

not exceed 1000 Å<sup>3</sup>. 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-interactive 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

- Paszkwicz, W. (1987a). *J. Appl. Cryst.* **20**, 161-165.  
 Paszkwicz, W. (1987b). *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).*

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**Professor Sir Jack Lewis**, Professor of Chemistry at the University of Cam-

bridge, 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

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### 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.*

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### 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