



# CRYSTALLOGRAPHY NEWS

BRITISH CRYSTALLOGRAPHIC ASSOCIATION

No. 6      SEPTEMBER 1983

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Autumn brings with it meetings of individual Groups, and in particular the first solo meetings organised by the two new Groups - the Biological Structure on 22nd September and the Industrial on 10th November. In August, the 8th ECM was held in Liège - a fuller account is included in this issue. The BCA had nominated Dr Olga Kennard to represent UK crystallographers on the European Crystallographic Committee, which met during this conference.

Next year in August, the 13th Congress and General Assembly of the IUCr will take place in Hamburg. I have been in touch with several travel firms to see if there are any advantages in arranging group travel to this meeting, as compared to the use of APEX fares which allow individuals to make their own arrangements. When 1984 prices have been fixed by the airlines, a more detailed announcement will be made in Crystallography News.

Now that the programme of seeking financial aid from Industry to help establish the BCA seems to have run its course, I will summarise its scope and results. By my count, a total of 195 companies were approached, of which 32 responded positively to give a total of £12,300 to the BCA. The individual donations varied from £1000 to £90. It is clear that a number of other companies would have helped were they not themselves in some difficulty. Several colleagues, in particular Dr Brian Isherwood, helped me in providing names of people to approach, and the letters were sent by our President. The massive task of typing all the initial letters, and dealing with any ensuing correspondence, was carried out by the President's secretary Mrs P. Batchelor - to whom the Association owes a debt of gratitude. This programme was the most important contribution to establishing a sound financial basis for the BCA.

Finally a word about membership. The By-laws state that new Ordinary Members paying their subscription between 1st October and the end of the year, do not have to pay any subscription for the ensuing calendar year. This is therefore a good time to seek new recruits, and with this in mind a pocket-size information pamphlet is being prepared for distribution to Groups or anyone who is interested.

Andrzej Skapski

BCA COORDINATING COMMITTEE

This committee was set up by the BCA to take over the coordinating functions hitherto carried out by the United Kingdom Crystallographic Council (which has now been dissolved). It had its first meeting on 27th June under the chairmanship of Dr. S.C. Wallwork, who was the last chairman of the UKCC. Most of the organisations formerly represented on the UKCC have agreed to be represented on the new Coordinating Committee and there are a number of new representatives, including those of the Industrial Crystallography Group and the Biological Structure Group recently set up by the BCA. The situation is still slightly fluid but at present there are at least 14 representatives and a complete list will be published in the next issue of 'Crystallography News'.

The main purpose of the committee is to alert its associated organisations to possible clashes of dates and topics, when planning meetings of possible crystallographic interest. To assist this process, the chairman has prepared and circulated to these associated organisations, a computer listing of a wide range of future meetings planned by all the bodies concerned. This includes all the tentative plans as well as firm meetings, since it is only the former that can be changed if any serious clashes are detected. Being held in a computer file, this list can be modified and up-dated very readily and it is hoped to distribute revised lists about four times a year. The spin-off from this process is that there is a wider interchange of information among member organisations, with the chance of enhanced publicity.

It is felt that this interchange of meetings information by post will be sufficient for the normal business of the committee, but there will be an annual meeting of representatives in addition, probably associated with the annual meeting of the BCA.

S.C. Wallwork



PHYSICAL CRYSTALLOGRAPHY GROUP OF THE INSTITUTE OF PHYSICS AND THE BRITISH  
CRYSTALLOGRAPHIC ASSOCIATION

COMMITTEE FOR 1ST OCTOBER 1983 - 30TH SEPTEMBER 1984

CHAIRMAN:	Professor M.M. Woolfson, University of York
VICE-CHAIRMAN:	Dr. B.T.M. Willis, AERE Harwell
HON. SECRETARY & TREASURER:	Dr. J.C. Halfpenny, Napier College
COMMITTEE:	Mr. C. Dineen, GEC Hirst Research Centre (Coopted)
	Dr. R.H. Fenn, Portsmouth Polytechnic (Coopted)
	Dr. I.F. Ferguson, UKAEA Springfields
	Dr. P.F. Fewster, Philips Research Laboratories
	Dr. A.M. Glazer, Clarendon Laboratory (Coopted)
	Mrs. M.A.G. Halliwell, British Telecom Research Labs.
	Dr. J.R. Helliwell, University of Keele/Daresbury Laboratory
	Dr. M.T. Hutchings, AERE Harwell
	Dr. C.J.E. Kempster, UMIST
	Prof. A.J. Leadbetter, Rutherford Appleton Laboratory
	Mr. P.B. McAllister, BICC
	Dr. A.M. Moore, Royal Holloway College (Coopted)
	Dr. R.W.H. Small, University of Lancaster (Coopted)
	Dr. A.J. Smith, University of Sheffield

INDUSTRIAL GROUP OF BRITISH CRYSTALLOGRAPHIC ASSOCIATION

Autumn Meeting 1983 : Crystallography in Industry

Thursday, 10th November, BP Research Centre, Sunbury-on-Thames

PROGRAMME

10.00	REGISTRATION AND COFFEE
10.30	Introduction
10.40	X-Ray Diffraction at BP - G.W. Smith and D. Wood
11.15	Crystallography of Industrial Zeolite Powders B. Beagley, J. Dwyer - UMIST
11.40	Neutron Diffraction Studies of $UO_2$ B.T.M. Willis - Harwell
12.05	Measurement of Internal Stress Using High Resolution Neutron Diffraction - A.J. Allen, M.T. Hutchings, C.G. Windsor - Harwell
12.30 - 13.45	LUNCH
14.00	Solving Laue Diffraction Patterns by Microcomputer P. Fewster - Philips Research Laboratories
14.20	The Role of X-ray Topography in the Study of the Growth of High Purity Quartz - J.M. Holt, D.F. Croxall GEC Hirst Laboratories
14.40	Analysis of Crystallites in Thin Oxide Films Using Combined EDA and Microdiffraction in a STEM - I.F. Ferguson Springfields Nuclear Power Development Laboratories.
15.00	TEA
15.15	<u>Workshop</u> : Diffraction Problems in Industry Topics will include:- (a) "The Right Tool for the Job" - Competing Analytical Techniques (b) Cost Effectiveness (c) Expediency Versus Rigour (d) -----?

Conference fee, including lunch and refreshments is:-

Member of Industrial Group of the BCA	£12.00
Non-Members	£15.00
Students	£ 7.00

The registration form is included in this issue of the newsletter



## SOLID STATE PHYSICS CONFERENCE

14-16 DECEMBER 1983

Department of  
Experimental Psychology  
University of Oxford



The Physical Crystallography Group is organizing a Symposium on DIFFRACTION STUDIES OF MATERIALS as part of the conference.

The Symposium runs from 09 45h on Wednesday 14 December through to midday on Thursday 15 December and includes two Plenary Talks by Professor Sir Peter Hirsch, FRS (Chairman, UKAEA) and Professor A Authier.

Offers of contributed papers for the Symposium should be sent to:

Dr C Dineen  
GEC Hirst Research Centre  
East Lane  
Wembley  
Middlesex HA9 7PP

by 1 November 1983.

The Registration Fees for the conference are:

Members	£15 for 1-day:	£28 for 3-days
Student Members	£10 " "	£18 " "

Further details and registration forms may be obtained from:

Mr M Wells  
Clarendon Laboratory  
Parks Road  
Oxford OX1 3PU

## BCA MEETING - NOTTINGHAM UNIVERSITY

2nd - 5th April, 1984

The Spring Meeting of the BCA will be held at Nottingham University, which is on a large open parkland campus 2 miles west of Nottingham. The scientific sessions will be based in the Chemistry Department and accommodation has been arranged in nearby Lenton Hall. Being roughly in the middle of England it is readily accessible by road (M1), rail and air (East Midlands Airport). An important point to note in the timing is that this is not the traditional week before Easter. Easter is so late in 1984 that to have held the conference then would have trespassed into Scottish University terms!

The conference will follow the same successful format as this year's at Royal Holloway College, with consecutive sessions organised by the constituent groups of the BCA. However, the changes have been rung by varying the sequence of the presentations. After registration and lunch on Monday 2nd April, the first afternoon will be devoted to the Physical Crystallography Group. Tuesday morning is the turn of the Industrial Group with the Chemical Crystallography Group on Wednesday morning and finally the Biological Structures Group are on Thursday morning. In addition, there will be poster sessions, ad hoc meetings, a plenary lecture, conference dinner, etc. Each group has appointed a representative on the Steering Committee to organise its own sessions. These are: Chemical Crystallography - David Russell (University of Leicester); Physical Crystallography - Paul Fewster (Philips Research, Redhill); Biological Structures - Guy Dodson (University of York); Industrial Crystallography - Keith Bowen (University of Warwick) and John Harding (British Rail, Derby). The local organiser is Mike Begley from the Chemistry Department at Nottingham University. Full details and registration forms will be included in the December issue of 'Crystallography News'.

M.J. Begley.



INTERNATIONAL SCHOOL OF CRYSTALLOGRAPHY

Erice, Trapani, Sicily - April 7-19, 1984

10th Course: Direct Methods of Solving Crystal Structures

Topics

The fundamental principles of direct methods, structure factor algebra, multiresolution methods, symbolic addition methods, from a partial to a complete structure, phase extension and refinement, phase invariants and seminvariants: theory and application, determinantal methods, maximal entropy and direct methods, and direct methods in macromolecular crystallography.

Lecturers

G. Allegra, P. Beurskens, G. Bricogne, C. Giacovazzo, H. Hauptman, I. Karle, J. Karle, J. Kroon, P. Main, D. Sayre, H. Schenk, G. Sheldrick, G. Tsoucaris, D. Viterbo, and M. M. Woolfson.

General Information

Persons wishing to attend the Course should write to:

L. Riva di Sanseverino  
Executive Secretary  
International School of Crystallography  
Piazza Porta San Donato, 1  
40127 Bologna, Italy

The closing date for application is October 31, 1983.

Fees

The total fee including full board and lodging (arranged by the School) is 1,200 Swiss Francs. Thanks to the generosity of the sponsoring institutions, partial support can be given to those students who need financial help, but the amount required must be specified and justified in the application letter.

AMERICAN  
CRYSTALLOGRAPHIC  
ASSOCIATION

The American Crystallographic Association (ACA) was founded in 1949 through a merger of the American Society for X-Ray and Electron Diffraction (ASXRED) and the Crystallographic Society of America (CSA). The objective of ACA is to promote interaction among scientists who study the structure of matter at atomic (or near-atomic) resolution. These interactions will advance experimental and computational aspects of crystallography and diffraction. They will also promote the study of the arrangements of atoms and molecules in matter and the nature of the forces that both control and result from them.

The present-day crystallographer, like his predecessors, is interested in the form and symmetry of ideal crystals, as well as in the growth of crystals and the measurements of their physical properties. However, the range of his interests encompasses vastly more than this. He realizes that nearly all solid objects are more or less fully crystalline, and he uses the powerful techniques of X-ray, electron and neutron diffraction to establish their cell dimensions and space groups and determine the positions of their constituent atoms in the unit cell. He is aware that actual crystals deviate more or less from ideal and he devotes much effort to diagnosing the nature and extent of the imperfections prevailing in the actual structure of crystals.

ACA members have made important and fundamental contributions to the several branches of physics, chemistry, geology, materials science, biochemistry, biophysics and computer science. For example, they have unravelled the atomic arrangements and molecular structures of such diverse substances as minerals, metals, alloys, building materials, antibiotics, proteins, nucleic acids, missile materials and polymers, as well as one-dimensional conductors and liquid crystals. A great many crystallographers are busy extending our fundamental knowledge in these areas, while a much greater number are engaged in technological applications.

Membership in the American Crystallographic Association is open to any person who is actively interested in the purposes of the Association and whose application is sponsored by two regular members. Student members are very welcome and their contribution to the life and vigor of the Association has always been important. The annual dues for students are \$7.50 as compared with \$20 for regular members. The benefits of membership are the same in both cases. These include: voting privileges, a newsletter that is published six times a year, an up-to-date ACA membership Directory and Constitution, programs and abstracts of all ACA meetings, a copy of the current volume of the *Transactions of the American Crystallographic Association*, and reduced prices for the *International Tables for X-ray Crystallography*, *Structure Reports*, *Journal of Applied Crystallography*, and *Acta Crystallographica* when purchased for the member's personal use only. Also, because ACA is a member society of the American Institute of Physics (AIP), ACA members receive *Physics Today*, a monthly publication of AIP.

The total membership of ACA is about 1700. National Meetings are held twice year, except for those triennial years when the summer meeting is replaced by a Congress of the International Union of Crystallography. There are four Special Interest Groups concerned with Applied Crystallography, Small Angle Scattering, Biological Macromolecules and Small Molecules respectively. ACA members may join as many of these as interest them. Each special Interest Group is responsible for organizing sessions at National Meetings at least every other year.



FORTHCOMING MEETINGS and COURSES

21 - 22 Sept. 1983 BCA Chemical Crystallography Group Meeting,  
Univ. College, Swansea.  
Dr R W H Small, Chemistry Dept., The University, Lancaster, LA1 4YA  
(see previous issue).

22 Sept. 1983 BCA Biological Structures Group Meeting,  
Univ. of Manchester,  
Dr D W L Hukins, Dept of Medical Biophysics, Univ. of Manchester,  
Manchester, M13 9PT (See previous issue).

21 - 23 October 1983 British Assoc. for Crystal Growth Annual  
Meeting, Chester  
Mr F W Ainger, Plessey Research (Caswell) Ltd, Allen Clark Research  
Centre, Caswell, Towcester, Northants, NN12 8EQ

10 November 1983 Crystallography in Industry: BCA Industrial  
Group, Sunbury on Thames  
G W Smith, Spectroscopy Branch, BP Research Centre, Chertsey Road  
Sunbury-on-Thames, Middx (see this issue).

14 - 16 December 1983 20th Annual Meeting on Solid State Physics  
Oxford  
Mr M R Wells, Clarendon Laboratory, Parks Road, Oxford OX1 3PU  
(see this issue - p.6)

1984

19 - 25 February 1984 7th International Biotechnology  
Symposium, New Delhi, India.  
The Secretary, 7th Int. Biotech. Symp., Biochemical Engineering  
Research Centre, Indian Institute of Technology, Hauz Khas,  
New Delhi - 11016 India.

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

2 - 5 April 1984 BCA Spring Meeting Nottingham  
Dr M Begley, Dept of Chemistry, Univ of Nottingham, University Park,  
Nottingham, NG7 2RD

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

26 April - 22 June 1984  
Spring College on Crystalline Semiconducting Materials and Devices  
Trieste, Italy.  
International College for Theoretical Physics, P O Box 586, I-34100  
Trieste, Italy.

21 - 25 May, 1984 ACA Spring Meeting, Lexington  
Prof D E Sands, Dept of Chemistry, University of Kentucky, Lexington  
KY 40506, USA

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

9 - 13 July 1984 MICRO 84 London  
The Royal Microscopical Society, 37/38 St Clements, Oxford OX4 1AJ

29 July - 4 August 1984 8th International Biophysics Congress,  
Bristol, England.  
Congress Secretariat, 8th Internat. Biophysics Congress, Meon  
Conference Services, Petersfield, Hants, GU32 3JN.

4 - 14 August 1984 27th International Geological Congress  
Moscow, USSR  
Secretariat of the Organizing Committee, 27th Internat. Geological  
Congress, Institute of the Lithosphere of the Academy of Sciences  
of the USSR, 22 Starometny, Moscow 109180.

9 - 18 August 1984 XIII I U Cr Congress, Hamburg  
Prof Dr H Saalfeld, Mineralog-Petrogr. Institut, Universität Hamburg,  
Grindelallee 48, D-2000 Hamburg 12, Fed. Rep Germany.

13 - 18 August 1984 8th European Congress on Electron  
Microscopy Budapest, Hungary,  
Congress Bureau, MOTESZ, Budapest, POB 32, H-1361, Hungary.

27 - 31 August 1984 6th General Conf. of the European  
Physical Society. Prague, Czechoslovakia  
Physical Section, Union of Czechoslovak Mathematicians & Physicists  
Na Slovance 2, 18200, Prague 8, Czechoslovakia.

11 - 13 Sept 1984 BCA Cruickshank Symposium  
Dr Brian Beagley, Dept of Chemistry, UMIST, PO Box 88,  
Manchester M60 1QD

17 - 21 September 1984 7th International Conference on  
Textures of Materials. Noordwijkerhout, The Netherlands  
ICOTOM 7, Netherlands Society for Materials Science, P O Box 390,  
NL-3330 AJ ZWIJNDRECHT, The Netherlands.

1985

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

24 May - 6 June 1985 The Determination & Interpretation of  
Small Structural Differences. Erice, Sicily.  
Prof L Riva di Sanseverino, International School of Crystallography  
Piazza Porta San Donato, 1, 40127 Bologna, Italy.

September 1985 8th European Crystallographic Meeting  
Turin, Italy  
Prof M Catti, Istituto di Mineralogia e Cristallografia dell'  
Università, Via S Massimo 22, 10123 Torino, Italy.



1986

10 - 19 June                      Synchrotron Radiation for X-ray Crystallography  
Erice, Sicily.  
Prof. L Riva di Sanseverino, International School of Crystallography,  
Piazza Porta San Donato 1, 40127, Bologna, Italy.

1988

30 May - 7 June 1988              Crystallography of Molecular Biology  
Erice, Sicily.                      Prof L Riva di Sanseverino,      International  
School of Crystallography,                      (see Bologna address above.)

1989

16 - 26 September 1989              X-ray Crystallography & Drug Action,  
Erice, Sicily.  
Prof. L Riva di Sanseverino, Intern Schl of Cryst, (see Bologna  
address above).



CRYSTALLOGRAPHY NEWS

For inclusion in the December issue, please send camera-ready  
copy by November 15th to the Editor, Dr Moreton Moore, Department  
of Physics, Royal Holloway College, Egham Hill, Egham, Surrey,  
TW20 0EX (0784-35351 ext. 36).