not exceed 1000 Å^3. The corresponding time for an IBM PC/AT and an IBM-compatible Schneider computer is about three times shorter. The program is much faster in the local case.

Software environment: *INDEXING* is written in Fortran77 using the Microsoft Fortran compiler 4.10 under MS-DOS3.10. No external library is required.

Hardware environment: The program runs on IBM-compatible PC/XT or PC/AT computers equipped with 640 Kbyte of memory and coprocessor. Use of hard disk is recommended.

Program specification: The present version of *INDEXING* indexes up to 50 peaks of hexagonal, tetragonal and orthorhombic patterns. Separate runs are performed for each system. Rhombohedral patterns may be solved with the hexagonal option, but solving them is more difficult and more time consuming. The full listing contains about 2800 lines of source Fortran code. This version of the program was successfully tested mainly with National Bureau of Standards' powder diffraction data. Previous non-interative versions have been routinely applied to data of different sources and quality on a Cyber73 computer since 1983.

Documentation: A tutorial is available as a machine-readable file. Example files and some on-line help facilities are included.

Availability: The program (including files containing user manual and input test examples) is available free of charge in executable form on two 360 or one 1200 Kbyte 5·25″ floppy disks supplied by the user.

Keywords: X-ray diffraction, powder-pattern indexing.

References

Paszkowicz, W. (1987*a*). *J. Appl. Cryst.* **20**, 161–165.

Paszkowicz, W. (1987*b*). *J. Appl. Cryst.* **20**, 166–172.

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. (1989). **22**, 187

Professor **Sir Jack Lewis,** Professor of Chemistry at the University of Cambridge, England, and Chairman of the Commission on Environmental Pollution, has been made a Life Peer.

Sir David Phillips, Professor of Molecular Biophysics at the University of Oxford, England, and Chairman of the Advisory Board for the Research Council, has been made a Knight Commander of the Order of the British Empire.

Dr **Qun Shen,** Postdoctoral Associate in Applied and Engineering Physics at Cornell University, USA, has received the 1988 Sidhu Award for his contributions to the development of experimental procedures for phase determination. The Sidhu Award was established as a memorial to one of the founders of the Pittsburgh Diffraction Conference and is presented to a scientist under 33 years of age who has made a significant contribution to the field of diffraction.

Professor **G. A. Somorjai,** Department of Chemistry, University of California, Berkeley, California, USA, has been awarded the Peter Debye Award in Physical Chemistry of the American Chemical Society. The award, sponsored by the DuPont Company, recognizes Gabor Somorjai's pioneering work and continuing leadership in surface science and heterogeneous catalysis research involving, among many other activities, the characterization of clean single-crystal surfaces and the determination of surface structures of ice, alkanes and amino acids grown epitaxially on metal single crystals.

International Union of Crystallography

J. Appl. Cryst. (1989). **22**, 187

Nominations for the Ewald Prize

The International Union of Crystallography is pleased to invite nominations for the Ewald Prize for outstanding contributions to the science of crystallography. The Prize is named after Professor Paul P. Ewald, in recognition of his significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography. Professor Ewald was the President of the Provisional International Crystallographic Committee from 1946 to 1948, the first Editor of the Union's publication *Acta Crystallographica* from 1948 to 1959 and the President of the Union from 1960 to 1963.

The Prize consists of a medal, a certificate and a financial award. It is presented once every three years during the triennial International Congresses of Crystallography. The first Prize was presented at the XIV Congress at Perth, Australia, in 1987. The second Prize, for which nominations are now being invited, will be presented at the XV Congress in Bordeaux, France, in July 1990.

Scientists who have made contributions of exceptional distinction to the science of crystallography are eligible for the Ewald Prize, irrespective of nationality, age or experience. The only exceptions are the current members of the Prize Selection Committee and the President of the Union, none of whom are eligible. No restrictions are placed on the time or the means of publication of the nominee's contributions. The Prize may be shared by more than one contributor to the same scientific achievement.

Nominations for the Ewald Prize should be submitted in writing, preferably using the Ewald Prize Nomination Form and accompanied by supporting documentation, to the Executive Secretary of the International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England, from whom copies of the Nomination Form, the names of the Selection Committee and advice on the submission of nominations may be obtained. **The closing date for nominations is 31 August 1989.**

M. NARDELLI, President — A. I. HORDVIK, General Secretary

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, BP166, 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**, 187–188

Molecular Mechanics Parameter Generation on the MITIE Superworkstation

Chemical Design is pleased to announce that the **MITIE supercomputing system** for molecular modelling has now taken on an important new role – as a **molecular mechanics parameter generator**.

Molecular mechanics is an important technique used by computational chemists to calculate the energy of molecular systems, and to determine accurate molecular geometries. However, to use this technique it is

essential to know the values of certain system-specific parameters, not all of which may be available from the literature.

Using the MITIE, it is possible to calculate the values of these unknown parameters *via* quantum mechanics. This procedure is extremely computer intensive, but thanks to the intrinsic speed of the T800 transputer chips contained in the MITIE, its parallel architecture, and a highly efficient automation procedure, the results can be calculated very rapidly and with minimum user involvement.

An entry-level MITIE system has a throughput eight times that of a VAX 8600 in typical quantum-chemistry applications, but costs only about £85 000 (price includes high-performance graphics terminal and Chem-X modelling software). A fully configured MITIE system offers up to 72 times the power of a VAX 8600 for less than half the price.

MITIE systems may be used either as stand-alone superworkstations or as compute-servers in a VAX network.

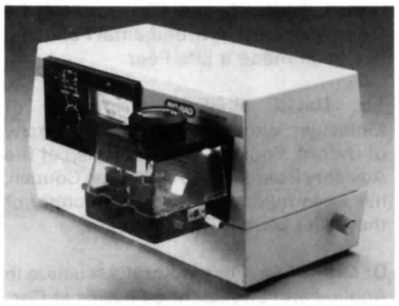
Founded in 1983, and with offices in both the US and the UK, Chemical Design is now established as the world's leading supplier of molecular modelling systems. The company's success is based largely on the reliability, flexibility and functionality of its state-of-the-art Chem-X modelling software, which has been installed at nearly 300 sites throughout the US, Europe and the Far East. Customers include divisions of virtually all the major multinational chemical corporations, as well as many leading academic research centres.

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

J. Appl. Cryst. (1989). **22**, 188

HL5400 Semiconductor Wire Bonder

The **HL5400 semiconductor wire bonder** is a small bench-top instrument designed to bond wires directly to semiconductor materials. A controlled current through the wire, which is usually 0·05 mm diameter gold, thermally alloys it to the semiconductor. The resultant bond consists of a small bead of metal with a short length of wire attached. The technique is applicable to silicon and



The HL5400 semiconductor wire bonder.

many compound semiconductors including GaAs and InP.

The instrument has a facility for fume extraction and provision for operation with an inert environment. The control panel provides for precise adjustment of the bonding conditions and a means of checking the resistance of the contact. The HL5400 can also bond wires to copper pads on printed circuit boards making this instrument a truly versatile bonder to complement many semiconductor characterisation techniques.

Mr R. Claridge, Bio-Rad Microscience Division, 53–63 *Greenhill Crescent, Watford Business Park, Watford, Herts WD*1 8*QS, England.*

J. Appl. Cryst. (1989). **22**, 188

3D Protein Modelling from Chemical Design

Chemical Design has recently developed an automated procedure which **constructs 3D models of proteins** from their amino acid sequences using sequence homology or similarity.

Information on the 3D structure of a protein is important because it allows interactions between small molecules and protein receptor sites to be modelled (crucial in the rational design of drugs and agrochemicals). Since the amino acid sequences of many receptors of physiological importance are known, but their 3D structures are not, a method which converts one into the other is clearly of great value.

The Chemical Design software is based on an approach developed at Birkbeck College, London, in which a 3D model of a protein is constructed by comparing its amino acid sequence with sequences occurring in other proteins of known 3D structure. The method is dependent on a high level of similarity between the proteins.

Chemical Design has automated and extended this procedure, allowing protein sequences to be matched and the corresponding 3D models to be built automatically. These models can then be refined further using techniques such as molecular mechanics or molecular dynamics.

This automatic technique has already been used successfully to build models where the sequence homology was as low as 20%, suggesting that many very useful protein models can be generated in this way.

With more than 280 installations of its Chem-X software worldwide, Chemical Design is the leading supplier of computer-aided molecular modelling systems. Customers include divisions of most multinational chemical corporations as well as many leading academic research centres. Chem-X is used in a wide variety of application areas, including drug design, agrochemicals, protein engineering, petrochemicals and polymers. In addition to the modular Chem-X system, Chemical Design also offers a range of powerful workstations and graphics systems customized for molecular modelling.

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.*

Books Received

The following book has 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**, 188

Morphology of crystals: Part A (Series in materials science of minerals and rocks). Edited by *I. Sunagawa.* Pp. xxii + 365. Dordrecht: Kluwer Academic Publishers, 1988. Price Dfl 220.00, US$ 99.00, £74.00. A review of this book, by H. E. Lundager Madsen, has been published in the February 1989 issue of *Acta Crystallographica,* Section A, pages 211–212.