computed and refined bell-shaped curves;

(xi) use of generalized coordinates to generate the structural model and possibility of introducing properly weighted restraints among them;

(xii) the quantity minimized is $\chi^2 = \sum w_i(I_{obs} - I_{calc})^2$ with $w_i$ set equal to (number of counts)$^{-1}$, and the disagreement factor is $R_3 = \chi^2/\sum w_i I_{obs}^2$; but another disagreement factor is also computed as $R'_3 = \chi^2/\sum w_i(I_{obs} - BKG)^2$ since, in the case of polymers, the background contribution from the amorphous phase is usually relevant and keeps $R_3$ unrealistically low;

(xiii) plot on the screen and, optionally, on a laser writer of both the structural model and of the results of the refinement in the form of observed + calculated profiles, background contribution and difference profile.

**Hardware environment:** The program was developed on an IBM PC/AT compatible with 80486/66 MHz microprocessor, mathematical coprocessor and at least 4 Mbytes of memory.

**Documentation and availability:** A zipped file DEBVIN.ZIP, with the executable version of *DEBVIN*, the instruction notes written with WORD 6.0 and stored as a PostScript file and a number of examples of input data, is available by anonymous FTP from ftp.cc.uniud.it in the directory DEBVIN. Further information is available by e-mail from sergio.bruckner@dstc.uniud.it.

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**Keywords:** Rietveld refinement, generalized coordinates

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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 Co-editors, should be sent to The Executive Secretary, 2 Abbey Square, Chester CH1 2HU, England.*

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### Gordon Cox 1906–1996

Sir Ernest Gordon Cox FRS died on 23 June 1996 at the age of 90. His career as a practising crystallographer lasted from 1927, when he joined Sir William Bragg's group at the Royal Institution, to 1960, when he left the University of Leeds to become Secretary of the UK Agricultural Research Council.

Cox graduated in physics at Bristol University. At the Royal Institution, Sir William Bragg suggested as his main task the crystalline structure of benzene. Even at 273 K the vapour pressure of benzene is very high. A special rotation camera, with a double-walled cylinder through which the cooling liquid was circulated, was constructed by C. J. Jenkinson the laboratory mechanic. X-ray measurements were made at 251 K. Cox showed that the evidence strongly favoured a flat-ring molecule with C–C about 1.42 Å.

In 1929 he was recruited by W. N. Haworth, the carbohydrate chemist, to the staff of the Chemistry Department of Birmingham University. Here he did pioneer work on the structures of sugars and coordination compounds of nickel, palladium, platinum and other metals. A highlight was the determination of the crystal structure of vitamin C, ascorbic acid, where his X-ray work was done in concert with the chemists. (Haworth received the Nobel Prize in 1937 for his investigations on carbohydrates and vitamin C.) Cox became increasingly interested in the determination of accurate structures from three-dimensional data. Pentaerythritol (1937) was followed by glucosamine hydrobromide (1939).

After scientific and military service in the Second World War, he was appointed in 1945 as one of the Professors of Chemistry at Leeds. There he built a very happy Department of Inorganic and Structural Chemistry and a strong all-round group in chemical crystallography. Based on his Birmingham experience, Cox was keenly aware that good results in chemical crystallography were dependent on developments in apparatus and computing. In the first years in Leeds, he took a particular interest in the design and production of a Weissenberg camera and in the use of Hollerith punched-card equipment. He was very quickly aware of the potentialities of electronic computers, and despatched one of his team to the first programming school at Cambridge in 1950, and thereafter to exploit the Ferranti Mark I machine in Manchester from 1952 onwards. The benzene story was completed by placing the crystallographer as well as the crystal inside a cold room. It led to the discovery of the librational correction to atomic positions (1955).

A stream of high-grade structure determinations flowed from his team, often setting standards for others to follow. Many analyses concerned relatively simple molecules, such as heterocyclic sulfur compounds, with the object of establishing reliable values for standard bonds. The work on stereochemistry of coordination compounds was considerably broadened, *e.g.* to include new organic compounds of platinum. Low-temperature work was extended down to 34 K. Cox led the bid for an ICL Pegasus computer for the University of Leeds. When it was installed in 1957, his crystallographers were immediately the largest users.

His administrative skills and good sense drew him increasingly into the general running of the university and onto outside committees. He was a member of the IUCr Commission on Crystallographic Apparatus from 1948–1957 and of the Commission on Crystallographic Data from 1954–1960. He was Chairman of the X-ray Analysis Group, the main precursor of the British Crystallographic Association, from 1956 to 1959.

He was a member of the national Agricultural Research Council from 1957–1960. This led to his departure from Leeds in 1960, when he was appointed Secretary (*i.e.* chief executive) of the ARC. He retired from this post in 1971. An especially moving tribute to his work there was paid by the politician Tam Dalyell MP in *The Independent* newspaper of 8 July 1996 – 'Never was there a more impressive, energetic advocate of the value to society of long-term serious scientific inquiry'.

DURWARD CRUICKSHANK

**Professor M. Vijayan**, Professor in the Molecular Biophysics Unit and Chairman of the Division of Biological Sciences, Indian Institute of Science, Bangalore, was presented with the Federation of Indian Chambers of Commerce and Industries (FICCI) Award on 10 December 1996, at a function in New Delhi, by the Prime Minister of India, for his outstanding contributions to biological crystallography. Professor Vijayan has served on the IUCr Commissions on Small Molecules and Biological Macromolecules, and

was the Chairman of the latter during 1993–1996. He is currently a member of the IUCr Subcommittee on the Union Calendar and a Co-editor of *Acta Crystallographica.*

## Notes and News

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On the occasion of fifty years of synchrotron radiation, the **European Synchrotron Radiation Society** (ESRS) is pleased to announce a prize to be awarded for an outstanding contribution to synchrotron radiation science. The prize of 1500 ecu will be presented at the International Conference on *Highlights in Synchrotron Radiation Research* organized by the European Synchrotron Radiation Facility and co-sponsored by the ESRS in Grenoble, 17–20 November 1997. It will be given to a person aged 35 years or younger (at the closing date) for work that has been undertaken in Europe after December 1994.

Applicants should send a summary of not more than 2000 words outlining the nature of the research, its significance and their contribution to it, together with any relevant reprints and the names of two referees, to Professor C. Norris, Department of Physics and Astronomy, The University of Leicester, LE1 7RH, UK [fax: +44 (0)116 252 2770; e-mail: ar9@le.ac.uk; WWW: http://fy.chalmers.se/esrs]. Closing date for submission: 1 August 1997.

## International Union of Crystallography

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### New *Software Reviews* section

A new *Software Reviews* section has been launched in the *Journal of Applied Crystallography*, to review some of the commercial and noncommercial software that is available to crystallographers. These reviews will take the form of helpful guides to the selection of software. Peter White, Director of the X-ray Facility at the University of North Carolina at Chapel Hill, has been appointed Software-Review Editor. Authors of software useful to crystallographers are invited to submit copies for review to P. S. White, Department of Chemistry, CB#3290 Venable Hall, University of North Carolina, Chapel Hill, NC 27599-3290, USA. Authors of software presented in all IUCr journals will be invited to submit copies for review.

### Software lists on the World Wide Web

Lists of software recently presented and/or reviewed in the *Journal of Applied Crystallography* are now available on the World Wide Web at the address http://www.iucr.ac.uk/journals/jac/software/, together with information about the availability of the software where this is known.

## 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, Dr A. M. Glazer, Editor Journal of Applied Crystallography, Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, England.*

*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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### American Ceramics Society *ceramicSOURCE 1997*

The American Ceramic Society (ACerS) has published ***ceramicSOURCE* 1997**, the Annual Company Directory and Buyer's Guide for the ceramics marketplace. From traditional to advanced ceramic applications, the *ceramicSOURCE* features listings of more than 2000 suppliers to ceramic manufacturers of products and components. Listings are cross-referenced geographically, alphabetically and by product offerings. The North American list price is US$ 45 and the international list price is US$ 65.

ACerS is an international association of scientists, engineers and industrialists who are active in the creation of new products, applications and research regarding ceramics and related materials. ACerS serves more than 12 000 members and subscribers in 80 countries with periodicals and books, meetings and expositions, continuing education courses and online technical information.

*The American Ceramic Society, Customer Service Department, PO Box 6136, Westerville, Ohio 43086–6136 (e-mail: customersrvc@acers.org; WWW: http://www.acers.org).*

## Books Received

*The following books have 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.*

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**Structural electron crystallography.** By DOUGLAS DORSET. Pp. xiii + 452. New York: Plenum Publishing Co., 1995. Price US$ 69.50. ISBN 0-306-45049-6. A review of this book, by Peter Goodman, has been published in the January 1997 issue of *Acta Crystallographica Section A*, page 102.

**Symmetry in chaos.** By M. FIELD and M. GOLUBITSKY. Pp. 230. Oxford University Press, 1996. Price £15.00 (Paper). ISBN 0-19-853688-7. A review of this book, by W. D. Whitehead, has been published in the March 1997 issue of *Acta Crystallographica Section A*, page 251.

**Metallomesogens – synthesis, properties and applications.** Edited by J. L. SERRANO. Pp. xix + 498. Weinheim: VCH Verlagsgesellschaft, 1996. Price DM 298. ISBN 3-527-29296-9. A review of this book, by Peter Maitlis, has been published in the April 1997 issue of *Acta Crystallographica Section B*, pages 323–324.

**Ordering and phase transitions in charged colloids.** Edited by A. K. ARORA and B. V. R. TATA. Pp. xi + 361. Weinheim: VCH Verlagsgesellschaft, mbH, 1996. Price DM 185.00. ISBN 1-56081-917-0. Colloidal dispersions have many interesting properties that 'almost mimic all the phases of condensed matter'. This volume covers a wide range of experimental and theoretical investigations into the title topic. Experimental techniques discussed include video microscopy, optical Bragg and Kossel diffraction, light scattering and ultra-small-angle X-ray scattering. Theoretical tools discussed include density-function theory, computer simulations and inversion methods. Both the 'repulsive' and the 'attractive–repulsive' schools of thought are represented.