitta. In 1961 he organized an international conference on 'Scientific Information in the Fields of Crystallography and Solid State Physics' at Kwansei-Gakuin University, Nishinomiya, as the President of the Crystallographic Society of Japan, with the support of the IUCr and other interested bodies.

Tokunosuké Watanabé was born on 28 February 1904, in Fukushima prefecture, a north-eastern district of Japan. Graduating from Tokyo Technical High School (predecessor of Tokyo Institute of Technology) in 1924, he entered Dr G. Asahara's laboratory at the Institute of Physical and Chemical Research, where he began his X-ray crystallographic studies. His first crystal-structure work on northupite and tychite, published in French, was approved by Professor Nitta, which gave him the opportunity to be taken as an assistant when Professor Nitta moved to the Faculty of Science, Osaka University, as Professor of Physical Chemistry.

Among his early structural studies with Professor Nitta, perhaps the best known to older colleagues will be the Fourier analysis of pentaerythritol published in 1938. He went one step further to study a high-temperature modification of pentaerythritol, which opened a new field of study, plastic crystals, as named by J. Timmermans. During World War II, he searched for thallium in Japanese sulfide mines, using spectroscopy and chemical analysis, which enabled him to start a series of crystal-structure studies on thallium complex salts soon after the end of the war.

In 1951 he was warmly accepted by Professor Ray Pepinsky to work in his laboratory at State College, PA, USA. He stayed there for two years, creating friendly relationships with the people there, and also with the scientists from other parts of the world who were staying or visiting at that time. It opened a road by which a number of young crystallographers from Japan followed him. In 1986 he was given the first Pennsylvania State University Medal as Pioneer Bridge Builder between Japan and the United States.

In 1964 he moved to the College of General Education of Osaka University and in 1965 opened a laboratory of

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.

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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*

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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