

Computer Program Abstracts

The category *Computer Program Abstracts* provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Following normal submission, a *Computer Program Abstract* will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 of the June 1985 issue of the *Journal* [*J. Appl. Cryst.* (1986), 18, 189–190].

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EDDA – program for predicting energy-dispersive powder diffraction spectra. By L. GERWARD, *Laboratory of Applied Physics III, Building 307, Technical University of Denmark, DK-2800 Lyngby, Denmark*, and J. STAUN OLSEN, *Physics Laboratory, University of Copenhagen, DK-2100 Copenhagen, Denmark*

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The crystallographic problem: The program finds Miller indices of all relevant Bragg reflections and solves the Bragg equation in terms of photon energy.

Method of solution: Integrated intensities of the powder diffraction lines are calculated using a simplified formula. Escape peaks are taken into account in the case of a germanium detector. The minimum input data consist of the parameters of the unit cell, the coordinates of the atoms in the unit cell, translational symmetry of the lattice, the energy range and the Bragg angle. The output is a listing of energies and intensities of diffraction peaks, fluorescence peaks and escape peaks. If one knows the peak shape and resolution (Buras, Niimura & Olsen, 1978) the predicted spectrum can be plotted. The Bragg angle can thus be optimized without wasting time at the X-ray source, which is particularly important in synchrotron radiation work.

Software and hardware requirements: The program is written in Fortran IV and has been run on an IBM3033 using 250 K storage. For a cubic structure the CPU time is about 1.5 s. Drawings have been made on an HP7475A plotter.

Documentation and availability: A listing of the program is available from one of the authors (LG) together with examples of predicted and observed spectra.

Reference

Buras, B., Niimura, N. & Olsen, J. S. (1978). *J. Appl. Cryst.* 11, 137–140.

Crystallographers

J. Appl. Cryst. (1987), 20, 324–325

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).

On 3 November 1986, **Walter Hoppe** passed away after a serious illness, which he suffered with admirable patience.

Primarily, W. Hoppe was known to the scientific community by his contributions to methods and instrumentation of X-ray structure analysis. In the sixties he turned to electron microscopy, extending crystallographic methods to electron diffraction. He dealt with three-dimensional imaging of periodic and mainly aperiodic structures under conditions of high resolution. His ideas covered instrumental as well as image-processing innovations.

Professor Dr A. Gieren writes that it would be impossible to cite all the contributions made by Hoppe to X-ray and neutron diffraction in detail, but his main fields of interest were thermal diffuse scattering, the convolution molecule method, phase determination, the shift product method, direct methods, the phase correction method, phase determination of protein structures, and last but not least the development of computer programs. He also developed the lable triangulation method for structure determination of aperiodic objects by neutron scattering, and, on the instrumentation side, a mechanical analogue computer for Fourier syntheses, the so-called Fourier synthesizer, film scanners and automatic single-crystal off- and on-line diffractometers.

Many structure determinations, especially of organic molecules, were performed in his laboratory during the pioneer days of X-ray structure analysis. At the end of the 1960's, he went into the new field of electron microscopy. He used the electron microscope like an X-ray diffractometer, transferring X-ray crystallographic methods to structure determinations with electron beams. He used crystallographic electron-microscope methods to produce three-dimensional pictures with almost atomic resolution. His special interest was the structure analysis of biological macromolecules. His methods for 3D-image reconstructions from 2D projections opened the door for investigations on the fine structure of aperiodic biological materials, which were inac-

cessible by other methods at this time. His goal was to push 3D electron microscopy to a stage of automation which is standard nowadays for X-ray structure analysis.

W. Hoppe was born on 21 March 1917 in Wallsee/Donau, Austria. Between 1936 and 1941 he studied chemistry at the German University of Prague and obtained his PhD in the laboratory of J. Böhm. The war brought him to Munich, where his collaboration with G. Scheibe had a great influence on his future scientific career. In Scheibe's laboratory at the Munich Technical University (TU) he was engaged in X-ray diffraction studies. At this time his first X-ray investigations of organic molecules were performed. In 1944 his '*Habilitation*' thesis was finished, which dealt with methodical aspects of X-ray structure analysis. Directly after the war, his experience in the field of photosensitive compounds, obtained in Scheibe's laboratory, enabled him to work as a consultant in the photochemical industry. From 1948 to 1953 he also worked in industry, in Switzerland, and was involved in the development of electrical computers. In 1953 he returned to Munich as Privatdozent at Scheibe's reconstructed Institute for Physical Chemistry at the TU Munich while at the same time he was a guest fellow of Bern University in 1953 and, from 1954 to 1957, a guest of the Institute of Mineralogy and Petrography at the ETH Zürich in the laboratory of F. Laves. In 1956 he became 'Diätendozent' at TU Munich and in 1958 was appointed as a professor. There followed a sabbatical in the MRC Molecular Biology Laboratory in Cambridge, England, where he became familiar with protein structure analysis. In 1959 he was appointed Head of the department for X-ray structure analysis at the former Max-Planck-Institut für Protein and Leather Research. In 1964 he became Director of this section. After the incorporation of this Institute into the Max-Planck-Institut für Biochemie in Martinsried/Munich he was the Head of the Department of Structure Analysis I until he retired in 1985.

W. Hoppe was a member of numerous scientific societies, in Germany and abroad. His scientific work was honoured in many ways; he was a fellow of the German Academy of Naturforscher Leopoldina in Halle and the Bavarian Academy of Sciences. He had also been a member of the Commission on Crystallographic Apparatus of the IUCr.

All who have known Walter Hoppe will remember his strong personality. We will miss his stimulating and critical remarks in discussions, which he usually started very innocently with the remark 'I want to make only a short comment'. In fact this was the signal for a long scientific discussion.

As a result of a suggestion from the Bragg Lecture Fund committee, the Kathleen Lonsdale Lectures have been established by the British Crystallographic Association to commemorate her achievements. These lectures are intended to educate the public in the science of crystallography and will be given at the annual meetings of the British Association. The first one will be at 2 p.m. on 27 August 1987 at the British Association meeting in Belfast, Northern Ireland, and will be open to the public. The lecture will be given by Professor **David Blow** and the title of the lecture is 'Protein Crystallography Applied to Medicine and Industry'.

The Chemistry award of the Wolf prize this year will be shared by two macromolecular crystallographers: Professor Sir **David Phillips**, Laboratory of Molecular Biophysics, Department of Zoology, University of Oxford, England, and Professor **D. M. Blow**, Blackett Laboratory, Imperial College of Science and Technology, London, England. They are cited for their pioneering contributions to the understanding of enzymatic catalysis through the study of enzyme structure by X-ray diffraction. The award, which is considered in the class of the Nobel, Lasker and Welch prizes, will be presented in the late spring in Israel.

Dr **M. F. Perutz**, MRC Laboratory of Molecular Biology, Cambridge, England, and Sir **John Kendrew**, St John's College, Oxford, England, were presented the 1987 Distinguished Service Award of the Miami Winter Symposium in honour of their contributions toward promoting international cooperation between biological scientists. In particular, they were cited for their support of the founding and growth of the European Molecular Biology Organization, now in its 24th year. In 1962, Dr Perutz and Sir John Kendrew jointly received the Nobel Prize in medicine, Dr Perutz for his work on determining the three-dimensional structure of hemoglobin through X-ray diffraction and Sir John for similar work on myoglobin.

International Union of Crystallography

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The Ewald Prize

The first Ewald Prize for outstanding contributions to the science of crystal-

lography has been awarded jointly to Professor **J. M. Cowley** and Dr **A. F. Moodie**, for their outstanding achievements in electron diffraction and microscopy, especially for their fundamental contributions to the theory and technique of direct imaging of crystal structures and structure defects by high-resolution electron microscopy.

Their pioneering work on the dynamical scattering of electrons was reported in a series of papers in *Acta Crystallographica* and other journals from 1957 onwards. A theory of Fourier images led them to the multi-slice formulation of the scattering of an electron wave in its passage through a crystal. This formulation is able to take into account many hundreds of scattered beams, and has become the basis of widely used computer programs. The theory allows the electron micrographs, obtained with modern high-resolution instruments, to be reliably and quantitatively interpreted, and used for the determination of the structures of both perfect crystals and crystals containing defects.

Professor Cowley and Dr Moodie, together and separately, have made many further contributions to theory, methods and results in electron diffraction and microscopy. Their work has often stressed a unified approach to diffraction and microscopy through physical optics. An overview of the whole field may be found in Professor Cowley's book *Diffraction Physics* [(1981). Amsterdam: North-Holland].

John Maxwell Cowley, born in Australia in 1923 and a graduate of Adelaide University, was formerly a Chief Research Scientist at the Division of Chemical Physics, CSIRO, Melbourne, Australia. Later he was Professor of Physics at the University of Melbourne, and since 1970 has been the Galvin Professor of Physics at Arizona State University, Tempe, USA.

Alexander Forbes Moodie, born in Scotland in 1923, graduated from St Andrews University in 1948. Since then he has been a member of CSIRO in Australia where he is a Chief Research Scientist at the Division of Chemical Physics. This Division was incorporated into the Division of Materials Science and Technology at the end of 1986.

The presentation of the Ewald Prize, which consists of a medal and a certificate for each awardee and a shared award of US \$20 000, will take place at the Opening Ceremony of the XIV International Congress of Crystallography at Perth, Western Australia, on 12 August 1987. An honorary medal will also be presented to the Ewald family during the ceremony.

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.

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Radix Databox 8K

Radix Instruments announces an upgraded version of its Databox automation system for X-ray diffraction: the **Databox 8K**. This new unit features over 8000 channels of data memory and expanded control capabilities, including a sample changer option.

The Databox, an intelligent stepper-motor-controller integrated with a timer/scaler and data memory, fits in a two-wide NIM module, and is capable of automating both X-ray diffractometers and scanning spectrometers. The user programs the Databox via an RS232 port using a simple and self-documenting command language.

For only US \$4000, the Databox is an extremely cost effective and easy-to-use solution to X-ray automation needs. The Databox has proven to be an extremely reliable laboratory tool, with many accumulated unit years of trouble-free operation in the field.

Along with the Databox, Radix also now offers **XRD analysis software** from Materials Data, Inc., which runs on any IBM PC or compatible. These two packages, **Micro-ID** and **Micro-Peak**, allow full data reduction and search/match on any JCPDS subfile. Both software packages, when purchased together with the Databox, cost US \$4995, plus the JCPDS subfile license fee. University discounts are available.

Radix Instruments, Inc., 1019 Stratford Avenue, South Pasadena, California 91030, USA

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Polaron Semiconductor Cryostats

Polaron Equipment, a division of Bio-Rad Laboratories, announce a range of liquid nitrogen and helium cryostats suitable for semiconductor materials testing.

The **DL4960 liquid nitrogen cryostat** uses a horizontal continuous-flow liquid