computed and refined bell-shaped curves;
(x) use of generalized coordinates to
generate the structural model and pos-
cibility of introducing properly weighted
curves;
(xii) the quantity minimized is \( \sum w_i (|I_{obs} - |I_{calc}|)^2 \) with \( w_i \) set equal to
(number of counts) \(^{-1} \), and the disagree-
ment factor is \( R_3 = \sqrt{\sum w_i (I_{obs} - I_{calc})^2} \); but
another disagreement factor is also com-
cuted as \( R_3 = \sqrt{\sum w_i (|I_{obs} - BKG|)^2} \) since,
in the case of polymers, the back-
ground contribution from the amorphous
phase is usually relevant and keeps \( R_3 \)
unrealistically low;
(xiii) plot on the screen and, op-
tionally, on a laser writer of both
the structural model and of the re-
sults 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 mi-
croprocessor, mathematical coprocessor
and at least 4 Mbytes of mem-
ory.

Documentation and availability: A zipped file DEBVIN.ZIP, with the ex-
cutable version of DEBVIN, the in-
struction 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@dsc.uniud.it.

The authors thank Professor A. Sironi
and Dr N. Masciocchi for helpful dis-
cussions.

Keywords: Rietveld refinement, gener-
alized coordinates

References
Brückner, S. (1988). Chim. Ind. 70,
48–53.
Iannelli, P. & Immirzi, A. (1988). Macrom-
olecules, 21, 768–773.
Iannelli, P. & Immirzi, A. (1989). Macrom-
olecules, 22, 196–200.
Iannelli, P. & Immirzi, A. (1989). Macrom-
olecules, 22, 200–205.
2378–2385.
Meille, S. V., Brückner, S. & Lando, J. B.
Millini, R., Perego, G. & Brückner, S.
239–244.
Perego, G., Cesari, M. & Allegra, G.
Trifoggi, M., De Rosa, C., Aur Emma,
Macromolecules, 27, 3553–3559.

Crystallographers

This section is intended to be a series of short para-
graphs dealing with the activities of crystallographers,
such as their changes of position, promotions, as-
sumption 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.


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
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 in-
terested 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 crys-
tallography. 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
Hollenth 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 stereo-
chemistry 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 transferred to it.

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
Tan Dalley MP in The Independent
ewspaper 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 contri-
butions 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


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


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 in 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.


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 ceramic-SOURCE 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 12000 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: customerserv@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.


