



# CRYSTALLOGRAPHY NEWS

BRITISH CRYSTALLOGRAPHIC ASSOCIATION

No. 5

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## BCA NEWS

The 1983 Spring Meeting at Royal Holloway College showed that the level and quality of the Durham Inaugural Meeting could be sustained. Some 180 people attended, and took part in a varied and interesting programme, of which Dr Klug's plenary lecture was one of the highlights. What is more, the meeting produced a small financial surplus. We particularly thank the chief organiser, Dr Moreton Moore, for his hard work in ensuring the success of the first Spring Meeting organised by the BCA.

One event associated with the meeting was a special lecture for young children from neighbouring schools, which was given by our Treasurer. ( Although it was not meant for the more mature participants, some of us tried to look small, and spent an enjoyable hour listening! ). This involvement of youngsters in the Spring Meeting is something we hope will remain a feature of subsequent meetings.

The 1983 Spring Meeting also saw the retirement of Professor Dorothy Hodgkin as Vice-President of the BCA. We are indebted to her for her support in the crucial period both before and after the foundation of the BCA. Professor Hodgkin, however, still retains a close link as one of the Trustees of the Association.

After the various elections held at the Spring Meeting, and the creation of two new Groups, the composition of the Council is as follows:

President	Professor Sir David Phillips FRS
Vice-President	Professor D.W.J Cruickshank FRS
Secretary	Dr A.C. Skapski
Treasurer	Professor C.A. Taylor
Ordinary members	Mr J.W. Harding
	Dr Olga Kennard
	Professor J. Zussman
Group	Dr Ruth H. Fenn (Physical Crystallography Group)
representatives	( from October 1983 - Dr Joan C. Halfpenny )
	Dr R.W.H. Small (Chemical Crystallography Group)
	Dr R. Diamond (Biological Structure Group)
	Dr B.J. Isherwood (Industrial Group)
Co-opted members	Dr A.M. Moore (Editor of Crystallography News)
	Dr S.C. Wallwork
	Professor A.J.C. Wilson FRS
ex-officio	Professor D.M. Blow FRS (Chairman of BNCC)

As is customary, autumn will see individual Group meetings, including the first independent meetings organised by the two new Groups. Meanwhile, preparations for the 1984 Spring Meeting in Nottingham have started in earnest. The organising committee,



led by Dr Michael Begley, has had its first meeting and there is now a tentative programme.

As regards 1985, although the dates have not yet been finalised, the Spring Meeting will be held in Bristol.

On the radiation safety front, we live in interesting times. Hardly had the President sent off the BCA response to the HSE Consultative Document "The Ionising Radiations Regulations 198-", when I received a new Consultative Document. This has been passed to our Radiation Safety Committee for consideration. It is entitled "Draft guidance notes for the protection of persons exposed to ionising radiations in research and teaching", and is issued jointly by the Health & Safety Executive and the National Radiological Protection Board. Although a BCA response will be prepared, individuals or groups should feel free to submit their comments directly to the NRPB, if they so wish. The document is published by the HMSO, price £6-00 ( ISBN 0 11 883470 3 ), and the NRPB deadline for comments is 1st September, 1983.

Finally, the Association joins in congratulating Professor J.M. Robertson on the award of the Aminoff Gold Medal and Prize of the Royal Swedish Academy of Sciences. Fuller details are given elsewhere in this issue.

Andrzej Skapski



BCA LOGO

I hope you will have noticed our brand new logo on the front cover. The design is based on a primitive Bravais lattice, which is something fundamental to all areas of crystallography, and was adopted as the official BCA Logo at the Council meeting held on 31st March, 1983.

By the end of the Logo Competition at the Spring Meeting, I had 30 entries (one arrived on the first day of the meeting from Teheran!). My thanks to all those who sent in their designs.

The logos were on display throughout the meeting, and judging was entrusted to our President. He in turn convened an ad hoc panel of 6 members, representing different areas of crystallography, to help resolve this weighty matter.

There were two similar designs which were particularly liked, and the decision of the panel was that the BCA Logo should lie somewhere between these two entries, and that the bottle of Lagavulin should go to our Editor, Moreton Moore. It was with great pleasure that I was able to present Moreton with his prize at the Conference Dinner.

Andrzej Skapski



## DONATIONS TO THE BCA

The following generous donation from Industry is gratefully acknowledged.

Ilford Pension Trust Ltd      £250

This fifth list records donations received in the period March - May 1983.

## CRYSTALLOGRAPHERS IN THE NEWS

Professor Dorothy Hodgkin, OM, FRS was awarded the 1982 Lomonosov Gold Medal of the USSR Academy of Sciences and visited the USSR in March to receive it.

Professor J Monteath Robertson, CBE, FRS has been awarded the 1983 Aminoff Medal of the Royal Swedish Academy of Sciences in recognition of his achievements in developing chemical crystallography as a general and most powerful method of elucidating the structures of organic molecules. Gregori Aminoff (1883-1947) was, from 1923, Professor of Mineralogy at the Museum of Natural History, Stockholm and was a pioneer in applying crystal diffraction of X-rays and electrons to minerals and other inorganic substances. The presentation will be made in Stockholm on 1st June. Previous recipients were P P Ewald (1979), Sir Charles Frank (1981) and Gunnar Hägg (1982).

Our congratulations go to all those elected Fellows of the Royal Society, including Professor Sivaramakrishna Chandrasekhar (Liquid Crystals Laboratory, Raman Research Unit, Bangalore, India) and Dr Richard Henderson (MRC Laboratory of Molecular Biology, Cambridge).

## PROFESSOR A J C WILSON

Professor Arthur Wilson retired on 30 September 1982 after 17 years as Professor of Crystallography in the Department of Physics at Birmingham.

Arthur Wilson was born on 28 November 1914 in Springhill, Nova Scotia, and was educated at King's Collegiate School, Windsor Nova Scotia (1922/30) and at Dalhousie University, Halifax (1930/36). It was here that he started his academic career and in 1936 he was awarded the degree of MSc for his study, under the direction of Professor Howard Bronson, of the heat capacity of Ag, Ni, Zn, Cd and Pb as a function of temperature. He then joined Professor Hans Mueller's group at the Massachusetts Institute of Technology, where he proceeded to a PhD in 1938 with a thesis on the anomalous thermal behaviour of the ferroelectric Rochelle Salt. While at MIT he was awarded an 1851 Exhibition and a year later, in 1938, he went to St John's College and the Cavendish Laboratory, Cambridge. This was the year in which Sir Lawrence Bragg succeeded Lord Rutherford as the Cavendish Professor of Experimental Physics.



During the remaining two years of his scholarship, Arthur Wilson made accurate measurements of the thermal expansion of Al and Pb (the same samples as had been used for the heat-capacity measurements), which led to the award of a second PhD in 1942. It was through this work at the Cavendish Laboratory, and the influence of Bragg and Henry Lipson, that he acquired a life-long interest in the no-man's land of X-ray Crystallography.

Initially his contribution to crystallography was mainly confined to three aspects of the subject. His work on thermal expansion involved the measurement of precise lattice parameters which led naturally to a general investigation of experimental and other contributions to the position, shape and intensity of X-ray diffraction lines. He also became interested in crystal imperfections through a study of stacking faults in Co (1941/2) and the alloy  $\text{Cu}_3\text{Au}$  (1943), whence followed a continuing interest in small, distorted or otherwise imperfect crystals. His book "X-ray Optics" (1949, second edition 1962) has been the starting point for much subsequent research in this field and it is still a definitive work on the subject. These two aspects relate to the study of polycrystalline samples, but the third and perhaps most significant contribution was to the determination of structures from single-crystal data. In 1942, together with Henry Lipson, he was asked to comment on a letter submitted to *Nature* in which Professor YU of China claimed that absolute intensities of X-ray diffraction peaks could be derived from relative ones. Arthur Wilson devised a simple procedure based on statistical ideas, applied it to copper sulphate and the alums, and published the work alongside YU's contribution. The practical importance of the method was not realised for several years, but the 1942 note in *Nature* eventually became one of the most frequently cited papers on any aspect of crystallography, or indeed on chemical topics generally.

He left Cambridge in 1945 and went to the Department of Physics at University College, Cardiff, as a lecturer. In 1946 he became a senior lecturer and in 1954 was appointed Professor of Physics and Director of the Viriamu Jones Laboratory, a post he held until 1965. At Cardiff he founded a school of organic crystal chemistry which rapidly achieved worldwide recognition for its work on alkaloids such as ephedrine to harmine, on a number of terpenoids such as longifolene, and on amino-acid derivatives. Dr D Rogers, later Professor of Chemical Crystallography at Imperial College, London, was associated with the structural work and former research students from this period who subsequently established crystallographic laboratories elsewhere include Professor Sir David Phillips, FRS, of the Department of Zoology at Oxford, Professor Eric Stanley of the Department of Physics at the University of New Brunswick, and Professor Sukeaki Hosoya of the Institute for Solid State Physics at the University of Tokyo. In the late 1940s Arthur Wilson revived his interest in the statistical use of diffraction data and showed how the symmetry elements of a structure can be deduced from the observed intensities (1949). These elements include a centre of symmetry, which had previously been thought impossible to detect by X-ray methods. Sir Lawrence Bragg said of this discovery "Like all brilliantly original ideas, it seems so obvious when pointed out!"



The availability of commercial powder diffractometers about 1950 resulted in a dramatic improvement in the quality of powder data, and a second group was formed at Cardiff to exploit the new device. On the instrumental side, Dr E R Pike, FRS, now at R.S.R.E. Malvern and then a research student in the group, designed and built the first fully automatic powder diffraction system in the late 1950s. Improved data led to the introduction of the centroid (1959) and variance (1962) as accurate measures of the position and breadth of a diffraction line. The former, studied by E R Pike and B W Delf, meant that lattice parameters could be determined with far greater precision and the latter, developed by J I Langford, became a powerful technique for studying crystallite size and shape, microstrain, structural 'mistakes' and other imperfections. Development of this use of line-profile moments has continued to the present day in a number of laboratories throughout the world, including that of Professor G B Mitra of the Indian Institute of Technology, Kharagpur, who worked at Cardiff in the late 1950s. The early work in this field was published in 'Mathematical Theory of X-ray Powder Diffractometry' in 1963, with translations into French (1964) and German (1965). Together with H S Peiser and H P Pooksby, Arthur Wilson was also editor of 'X-ray Diffraction by Polycrystalline Materials' (1955, revised 1960) and lecture courses he gave at Cardiff formed the basis of 'Elements of X-ray Crystallography' (1970). The powder group at Cardiff also collected and edited accurate diffraction data for inclusion in the powder data file of the American Society for Testing & Materials\* until 1975.

In addition to pursuing the three lines of research engendered at Cambridge, Arthur Wilson acquired an interest in editing and in the general field of presenting and disseminating scientific information. In 1948 he became the first editor of *Structure Reports*, published by the International Union of Crystallography. *Structure Reports* succeeded *Strukturbericht*, which had been discontinued at the outbreak of World War II and, in addition to dealing with current volumes, he had the onerous task of editing a backlog of data covering the years 1940 to 1947. This work, which continued until 1960, initiated an active involvement in the affairs of the IUCr which has continued to the present day. Since about 1951 he has also been a member of the Abstracting Board of the International Council of Scientific Unions, either as an observer or an IUCr representative or Vice-President. From 1960 to 1977 he edited *Acta Crystallographica* and was Chairman of the IUCr's Commission on Journals. In 1963 he was elected a Fellow of the Royal Society in recognition of his substantial contribution to most branches of X-ray crystallography, and he is currently an associate editor of the Society's *Proceedings and Transactions*.

At the instigation of Professor Philip Moon, FRS, he was appointed to the newly-created Chair of Crystallography at the University of Birmingham in 1964 and he joined the Physics Department in 1965. At Birmingham he continued to pursue his former research interests and editorial activities, and few aspects of crystallography, single-crystal or powder-methods, have not been covered in the 300 or so papers, articles, etc. he has published to date. During his years at Birmingham he was Visiting

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\* The file has since been taken over by JCPDS-International Centre for Diffraction Data.



Professor at the Georgia Institute of Technology, USA (1965, 1968 and 1971) and at the University of Tokyo (1972) and was a co-author of 'X-Ray Diffraction' (1974). He has been a member of the Executive Council of the IUCr and was its Vice-President from 1978 to 1981. Recently he has been involved in the formation of the British Crystallographic Association and became a founder member at the inaugural meeting at the University of Durham in 1982.

On 17 November 1982 Arthur Wilson was made Emeritus Professor of the University of Birmingham and he has now returned to Cambridge where he will continue the editing of the revised *International Tables for Crystallography* at the Crystallographic Data Centre of the University Chemical Laboratory.

J Ian Langford

January 1983

TREVOR JOHN KING: 1921 - 1983

During the period in which Trevor King's research was centred on crystallography, he became very well known in the field, both nationally and internationally. There will be many, therefore, who will be saddened by his untimely death on 12th April, 1983.

After some 22 years of pure organic research, Trevor realised in about 1965 that crystallography provided not only the most unambiguous, but also the most rapid, method of discovering the chemical structure of any new organic material. He therefore set about learning crystallographic techniques by carrying out one or two crystal structure determinations under the direction of his colleague, Stephen Wallwork. In his characteristically brilliant way, he picked up the techniques very rapidly and was soon using them independently with considerable success. In 1968, the Nottingham Chemistry Department acquired its first complete package of crystallographic programs but Stephen Wallwork's new Institute of Physics Crystallography Group commitment prevented him from undertaking the implementation of the programs on the Nottingham computer. Trevor King, therefore, took on the job with no previous knowledge of computing. He not only quickly succeeded in this task, but immediately wrote some necessary ancillary programs. He rapidly became the Chemistry Department's acknowledged computer expert and continued as such until his death.

This intellectual feat of transition from the heights of non-mathematical organic chemistry to the theoretical complexities of crystallography and computing no doubt contributed to his recognition by the University in appointing him to a personal Chair of Chemistry in 1973. He went on from strength to strength, attending the first Summer School on Direct Methods in Crystallography in Parma in 1970 and applying his newly-gained knowledge with considerable success from then



on. Soon, organic chemists from all over the world were sending him crystals in order to solve their intractable chemical problems. Trevor had always loved wrestling with problems and helping other people to solve them, so he accepted these tasks willingly. This inquisitive and generous attitude also meant that he spent a high proportion of his time helping colleagues, research students and undergraduates with their own crystallographic and computing problems.

In spite of making himself so readily available, Trevor managed to do a tremendous amount of personal research. (He very rarely had any research students). He believed in keeping the diffractometer working full-time and would not hesitate to return to the Department in the small hours of the morning to reset the apparatus for a new batch of measurements. His urge towards efficiency, and his curiosity to know just how quickly structural information could be acquired crystallographically led him to keep breaking his own speed record until, as the ultimate, he once reduced the time from mounting the crystal to obtaining a refined complex structure to 48 hours. In this connection, he was a great advocate of the idea of matching the accuracy of a structure determination to the nature of the information required from the results (high accuracy for determination of absolute configuration or accurate molecular geometry but low accuracy if only the nature of the molecule and its qualitative stereochemistry are required).

In recent years, Trevor's other special gifts of great wisdom and skilful diplomacy were more fully recognised by the University when it appointed him simultaneously a Pro-Vice-Chancellor and Head of the Chemistry Department in 1978. It was towards the end of his period in these two offices that he lost his voice and had to chair meetings in a whisper. For this reason, he resigned from the post of Vice-Chairman of the Chemical Crystallography Group. It led to an operation in July 1982 and he had largely perfected the art of speaking with another part of his throat when he had to have a second operation in April 1983, which, unfortunately, could not prevent his death. His courage in coping with these speech problems and in continuing with his teaching and research until a few days before his death was entirely in keeping with his personality and is an inspiration to everyone associated with him. His passing is a great loss to his family and friends, to the University of Nottingham, and to British Science in general.

The University of Nottingham and Trevor's family are hoping to establish a prize and a medal in his memory, for distinguished laboratory work by final-year undergraduate students. Anyone wishing to contribute to the endowment of this prize is invited to write to Mr. P.W. Lemeunier, Department of Chemistry, University of Nottingham, Nottingham NG7 2RD.

S.C. Wallwork.



## British Crystallographic Association Meeting

The British Crystallographic Association held their Spring Meeting at the Royal Holloway College of the University of London, 28-31 March 1983. Besides being a successful meeting in which groups of diverse scientific interests were brought together in worthwhile symposia, it was also an historic one marking the realization of the purposes for forming the British Crystallographic Association at a meeting at the University of Durham in April of 1982. There formerly had been two groups, a Crystallography Group associated with the Institute of Physics and a Chemical Crystallography Group associated with the Royal Society of Chemistry. These groups have come together to form the British Crystallographic Association and at the same time have retained their respective associations with the Institute of Physics and the Royal Society of Chemistry.

The meeting consisted of symposia on Biological Structures, Physical Crystallography, Industrial Crystallography and Chemical Crystallography. In the symposium on biological structures organized by R. Diamond, the topics were sources and instrumentation (U. W. Arndt), heavy atom location and phasing (D. M. Blow), interpretation and refinement (D. S. Moss), crystallographic contributions to understanding enzymes (D. Phillips), crystallographic contributions to understanding nucleic acids (D. Kennard) and crystallographic contributions to understanding viruses (A.C. Bloomer). In the symposium on physical crystallography organized by J. Helliwell, the topics were x-ray anomalous dispersion (M. Hart), x-ray absorption near edge structure (P. Durham), direct methods and anomalous dispersion (J. Karle), use of spallation neutron sources (C. Windsor), molecular



dynamics in framework silicates (M. Dempsey) and topography (K. Bowen). In the symposium on industrial crystallography organized by G. Smith, the topics were single crystal castings (C. Baxter), topography of semiconductor crystals (M. Lyons with M. Helliwell), strain measurement and dopants in semiconductors (P. Fewster), crystallography of Bragg cells (B. Isherwood), portland cement (W. Guttridge), powder diffractometry used to determine polymer morphology (P. B. McAllister with T. J. Carter), catalysts (D. G. Puxley) and powder diffractometry in forensic science (D. Rendle). In the symposium on chemical crystallography organized by M. B. Hursthouse, which concerned practices and problems of crystal structure determination, the topics were data collection procedures (W. Clegg), problems in direct methods (C. J. Gilmore) and techniques in structure determination and refinement (G. M. Sheldrick) followed by a panel discussion in which the organizer and speaker were joined by M. G. B. Drew and D. J. Watkin.

Along with the symposia were very fine poster sessions at noncompeting times on similar topics. The posters were displayed in a huge art gallery surrounded by beautiful Victorian paintings.

Among the highlights of the meeting were a plenary lecture on Structural Analysis of Macromolecular Assemblies by Aaron Klug, the most recent Nobel Laureate in Chemistry, and an organ recital in the ornate Chapel. In addition to those already named, there were many distinguished members of the British crystallographic community present and it was a great pleasure for me to meet old friends once again and renew old acquaintances.

The Royal Holloway College is a very fine facility for holding meetings. It is a very large, comfortable, picturesque and well-preserved example of



Victorian architecture. All the requirements of lodging, meeting rooms, and places for socializing are in one place, affording the conveniences that are missing when lodging and meeting place are at large distances apart. The organizer, A. Moreton Moore, did a first-rate job in effecting a memorable meeting.

J. KARLE

President of the International  
Union of Crystallography

8.

AUTUMN MEETING OF THE BIOLOGICAL STRUCTURE GROUP  
OF THE BRITISH CRYSTALLOGRAPHIC ASSOCIATION

on "Structural studies of crystalline and  
non-crystalline biological materials"

To be held at the Medical School  
University of Manchester on Thursday 22nd September 1983  
from 9.30 a.m. - 5.30 p.m.

Submitted contributions are requested on all aspects of Biological Structure Studies, including both methods and results.

There will be two invited lectures of 50 minute duration. Also, twelve 15 minute oral contributions will be selected from submitted abstracts. There will be a lunchtime poster session from 12.30 - 2.30 p.m.

Deadline for submission of abstracts is 1 July 1983 and these should be sent to one of the organisers: Dr D.W.L Hukins, Department of Medical Biophysics, University of Manchester, Manchester M13 9PT or Dr. J.R. Helliwell, SERC, Daresbury Laboratory, Daresbury, Warrington WA4 4AD from whom further particulars and registration forms can be obtained.

Accommodation for the night of 21st September will be available. Deadline for registration for participants requiring accommodation is 18th August, otherwise the deadline is 16th September (registration forms to D.W.L Hukins).



9.

## Chemical Crystallography Group

### Autumn Meeting 1983

The programme for this meeting, to be held at University College Swansea, during the RSC Autumn Meeting, is given below.

Titles for contributions to the Poster Session, on any area of Chemical Crystallography, should be sent to Dr. R.W.H. Small, Chemistry Department, The University, Lancaster, LA1 4YA, before 31 August 1983.

Full details of the RSC Autumn Meeting (for which part attendance is possible) may be obtained from Dr. John F. Gibson, The Royal Society of Chemistry, Burlington House, London W1V 0BN.

### Programme

Wednesday 21 September 14.30 - 17.00

General Poster Session

Thursday 22 September 9.00 - 13.00

### Chemical Processes in the Solid State

The Control and Design of Reactions within Organic Solids.  
Dr. W. Jones, University of Cambridge.

Computer Simulation and Neutron Diffraction Studies of Complex and Disordered Crystals.  
Dr. C.R.A. Catlow, University College, London.

Organic-Inorganic Molecular Composites. Physical Properties and Chemical Reactions.  
Dr. P. Day, University of Oxford.

X-ray Topographic Studies of Substructural Changes During the Initiation and Progress of Chemical Reactions in Crystalline Solids.

H.L. Bhat, M. Dudley, K. Gillespie, D.B. Sheen and J.N. Sherwood, University of Strathclyde.

The Low Temperature Crystal Structure of  $[\text{NH}_4]_2[\text{Cu}(\text{OH})_2]_2[\text{SO}_4]_2$  by X-Ray Diffraction and  $[\text{ND}_4]_2[\text{Cu}(\text{OD})_2]_2[\text{SO}_4]_2$  by Neutron Diffraction - A Fluxional  $\text{CuO}_6$  Chromophore.

N.W. Alcock, University of Warwick.

A. Hewat, Institute Max von Laue-Paul Langevin.

Mary Duggan, Angela Murphy, Suresh Tyagi and

B.J. Mathaway, University College Cork.



Chairman's Comments

"The Industrial Group of the BCA is now legitimate"

A Inaugural AGM

The AGM of the embryonic Group was held on March 30 during the Spring Conference of the BCA at Royal Holloway College. Approximately 50-60 people attended, an impressive number for an AGM. The principal items of business were:

(i) Adoption of the "Constitution and Rules" of the Group: The draft Rules were presented and, after some discussion, adopted by the meeting for submission to Council. They were subsequently approved by the Council of the BCA on March 31. Those wishing copies should contact either Ian Langford or myself.

(ii) Committee Elections: The following were elected unopposed to form the Committee:

Chairman	Brian Isherwood
Vice Chairman:	Glen Smith
Secretary/Treasurer:	Ian Langford
Ordinary Members:	Brian Bellamy
	Keith Bowan
	John Harding
	Ed Metcalfe
	Jeff Wilson

(iii) Plans for 1983/84: These are to be decided by the Committee, but it is intended that the Group will participate actively in the 1984 Spring Meeting, Nottingham and hold a one day meeting in the Autumn 1983 (See Notice below).

B Industrial Symposium; March 30th Royal Holloway College

I understand that a review of the Spring Meeting is to appear elsewhere in this Newsletter, so perhaps only brief comments on the Industrial Symposium are warranted here. This also avoids the necessity of making somewhat incestuous and arrogant remarks concerning the success of the Symposium. However, from numerous comments received it is apparent that, for many it was the highlight of the Meeting. Glen Smith and John Harding are to be congratulated for providing such an informative and entertaining day. It must have been gratifying for them to see that it was "standing room only" for the morning verbal session. The choice of Colin Baxter, Rolls-Royce, and of Walter Gutteridge, Cement and Concrete Research Association, as invited speakers to open the single and poly-crystalline sessions was particularly inspired. The Group was also well represented in the afternoon poster session, both in terms of the number and content of the posters. We will do well to maintain this standard.

On behalf of the Group I would like to thank Moreton Moore and his helpers for their calm and efficient organization, which contributed largely to the success of the Spring Meeting

"Come and join us"

Brian Isherwood



Industrial Group of the BCA

Autumn Meeting 1983 - Preliminary Notice

This meeting is to be held on Thursday 10th November 1983  
at the BP Research Centre, Sunbury-on-Thames,  
and will be entitled:

CRYSTALLOGRAPHY IN INDUSTRY

No specific topic has been selected for this first autumn meeting of the Group. Instead, papers are required on any aspect of the use of crystallographic techniques in industrial/technical applications. Please note that such techniques are not specific to X-ray diffraction and papers on electron diffraction and neutron diffraction will also be welcome.

Contributed papers are now invited. Provisional titles along with a short abstract (approximately 50 words) should now be submitted before 31st July 1983. Presentation time will be 15-20 minutes.

These should be sent to:

Mr G. W. Smith  
X-ray Laboratory, Spectroscopy Branch  
BP Research Centre  
Chertsey Road  
Sunbury-on-Thames  
Middlesex  
TW16 7LN

It is hoped that this first meeting of the Industrial Group will be an informal occasion and that the presentations will generate a lot of free discussion.

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The Applications of Synchrotron RadiationOne day Seminar at the BA Meeting - August 24 1983

Organizer - J.R. Helliwell, SERC, Daresbury Laboratory and University of Keele on behalf of the Institute of Physics Physical Crystallography Group.

Synchrotron radiation is finding wide ranging applications as a research tool in physics, chemistry and biology and increasingly in industry. Techniques such as X-ray and UV spectroscopy, microscopy, crystallography, topography, surface science and infrared studies benefit enormously from this bright, tunable light source. The seminar aims to cover the most recent results obtained at the U.K. synchrotron radiation source (SRS) at Daresbury Laboratory and to provide a more general background to this broad field of research activity.

The registration fee for the IOP Physical Crystallography Group Seminar is £5 (payable to "IOP"). Accommodation fees are as specified on the registration form (payable to "British Association").

To attend the BA meeting on additional days you need to be a member of the BA, the registration forms must be completed and the fees paid to the "British Association".

Further details from John Helliwell (0782-621111 x307) to whom cheques and forms should be returned.



## The Applications of Synchrotron Radiation (SR)

One day seminar at the BA meeting Brighton, August 24 1983

### TIME TABLE

10.00 - 10.30	Coffee
10.30 - 11.15	Professor M. Hart (Physics Dept., King's College, London). "X-ray optics and anomalous dispersion studies with SR".
11.15 - 12.00	Dr. K. Bowen (Engineering Dept., Warwick). "Topography with SR".
12.00 - 12.45	Dr. P. Duke (SERC, Daresbury) "X-ray microscopy with SR".
12.45 - 13.45	LUNCH
13.45 - 14.30	Dr. N. Greaves (SERC, Daresbury) "EXAFS".
14.30 - 15.15	Dr. G. Thornton (Chemistry Dept., Manchester) "Surface Studies with SR".
15.15 - 16.00	Dr. I. Munro (SERC, Daresbury). "UV spectroscopy and molecular dynamics studies with SR".
16.00 - 16.45	Dr. J.R. Helliwell (Physics Dept., Keele and SERC Daresbury) "The study of protein structures and the use of SR".
16.45 - 17.30	Dr. J. Bords (European Molecular Biology Laboratory, Hamburg). "Time resolved X-ray scattering studies with SR"

Further information and registration forms from:

Dr. John Helliwell, Dept. of Physics, University of Keele, Keele,  
Staffordshire, ST5 5BG. (Tel. no. 0782-621111 x307).



This meeting, sponsored by the Deutsche Forschungsgemeinschaft (DFG) and Freie und Hansestadt Hamburg, will be held 9-18 August 1984 at the Congress Centrum Hamburg, Hamburg, Federal Republic of Germany.

You are cordially invited by the Arbeitsgemeinschaft Kristallographie (AGKr) of the Federal Republic of Germany to attend the XIIIth Congress and General Assembly of the International Union of Crystallography to be held in Hamburg at the Congress Centrum Hamburg (CCH). Registration will begin on Wednesday, 8 August 1984. The sessions will continue until 18 August.

#### Programme

The scientific programme will include invited general lectures, invited oral papers and open Commission meetings. Most contributed papers will be presented in poster sessions. Commercial and non-commercial apparatus will be exhibited and crystallographic data file demonstrations are planned.

#### Subjects

The congress will cover recent advances in all aspects of crystallography. It is anticipated that the following areas will be represented:

##### 1. General Topics

- Anomalous scattering
- Atomic scale mechanisms of physical, chemical or biological properties
- Applied crystallography
- Computing statistics
- Crystal chemistry
- Crystal physics
- Crystal growth and morphology
- Diffraction theory
- Dynamical diffraction
- Education and data retrieval
- Electron density studies
- Electron diffraction and microscopy
- EXAFS and near-edge spectroscopy
- Instrumentation and apparatus
- Lattice dynamics
- Materials research
- Methods of structure determination
- Neutron diffraction
- Phase transitions
- Powder diffraction
- Resonance studies
- Real and ideal crystals
- Small angle scattering
- Synchrotron radiation and applications
- Symmetry and related topics
- Techniques



## 2. Structural Studies

Biological materials (proteins, viruses, membranes, drugs, etc.)

Coordination compounds

Glasses and amorphous materials

Industrial materials

Inorganic and intermetallic compounds

Liquid crystals

Magnetic structures

Minerals

Organic compounds

Organo-metallic compounds

Polymeric materials

Surfaces, interfaces and films

A Workshop on the X-ray Powder-Diffraction File is planned for 8 August 1984.

### Committees

Organizing: Professor H. Saalfeld, Hamburg (Chairman) with the assistance  
the Gesellschaft Deutscher Chemiker

Programme: Professor U. Bonse, Dortmund (Chairman)

### Accommodations

Reservation will be arranged by a special travel agency. A limited number of student dormitories and camping facilities may be available. Detailed information will be given in the second circular.

### Further Information

A second circular with a call for papers, more details of the programme, the general arrangements and registration forms will be distributed in the Autumn of 1983. Those wishing to receive the second circular should write to:

Gesellschaft Deutscher Chemiker  
Abteilung Tagungen Postfach 90 04 90  
D-6000 Frankfurt/Main 90 F.R.G.

### Associated Meetings

1. A Symposium on Neutron Scattering will be held on 6-8 August 1984 at the Hahn-Meitner-Institut, West Berlin. Organization: Prof. W. Saenger, Institut für Kristallographie, Freie Universität Berlin, 1000 Berlin 33, F.R.G. Programme: Dr. M. S. Lehmann, Institut Laue-Langevin, Avenue des Martyrs, BP 156, 38042 Grenoble, France.
2. An International Summer School on Crystallographic Computing is planned for 30 July - 8 August 1984 at the Max-Planck-Institut für Kohlenforschung, Mulheim/Ruhr. Organizing Committee: Prof. H. Burzlaf, Prof. C. Kruger, Prof. G. Sheldrick. For information: Prof. H. Burzlaff, Institut für Institut für Angewandte Physik, Universität Erlangen-Nürnberg, Loewenichstrasse 22, D-8520 Erlangen, F.R.G.



3. A Symposium on Small Angle Scattering and Related Methods will be held on 20-23 August 1984 at DESY, Hamburg. Organization: Prof. H. Stuhrmann, c/o EMBL, DESY, Notkestrasse 85, D-2000 Hamburg 52, F.R.G. (together with Prof. P. W. Schmidt, Columbia, MO, USA).
4. A Symposium on Metals and Intermetallic Compounds is planned for 20-24 August 1984 at the Technische Hochschule Aachen. Information: Prof. W. Bronger, Institut für Anorganische Chemie der Technischen Hochschule Aachen, Templergraben 55, D-5100 Aachen, F.R.G.
5. An International Summer School on Symmetry-Related Crystal Structures: Group-Subgroup Relations is planned for 20-24 August 1984. Location: In the western region of the Federal Republic of Germany. For further information write to Prof. W. E. Klee, Institut für Kristallographie der Universität, Postfach 63 80, D-7500 Karlsruhe, F.R.G.

The Schweizerische Gesellschaft für Kristallographie has announced that it will hold the "Paul Niggli Symposium über geometrische Kristallographie und ihre morphologisch stereochemischen Anwendungen" on 6-7 August 1984 in Zurich. For further information can be obtained from Prof. W. Nowacki, Mineralogisch-Petrographisches Institut der Universität, Balzerstrasse 1, CH-3012 Bern, Switzerland.

For further information on the XIIIth Congress and General Assembly contact:

Gesellschaft Deutscher Chemiker  
Abteilung Tagungen  
Postfach 90 04 90  
D-6000 Frankfurt/Main 90  
Federal Republic of Germany

### 13. INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY VOLUMES B AND C

As the International Tables are of considerable importance to crystallographers, the following Memorandum and tentative Table of Contents, which have been received via the Royal Society, are being published in "Crystallography News".

The Editors of the proposed new volumes are:

#### for Vol. B

Professor U Schmueli  
Department of Chemistry  
Tel Aviv University  
Ramat Aviv  
69 978 TEL AVIV, ISRAEL.

#### for Vol. C

Professor A J C Wilson FRS  
Crystallographic Data Centre  
University Chemical Laboratory  
Lensfield Road  
CAMBRIDGE, CB2 1EW, England

The Editors invite comments on the scope and arrangement of the two volumes. The comments should be sent to the appropriate Editor, with a copy to the other Editor (by airmail), and should be received by the deadline of 30th June, 1983.



## INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY

### Memorandum on Volumes B and C

#### Introduction

The Commission on International Tables began a thorough revision of the existing Volumes I-IV in the early 1970s. By 1981 it had completed a new Volume A on direct space entitled Space-Group Symmetry, which is now in course of publication. Volume A covers in greater detail the content of the first part (approximately pages 6-352) of Volume I. It amounts to about 830 pages, and is thus twice the average size of the existing volumes I-IV, although its content corresponds only to the first part of the first volume.

No Editor was appointed and no Commission was elected at the Twelfth General Assembly held in Ottawa in August 1981, though the previous Chairman of the Commission and his collaborators continued with seeing Volume A through the press. A.J.C. Wilson was invited to attend a meeting of the Executive Committee of the International Union of Crystallography on 27 July 1982, during which future work on the International Tables was discussed. It was confirmed that two further volumes of the revision should be undertaken:

Volume B: Reciprocal Space

Volume C: Mathematical and Physical Tables.

Volume B would contain a revision and expansion of the remaining part of Volume I (pages 353-541), together with new material and a revision and expansion of certain parts of the existing Volumes II-IV that would appear more appropriately under the heading of Reciprocal Space.



Volume C would contain those mathematical and physical parts of Volumes II-IV that are still useful, revised and edited as necessary. With the obsolete and the dubiously useful parts of Volumes II-IV omitted, it is hoped that the number of pages in each of Volumes B and C will not exceed that of Volume A. The Executive Committee invited A.J.C. Wilson to become Chairman of the Commission and Editor of Volume C, and these invitations were accepted. The Chairman invited U. Shmueli to become Editor of Volume B; he has accepted and the Executive Committee has confirmed his appointment.

Since the planning undertaken by the Commission in the 1970s, there has been a considerable development in the power and accessibility of computers. It could, therefore, be argued that there is now no real need for extensive tables that could be generated on demand by computer, and thus most of Volume B and much of Volume C could consist of readily accessible programs or references to programs. There would, of course, be a continuing need for the physical tables of Volume C, and the explanatory parts of the Tables. The Editors do not share this extreme view, and set forth below the assumptions that will guide the choice of material for the two volumes. Comments from the recipients of this memorandum will be welcomed.

It is the intention of the Editors that all sections should have a handbook rather than textbook character, and should include the relevant tabular material. Each chapter will be provided with an introduction that summarizes the relevant concepts and constitutes a link between the chapter and the specialist publications on the topic. Contributors will



be asked to provide full references, both to articles and to available documented computer programs. Inclusion of relevant computing considerations will be encouraged. Realization of the Editors' intentions will depend, of course, on the willing cooperation of those invited to contribute.

#### Volume B: Reciprocal Space

The purpose of Volume B of the International Tables for Crystallography is to present the user with competent and useful accounts of the various aspects of reciprocal space in crystallographic research. The proposed layout of this volume is still tentative, and the main guideline in its conception is the desire to present a broad range of aspects of reciprocal space while maintaining the usefulness for crystallographic studies of the topics covered. A tentative Table of Contents is given on page 9.

The first part of the planned volume, 'General Relationships and Techniques', starts with an introduction to the concepts and mathematical relationships that will be used in the remaining parts of the book. Next, the structure factor, the most important function in the present context, is discussed and is accompanied by the tabular material usually needed in structure-factor calculations. This section is followed by a compendium of techniques for Fourier summations, traditional as well as modern, and their applications to several topics of importance, including new approaches to differential synthesis, general-plane sections, and accurate representation of electron-density contours. This part of Volume B is concluded by a section on symmetry in reciprocal space, which is to be a modern version of the structure-factor tables that appear in



the second part of the present Volume I (1959). It is proposed to enrich these tables with additional information on the phase relationships between symmetry-related reflexions, linearized products of trigonometric structure factors, and other relevant data. The size of these tables will be kept within reasonable bounds by making use of relationships common to several space groups.

The second part of Volume B is devoted to methods of crystal-structure determination that are intimately connected with reciprocal space. This part starts with a survey of statistical properties of the weighted reciprocal lattice, usually referred to as 'intensity statistics', and their applications to the determination of crystal symmetry. Both asymptotic and generalized statistics will be summarized. This chapter is followed by a summary of expressions and procedures employed in direct methods of phase determination, with particular attention to generally available computer programs. The second part is concluded with two chapters that deal with automated applications of Patterson techniques and methods of solution of the phase problem by the use of isomorphous-replacement procedures. The second part of Volume B is thus intended to be of service to scientists interested in single-crystal structure determination.

Part 3 is concerned with applications of reciprocal space as a mathematical device leading to concise representations of relationships that are of importance in the interpretation of the results of a crystal-structure determination. The basic tensor algebra, as introduced in chapter 1.1, is here applied to expressions for interatomic distances,



interbond angles, dihedral angles, and the deviations of atoms from the best plane of a specified group. Another application is concerned with model building, such as the systematic generation of structural fragments with predetermined orientations and locations in a unit cell of given dimensions and symmetry. The last chapter of this part concerns the use of reciprocal space in convergence-acceleration techniques, of importance in various energy calculations that appear in the interpretation of static and dynamic aspects of crystal structures.

The last part of Volume B deals with a range of topics associated with the occurrence of measurable intensity smeared out over appreciable regions of the diffraction pattern. These range from thermal diffuse scattering, which is present in the diffraction pattern of any single crystal; disorder scattering, which likewise manifests itself in the appearance of streaks (sometimes modulated) of diffracted intensity; through patterns that may be due to imperfect crystallinity (e.g. helical polymers); preferred orientation or small size of crystallites (e.g. in metals); to low-dimensional crystals (e.g. nematic or smectic mesophases), which also produce effects that can be interpreted in terms of reciprocal space rather than reciprocal-lattice vectors. This part is concluded with a chapter on the technique of small-angle scattering, which plays an important role in the experimental investigation of the scattering produced by large periodicities or quasi-periodicities.

#### Volume C: Mathematical and Physical Tables

Volume B consists to a great extent of new material, and could thus be planned a priori. Volume C, on the other hand, is conceived as a revision of the existing Volumes II-IV, and presents a different



problem in planning. The existing volumes were produced at intervals of several years, so that there is a certain overlap of content and some inconvenience of arrangement. The inconvenience of arrangement was to some extent determined by an attempt to place material unlikely to require revision (basic theory, mathematical background, mathematical tables) in Volumes I and II, and material subject to change in the light of new experimental results and the development of new techniques in Volume III. It was thus envisaged that Volumes I and II would remain unchanged for many years, whereas new editions of Volume III would appear at frequent intervals. A basic revision of Volume III never, in fact, took place, though some of Volume IV can be regarded as a revision of parts of it.

The material in the existing Volumes II-IV may be roughly classified as:

- a. Tables of elementary functions (sine, cosine, ...).
- b. Tables of simple functions of frequent occurrence (polarization factor, extrapolation functions, ...).
- c. Basic mathematics.
- d. Basic statistics.
- e. Mathematics with specific crystallographic applications.
- f. Statistics with specific crystallographic applications.
- g. Computational techniques.
- h. Experimental techniques.
- i. Tables of physical properties.
- j. Direct methods.
- k. Miscellaneous material.



The treatment of each of these types of material will be discussed in turn.

a,b. Elementary and simple functions

Full tables of elementary functions and of simple combinations of them are not needed by crystallographers in well equipped institutions, as comprehensive packages of crystallographic computer programs would be used as a routine. It is likely that crystallographers would possess or have access to a microcomputer or a programmable pocket calculator, even in badly equipped institutions. It is therefore proposed that the tables of elementary functions be eliminated entirely, and a number of entries (but not the number of significant digits) in the tables of simple functions be reduced by a factor of ten or more. These skeleton tables would have two purposes: to give users an immediate appreciation of the trend of the function, and to give a check that the program entered into a computer or calculator is working properly. The former purpose would be served by a graph or a table with a reduced number of significant digits, but the latter requires adequate precision.

c,d,e,f. Mathematics and Statistics

Volume II contains a long section (95 pages) of fundamental mathematics and statistics. With alterations in university curricula and the appearance of crystallographic textbooks it is doubtful whether such a section is now appropriate material for the International Tables. It is proposed, therefore, that the elementary material (algebra, trigonometry, geometry, calculus) be omitted entirely, and that the more advanced parts be developed as required in the sections dealing with their crystallographic applications. Many of these sections will be in Volume B rather than C.



g,h,i. Computational and Experimental Techniques; Physical Properties

The need for sections on computational techniques, experimental techniques, and physical properties remains as great as ever, but many of the existing sections are obsolescent, and some techniques of current importance are not mentioned at all. Bringing these sections up to date will be an important part of the revision; much of the computational material will now appear in the chapters to which it relates.

j. Direct methods.

Like some of the material discussed in the preceding paragraph, direct methods for phase determination are more appropriately placed in Volume B. Refinement of parameters, however, will remain in Volume C.

k. Miscellaneous material

Some minor tables not readily accessible elsewhere will be retained, and possibly a few new ones will be added.

Proposed content of Volume C

A tentative Table of Contents, prepared in accordance with the above considerations, is given on page 10-12. The proposed treatment of existing sections of Volumes II-IV is given on pages 13-14.

A.J.C. Wilson

U. Shmueli

2 May 1983



## **Tentative Tables of Contents**

### **VOLUME B: RECIPROCAL SPACE**

#### **Part 1. General Relationships and Techniques**

B.1.1 Reciprocal Space in Crystallography

B.1.2 The Structure Factor

B.1.3 Fourier Methods

B.1.4 Symmetry in Reciprocal Space

#### **Part 2. Reciprocal Space in Single-Crystal Structure Determination**

B.2.1 Statistical Properties of the Weighted Reciprocal Lattice

B.2.2 Direct Methods

B.2.3 Patterson Techniques

B.2.4 Isomorphous Replacement

#### **Part 3. Dual Bases in Crystallographic Computing**

B.3.1 Distances, Angles and their Standard Deviations

B.3.2 Best-Plane Calculations

B.3.3 Model Building

B.3.4 Reciprocal-Lattice Summations

#### **Part 4. Diffuse Scattering and Related Topics**

B.4.1 Thermal Diffuse Scattering

B.4.2 Disorder and Diffuse Scattering

B.4.3 Small Crystallite Size and Texture

B.4.4 Strain

B.4.5 Diffraction by Polymers

B.4.6 Scattering from Mesomorphic Structures

B.4.7 Small-Angle Scattering



## VOLUME C: MATHEMATICAL AND PHYSICAL TABLES

Part 1. Crystal Geometry

- C.1.1 Summary of General Formulae
- C.1.2 Application to the Crystal Systems
- C.1.3 Twinning

Part 2. Diffraction Geometry and its Practical Realization

- C.2.1 Classification of Experimental Techniques
- C.2.2 Single-Crystal Techniques
- C.2.3 Powder and Related Techniques
- C.2.4 Energy-Dispersive Techniques
- C.2.5 Small-Angle Techniques

Part 3. Preparation and Examination of Specimens

- C.3.1 Selection of Crystals
- C.3.2 Measurement of Density
- C.3.3 Measurement of Optical Properties
- C.3.4 Measurement of Electrical and Magnetic Properties
- C.3.5 Mounting and Setting of Specimens

Part 4. Production and Properties of Radiations

- C.4.1 Radiations used in Crystallography
- C.4.2 X-rays
  - C.4.2.1 Generation of X-rays
  - C.4.2.2 Wavelengths of Emission Spectra
  - C.4.2.3 Absorption Spectra, EXAFS etc.
  - C.4.2.4 Absorption Coefficients
  - C.4.2.5 Filters and Monochromators



C.4.3 Electron Beams

C.4.4 Neutron Beams

C.4.5 Atomic and Molecular Beams

Part 5. Determination of Lattice Parameters

C.5.1 Scattering Angles

C.5.1.1 Skeleton Tables of  $d$  vs  $\sin\theta$  and  $\theta$

C.5.1.2 Instrument Calibration and Correction of Systematic Errors

C.5.1.3 Thermal Expansion

C.5.2 Determination of Unit Cell and Refinement of Lattice Parameters

Part 6. Physics of Diffraction

C.6.1 Intensity of Diffracted Radiation

C.6.2 Lorentz-Polarization and other Trigonometrical Factors for the  
Various Techniques

C.6.3 Absorption Corrections

C.6.4 Primary and Secondary Extinction

Part 7. Measurement of Intensities

C.7.1 Detectors for X-rays

C.7.1.1 X-ray Film

C.7.1.2 Geiger Counters

C.7.1.3 Proportional Counters

C.7.1.4 Scintillation Counters

C.7.1.5 Energy-Dispersive Devices

C.7.1.6 Position-Sensitive Detectors

C.7.2 Detectors for Electrons

C.7.3 Detectors for Neutrons and other Radiations

C.7.4 Densitometry

C.7.5 Counting Circuits



### C.7.6 Correction of Systematic Errors

C.7.6.1 Absorption

C.7.6.2 Extinction

C.7.6.3 Thermal Diffuse Scattering

C.7.6.4 Compton Scattering

C.7.6.5 White Radiation and other Sources of Background

### C.7.7 Statistical Fluctuations

## Part 8. Refinement of Structural Parameters

C.8.1 Refinement by Least Squares

C.8.2 Other Refinement Methods

C.8.3 Constraints and Restraints in Refinement

C.8.4 Detection and Treatment of Systematic Errors

C.8.5 Statistical Significance Tests

C.8.6 Determination of Electron Density and other Scattering Densities

## Part 9. Basic Structural Features

C.9.1 Close Packing of Spheres and Ellipsoids

C.9.2 Layer Stacking

C.9.3 Typical Interatomic Distances

C.9.3.1 Metals

C.9.3.2 Inorganic Compounds

C.9.3.3 Organic Compounds

C.9.3.4 Organometallic Compounds

C.9.3.5 Hydrogen Bonds

C.9.3.6 Short 'Non-Bonded' Distances

C.9.4 Typical Inter-Bond and Conformation Angles

## Part 10. Precautions Against Radiation Injury



## APPENDIX: TREATMENT OF EXISTING SECTIONS OF VOLUMES II-IV

### II.2 Fundamental Mathematics

There will be no section with the title Fundamental Mathematics; the less elementary parts will be incorporated in the appropriate places, mainly in Volume B.

### II.3 Crystal Geometry

The same considerations apply to some of the section Crystal Geometry, but much of it must be retained, particularly the treatment of twinning.

### II.4 Diffraction Geometry

A section on diffraction geometry is very necessary, but the present one, even taken in conjunction with the supplementary material in Volumes III and IV, needs modernization. Many of the tables can be reduced to about one-tenth of their present size.

### II.5 Physics of Diffraction Methods

Some modernization of the section Physics of Diffraction Methods is required, and the tables will be shortened.

### II.6 Fourier Synthesis and Structure Factors

The basic theory of Fourier series and structure factors will appear in Volume B. Section 6.4, on refinement of structural parameters, will be modernized and enlarged.

### II.7 Special Topics

Statistical methods (7.2) and inequality relations (7.3) will form part of Volume B. Other topics are included in the planned Part 9 of Volume C.



## II.8 Miscellaneous Exponential and Trigonometric Tables

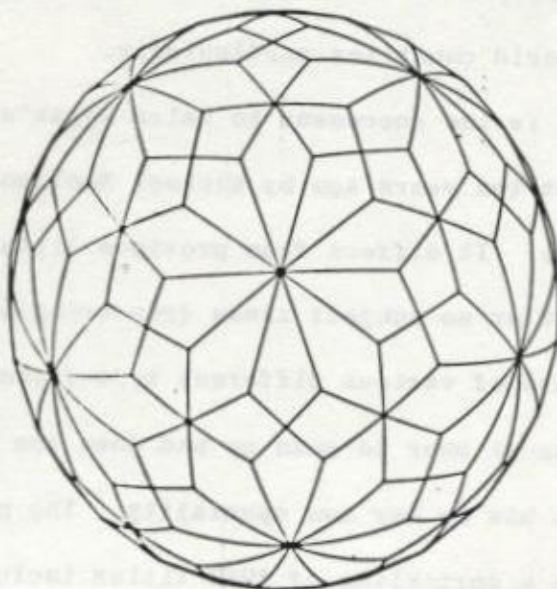
The tables of section 8 can all be generated easily by pocket calculator, and will be omitted.

### Volume III

The contents of Volume III, Physical and Chemical Tables, remain relevant, though much modernization and rearrangement will be required. Tables easily reproduced will be shortened, and parts of sections 3.3 and 5 will be transferred to Volume B.

### Volume IV

Volume IV is essentially supplementary to Volumes II and III, and in general its contents will simply be taken into account in the revision of the corresponding sections of the earlier volumes. Section 5, Thermal-Motion Analysis, is relevant both to Volume B and Volume C, and section 6, Direct Methods, will be taken into account in Volume B.





INTERESTED IN BOOKS?

Anyone with an interest in seeing the total range of currently available books on crystallography, and virtually all topics concerned with crystallography, can take advantage of the new, comprehensive Booklist recently produced by the IUCr. It has been published not as a separate booklet but in the Journal of Applied Crystallography (JAC), where it is in the December issue of the 1982 volume, running from page 640 to page 676. JAC can be found, of course, in any good library.

It is sometimes quite useful to have a document of this kind at hand, or on one's shelf, for reference. Copies of this new booklist can be obtained from the Chester office of the IUCr; however, as photocopying is nowadays so efficient, and so routinely available, the IUCr would prefer crystallographers who have such equipment in their institutions to make their own copies, if that is reasonably convenient. The Chester office will gladly supply copies to those who cannot easily make their own - to crystallographers in the developing, or Third World countries particularly.

This new booklist is the successor to Helen Megaw's list (of about 1965, which was updated about ten years ago by Michael Woolfson). The new list has about 1,200 entries. It differs from previous lists in having the books classified into some 30 or so subject areas (rendering it less tedious to consult), and in the use of various different type-faces, making it rather easy for a comparatively casual user to scan up and down the pages, to pick out what is interesting in his or her own speciality. The period covered is the decade 1970-1981, with a sprinkling of 1982 titles included. Incidentally, one book that's not in the list (because it has appeared only during the past month) is the reprint of James's classic, 'Optical Principles of X-ray Diffraction'.



BIDICS 1981

BIDICS 1981, the Bond Index of the Determination of Inorganic Crystal Structures published during 1981, is now available from:

Dr. I.D. Brown  
Institute for Materials Research  
McMaster University  
Hamilton, Ontario, Canada L8S 4M1

or

Polycrystal Bookservice  
P.O. Box 27  
Western Springs, Ill. 60558

price \$40. It contains references to 2619 papers reporting metals, inorganic and metal organic structures indexed according to the bonds present.

BIDICS 1981 will be the last volume in this series which started with BIDICS 1969 and which contains references to a total of over 24,000 crystal structure determinations. Most of the earlier volumes are still available.

In 1970, when BIDICS was first produced, the reference sources used by crystallographers to find information on crystal structures were 10-15 years out of date and there was an urgent need to provide an index to the current literature. The need was seen to be a temporary one since already the Cambridge File of organic crystal structures was showing that the future lay with computer databases. In the next few months the Inorganic Crystal Structure Database\* will become public and the Metals Data File shortly after. These, when fully operational, will permit a more complete and efficient retrieval of crystal structure data than BIDICS.

However, in spite of the advantages of computer searches there will continue to be need for a hard copy index to inorganic crystal structures, but this will be more effectively produced from the database itself. We are now working on such an index which, when published, will include additional keys such as oxidation state and coordination number, keys that it has not been feasible to provide in BIDICS. Further, the index will cover the complete inorganic crystallographic literature, not merely the literature of a single year. The publication date will be announced when the new index is ready.

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\* Enquiries concerning the Inorganic Crystal Structure Database and the Metals Data File should be directed either to Dr. H. Behrens, Fachinformationszentrum, Energie Physik Mathematik, Kernforschungszentrum, 7514 Eggenstein-Leopoldshafen 2 FRG, (FIZ) or Dr. G. Wood, Canadian Institute for Scientific and Technical Information, National Research Council of Canada, Ottawa, Canada (CISTI) as follows:

All enquiries from the Federal Republic of Germany to FIZ.

All Enquiries from Canada to CISTI.

In all other countries enquiries about the Inorganic Database to FIZ.  
Enquiries about the Metals File to CISTI.



## 16. CRYSTALLOGRAPHIC PROGRAMS ON MICROS

At the last session of the BCA Spring Meeting in Royal Holloway College, a member commented that he knew of some useful programs running on micros and asked whether there was any source of information about such programs. I propose to compile such a list and make it accessible on-line to users of the SERC computer network, and possibly publish it from time to time in Crystallography News.

Anyone who wishes to enter their program in the list should send me details as follows:

1. their name and address
2. the name of the program
3. a short description of what it does
4. which micro(s) it runs on
5. which operating system is used
6. how much core it needs
7. which language it is written in
8. state of available documentation
9. any other useful information, eg peripherals, monitor resolution.

We have a few programs running on the PERQ under the POS operating system. I understand Guy Dodson (York) is co-ordinating work on mounting further programs on PERQs which will be of use to the protein crystallography community.

K M Crennell  
Computing Division  
RAL

ATLAS CENTRE  
Chilton, Didcot,  
Oxfordshire OX11 0QX  
Telegrams: Ruthlab Abingdon  
Telex: 83159  
Tel: Abingdon (0235) 21900  
Extension: 6397

## 17. CRYSTALLOGRAPHY NEWS

Crystallography News is sent to a thousand crystallographers in the UK, and elsewhere, in March, June, September and December. Items for inclusion are welcome at any time, but to ensure inclusion in a particular issue, they should be sent to the Editor early in the month preceding publication: Dr Moreton Moore, Department of Physics, Royal Holloway College, Egham, Surrey, TW20 0EX.



FORTHCOMING MEETINGS (M) and COURSES (C)

1 - 5 August 1983 ACA meeting and Denver diffraction conference  
(M) Snowmass, Colorado, USA  
Prof. R. D. Witters, Dept of Chemistry, Colorado School of Mines,  
Golden, Co 80401, USA

1 - 10 August 1983 International School on Teaching Crystallography  
for Materials Science (C) Brasilia, Brasil.  
Prof S Caticha Ellis, Instituto de Fisica, UNICAMP - C.P. 1170.  
1130 Campinas, S P Brasil.

6 - 12 August 1983 41st Annual Mtg of the Electron Microscopy  
Society of America (M) Phoenix, Arizona.  
Dr C Ward Kischer, Dept of Anatomy, Health Sciences Center, Univ of  
Arizona, Tucson, AZ 85724, USA

7 - 10 August 1983 Applications of X-ray Topographic Methods to  
Materials Science (C) Snowmass, Colorado, USA  
Prof S Weissman, Dept of Mechanics and Materials Science, Rutgers  
University, Piscataway, New Jersey 08854, USA

8 - 12 August 1983 8th European Crystallographic Mtg. (M)  
Liège  
M Léon Dupont, Institut de Physique B5, Université de Liège au  
Sart-Tilman, B-4000 LIÈGE, Belgium.

16 - 19 August 1983 7th Intern. Conf. on High Voltage Electron  
Microscopy (M) Berkeley, California  
Mr K H Westmacott, Bldg 72, Room 127, Lawrence Berkeley Lab.,  
Berkeley CA 94720, USA

18 - 27 August 1983 Int. School on Crystallographic Computing (C)  
Kyoto, Japan.  
Prof. T Ashida, Dept of Applied Chemistry, Faculty of Engineering,  
Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464, Japan.

30 August - 2 Sept 1983 Electron Microscopy - EMAG 83 (M)  
Guildford  
Meetings Officer, IoP, 47 Belgrave Sq., London, SW1X 8QX.

30 August - 2 Sept. 1983 14th Mtg. of Crystallographers in  
Australia (M) C B Alexander Agricultural College, Tocal,  
Paterson, NSW  
H R Tietze, Department of Chemistry, University of Newcastle,  
NSW, 2308, Australia.

30 August - 2 Sept 1983 2nd Internat Conf on Databases (M)  
Cambridge  
Dr SM Dean, Dept of Computer Science, University of Aberdeen, AB9 2UB  
Scotland.



3 - 10 September 1983 5th International Summer School on  
Crystal Growth (C) Davos, Switzerland.  
Dr H Arend, Lab. für Festkörperphysik, ETH, CH-8093 Zürich, Switzerland

5 - 9 Sept 1983 10th Int Congress on X-ray Optics and Microanalysis  
(M) Toulouse  
ICXOM 10 - Secrétariat, Laboratoire d'Optique Electronique du CNRS,  
29 rue Jeanne Marvig, BP 4347, 31055 Toulouse Cedex, France.

5 - 10 Sept 1983 8th Iberoamericano Congress of Cryst. (M)  
Buenos Aires and La Plata  
Dr Maria A R de Benyácar, Avda. del Libertador 8250, 1429 Buenos Aires  
Argentina

12-14 September 1983 3rd National Conf. on Synchrotron Radiation  
Instrumentation (M) Upton, Long Island.  
Mr W Thomlinson, National Synchrotron Light Source, Brookhaven  
National Lab., Upton, Long Island, NY, USA

12 - 16 Sept 1983 7th Intern Conf on Crystal Growth (M)  
Stuttgart  
Dr K W Benz, Kristallabor., Physikalisches Institut der Universität,  
Pfaffenwaldring 57, 7000 - Stuttgart 80, Fed. Rep. Germany.

19-21 Sept 1983 3rd Hungarian Conf on Crystal Growth (M) Budapest  
HCCG-3, Eötvös Lorand Physical Society, Budapest, Pf 240, H-1368,  
Hungary.

20-23 Sept 1983 15th Europhysics Conf on Macro-Molecular Physics:  
the characterization of polymers in the solid state (M) Hamburg  
Prof Dr H G Zachmann, Abteilung Angewandte Chemie, Universität  
Hamburg, Martin-Luther-King-Platz 6, D-2000 Hamburg 13.

26-30 September 1983 Specialised course in Scanning Electron  
Microscopy (C) Cambridge  
The Administrator, Royal Microscopical Society, 37/38 St Clements,  
Oxford, OX4 1AJ

5 - 7 October 1983 41st Intern. Pittsburgh Diffraction Conf and  
3rd Canadian Crystallography Conf (M) Toronto, Ontario.  
Dr P R Sundararajan, Xerox Research Centre of Canada, 2480  
Dunwin Drive, Mississauga, Ontario L5L 1J9, Canada.

14-17 November 1983 Annual Meeting of the Materials Research  
Society, (M) Boston, Massachusetts  
EEM Hawk, 110 Materials Research Lab., University Park,  
PA16802, USA

14-16 December 1983 20th Annual Meeting on Solid State Physics  
(M) London Dr B T M Willis, AERE, Harwell, Oxon OX11 0RA

1984 19-23 March 1984 4th General Conf of the Condensed Matter Division  
of the European Physical Society (M) The Hague  
Mr F M Mueller, Physics Lab., Toernooiveld, NL-6525 ED Nijmegen,  
The Netherlands.



7-19 April 1984 International School on Direct Methods of Solving  
Crystal Structures (C) Erice, Sicily  
Prof L Riva di Sanseverino, Istituto di Mineralogia, Piazza di  
Porta San Donato 1, 40127 Bologna, Italy.

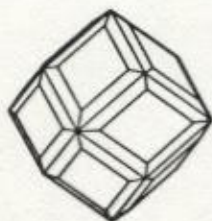
21-25 May 1984 ACA Spring Meeting (M) Lexington,  
Prof D E Sands, Dept of Chemistry, University of Kentucky, Lexington,  
KY40506, USA

3-6 July 1984 Intern Conf on Crystal Growth and Characterization  
of Polytype Structures (M) Marseilles.  
Dr A Baronnet, CRMCC, CNRS, Campus Luminy, Case 913, 13288,  
Marseille CEDEX 9, France.

9-18 August 1984 XIII IUCr Congress (M) Hamburg  
Prof Dr H Saalfeld, Mineralog-Petrogr. Institut, Universität Hamburg,  
Grindelallee 48, D-2000 Hamburg 12, Fed Rep Germany See this issue.

1985 11-14 February 1985 Characterization and Analysis of Polymers  
(M) Melbourne, Australia  
Dr J H O'Donnell, Polymer and Radiation Group, Dept of Chemistry,  
University of Queensland, Brisbane 4067, Australia.

September 1985 9th European Crystallographic Meeting (M)  
Turin, Italy. Prof M Catti, Istituto di Mineralogia  
e Cristallografia dell'Università, Via S Massimo 22, 10123, Torino, Italy.



#### RESEARCH ASSISTANTSHIP

A research assistantship in X-ray diffraction will be  
available from October 1983, for one year in the first instance,  
at the University of Edinburgh, on Scale 1A. The successful  
applicant will help in the development of high pressure  
crystallography, incommensurate structures and neutron diffraction.  
Applications from those holding, or about to hold, a PhD degree,  
and naming two referees, should be sent as soon as possible to  
Dr Richard Nelmes, Department of Physics, University of Edinburgh,  
Mayfield Road, Edinburgh, EH9 3JZ, Scotland.

