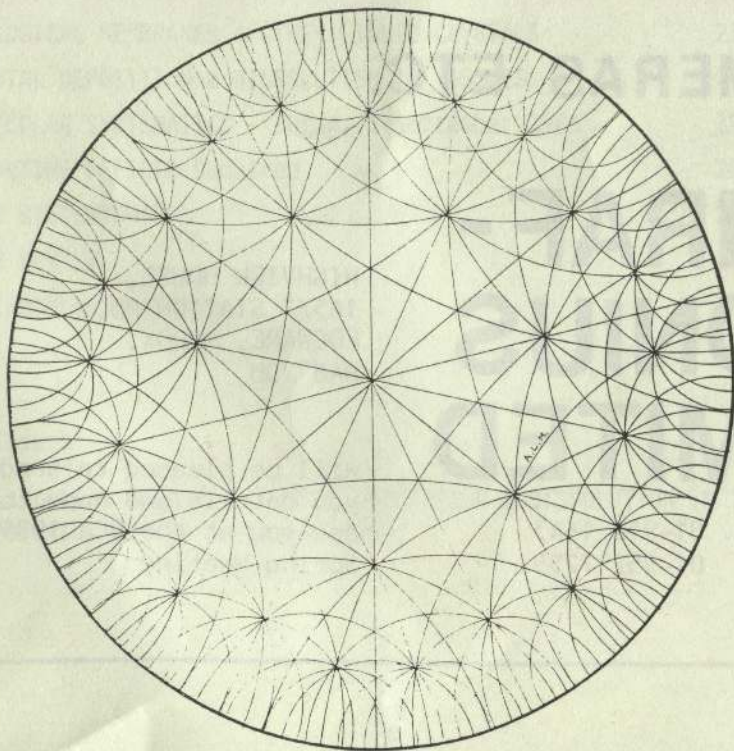




# CRYSTALLOGRAPHY NEWS

BRITISH CRYSTALLOGRAPHIC ASSOCIATION

No. 12 MARCH 1985



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will be pleased to send  
you details and hope to  
see you at the BCA 1985  
Spring Meeting

## CRYSTALLOGRAPHY NEWS

No. 12 March 1985

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### Enclosure

Registration form for CRYSTAL DEPOSITION & DISSOLUTION IN TISSUES  
Conference, 26-28 September 1985.

## COVER PICTURE

The picture reproduced on the cover was drawn by Dr Alan Mackay (Department of Crystallography, Birkbeck College) and it represents the packing of regular heptagons, each composed of seven equilateral triangles. It is shown in stereographic projection: (it is angle-true). Since in a plane the average coordination number is six, a coordination number of seven can only be achieved by curving the space, which is here hyperbolic. For equiangular triangles of unit area the radius of curvature is  $\sqrt{(-7/\pi)}$ . Sevenfold symmetry is quite possible in a lattice, but not in this world!

---

CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association. Camera-ready copy on A4 paper is welcome at any time, as well as line illustrations for the cover. Please ensure items for inclusion in the June issue are sent to the Editor by May 15: Dr Moreton Moore, Department of Physics, Royal Holloway College, Egham, Surrey, TW20 OEX. Telephone Egham 0784- (or from London 87-) 35351, extension 36. Telex 935504.

For details of advertisement rates please contact Mr S Sadler, Advertisement Manager, The Institute of Physics, Techno House, Redcliffe Way, Bristol, BS1 6NX, Telephone 0272-297481.

---

WANTED - Xray generator (sealed-tube type) in working (or close to working order for routine photographic experiments. Non-current model acceptable provided standard Xray tube and manufacturers spares are available. Please send brief details to: Department Administrator, Department of Chemistry, The University, Southampton SO9 5NH.

---

WANTED - Second-hand Xray powder equipment: high voltage generator, Hägg Guinier camera and diffractometer. Dr Peter G Bruce, Department of Chemistry, Heriot-Watt University, Riccarton, Edinburgh EH14 4AS (Tel: 031-449 5111) would be most interested to hear from anyone with such equipment for sale.

Full details and registration forms for the Bristol Spring Meeting were included with the December issue, and judging from the programme and registrations received so far all looks set for a very successful meeting.

Professor T.L. Blundell FRS has been coopted to join the Council of the BCA. Together with the recent addition of Professor M.M. Woolfson FRS, who as the new Chairman of BNCC becomes ex officio a member, the Council is now at full strength as allowed by the Constitution.

I would remind everyone that elections will take place at the Bristol AGM for Vice-President, Secretary, and one other Member of Council, and that the deadline for nominations to reach me at Imperial College is Friday, 22nd March 1985.

As part of 'BCA News', I have during the past few years introduced the Council, the various committees of the Council, and in general tried to explain the workings, both internal and external, of the Association. Looking back through past issues I notice that I have left out one group, namely the Trustees of the Association. At the request of the Charity Commissioners, the requirement for the BCA to have Trustees was incorporated in the Constitution, and in 1982 the Council appointed Professor Dorothy Hodgkin OM FRS, Professor Sir David Phillips FRS, Dr A.C. Skapski, and Professor C.A. Taylor, as the Trustees. The funds of the Association stand in the Association's name, and are held by the Trustees upon trust for the Association for the purposes and subject to the limitations of the Statutes and By-Laws.

This is the last 'BCA News' which I shall be writing, as my term of office as Secretary ends with the Bristol Spring Meeting. I would, therefore, like to take this opportunity to thank numerous colleagues for their help, encouragement, and forbearance, and to wish the new Secretary, whoever he or she may be, the best of success in this office.

Andrzej Skapski

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358/A01

## ANNUAL GENERAL MEETING

### TREASURER'S REPORT

The audited accounts of the Association for the year ended 31 December 1984 are given below. These are followed by accounts for the 1984 Spring Conference.

R. Hine

### ACCOUNTANTS REPORT

for the year ended 31st December, 1984.

We have examined the attached accounts on pages 1 to 3 and in our opinion they give a true and fair view of the receipts and payments of the Association for the year ended 31st December, 1984 and of the state of affairs of the Association at that date.

CARDIFF 11th February, 1985.

BEMAN GRAVELLE & THOMAS,

Chartered Accountants.

BRITISH CRYSTALLOGRAPHIC ASSOCIATION  
 RECEIPTS AND PAYMENTS  
 FOR THE YEAR ENDED 31ST DECEMBER, 1984.

1983			
£	£	£	£
<b>RECEIPTS</b>			
1,750.00	(receipts from industry)	-	
1,005.00	Receipts from members - (note 1)	1,482.90	
180.18	Deposit Account interest	96.86	
1,969.87	Investment Account interest	1,919.67	
587.80	Surplus on Spring conference	1,845.75	
200.00	(funds from U.K.C.C.)	-	
<u>5,692.85</u>		<u>5,345.18</u>	

<b>PAYMENTS</b>			
93.80	Stationery, postage and printing	259.29	
157.50	Newsletter	287.99	
49.94	Insurance	50.00	
63.10	Travelling expenses	51.34	
170.98	(advertising)	-	
-	Per capita payments to groups	180.00	
-	Prepayments for 1985 Spring conference	1,050.00	
62.35	(deficit on Radiation Projection Meeting)	-	
250.00	(float for Industrial Group)	-	
250.00	(float for Biological Structures group)	-	
<u>1,097.67</u>		<u>1,878.62</u>	
<u>£4,595.18</u>	<b>EXCESS OF RECEIPTS OVER PAYMENTS</b>	<u>£3,466.56</u>	

BRITISH CRYSTALLOGRAPHIC ASSOCIATION  
 BALANCE SHEET - 31ST DECEMBER, 1984.

1983			
£	£	£	£
754.77	CURRENT ACCOUNT	1,004.30	
1,361.68	DEPOSIT ACCOUNT	2,658.54	
<u>17,802.87</u>	INVESTMENT ACCOUNT	<u>19,722.54</u>	
<u>£19,919.32</u>		<u>£23,385.88</u>	
<u>£19,919.32</u>	<b>ACCUMULATED SURPLUS</b>	<u>£23,385.88</u>	

NOTES TO THE ACCOUNTS

1. The receipts from members include 1985 subscriptions received.

SPRING CONFERENCE AT NOTTINGHAM UNIVERSITY 1984

INCOME AND EXPENDITURE

	£	£
<u>INCOME</u>		
97 full fees @ 32.00	3104.00	
11 half fees @ 16.00	176.00	
39 one-day full fees @ 16.00	624.00	
8 one-day half fees @ 8.00	64.00	
7 non-member full fees @ 10.00	70.00	
2 non-member half fees @ 5.00	10.00	
102 Conference dinners @ 8.50	867.00	
Miscellaneous (overpayment)	0.10	
	<hr/>	
	4915.10	
Exhibition fees	1256.90	6172.00
	<hr/>	<hr/>
<u>EXPENDITURE</u>		
Coffees etc extra to accommodation charge		
168 @ 0.40	67.20	
Conference dinner 114 @ 6.50	741.00	
Lunches 521 @ 3.50	1823.50	
Projection facilities	35.50	
	<hr/>	
	2667.20	
VAT	400.08	3067.28
	<hr/>	
Speakers' expenses, accommodation etc.	643.43	
Conference secretary's expenses	71.79	
Conference booklets, badges etc.	151.71	
Labour for poster sessions	105.00	
Insurance	80.00	
Wine for conference dinner	110.00	
Concert singers, piano removal	89.10	1251.03
	<hr/>	
	4318.31	
Power supply for exhibition	6.90	
VAT	1.04	7.94
	<hr/>	
	4326.25	
	<hr/>	
Excess of income over expenditure		1845.75
		<hr/>

The Autumn meeting of the industrial group, held on 9 November 1984 at the Central Electricity Generating Board, North East Region Scientific Services Department was a great success. The varied and interesting programme organised by Drs Ed. Metcalfe (CEGB), Brian Isherwood (GEC), Brian Bellamy (UKAEA, Harwell) and John Harding (British Rail) attracted thirty eight members to Harrogate. Dr Richard Jack, Head of the Chemistry and Materials Division in welcoming the group to the CEGB complex at Harrogate told members that CEGB was at the forefront of scientific endeavour. Dr Ed Metcalfe (CEGB) presented the first paper. He described the organisational structure of CEGB in which some fifty five thousand people are employed. The facilities of eight research laboratories cope with the demands of this large organisation. Whilst the workforce is diminishing, the demand for electricity is increasing. Events such as the miners strike pose technical problems for the Board. Concentrating on the aspect of x-ray diffraction, Dr Metcalfe described some applications such as the characterisation of coal; study and identification of the phase changes which occur within the metal of turbine shafts and the detection of metal fatigue. The lattice parameter technique is widely used in the study of oxides and carbides.

Dr Derek Thompson (University of Newcastle) presented a fascinating paper on the topic of nitrogen in ceramics. Single crystals of such materials are not easy to produce but nevertheless Dr Thompson seems to have overcome the difficulty in the many examples of structures which he described. He showed how in the study of the polytypes in the Aluminium Silicon Oxygen Nitrogen system the metal to non-metal ratio was related to the ratio of the c-spacing to the number of layers in the polytype. Lattice parameter measurements allow one to relate the MX<sub>2</sub> layer concentration to the cell size. Using a series of trial and error approaches Dr Thompson showed how polytypes could be described by using layers of octahedra between the basic layers to tetrahedra. One dimensional lattice imaging was used to support his findings but in extending to the more demanding two dimensional imaging he showed some of the shortcomings relating to the detection of ordering. He completed his presentation with a description of a phase which he termed 'nitrogen mullite'. This phase exists in two forms (low and high). Again by applying a trial and error approach coupled with stereochemical requirements the structures were elucidated. TEM gave direct evidence of the faulting which occurs in the structure.

Dr Peter Doig (CEGB) described a mobile x-ray machine capable of producing precision data for use in the determination of stress in metal components. The equipment can be used either in a laboratory or in an industrial area. It comprises a Siemens transportable x-ray diffractometer in which the incident beam can be rotated with respect to the metal surface of the item being examined. A linear position sensitive detector records diffracted intensity data over an angular range of ten degrees (2-theta) and it takes only four minutes to obtain a value for the stress within a metal. Dr Doig described the computer software which he now uses and whilst fifty psi-steps can be handled he suggested that there was no real benefit in using more than ten such steps.

Dr David Dyson (British Steel Corporation) described a computer based procedure which he and Dr Steve Butler have devised to interpret electron diffraction patterns produced from compounds commonly detected in steels. The procedure is now widely used in their laboratories by persons who are not necessarily crystallographers, but who require to identify the inclusions etc. which they detect when using an electron microscope. The procedure is user interactive and all requests for specific information are

displayed on the VDU. By requesting information for four vectors the software will offer solutions which allow the user to identify the phase or phases which have produced the particular diffraction pattern.

Dr Craig Adams (Unilever Research) uses a 64k microcomputer to assist in the quantitative analysis of inorganic hydrates. The procedure includes the Chung approach in which overlapping profiles are used. Standard intensity data for one hundred and twenty standards have been collected and are stored by the computer. A least-squares procedure is used to determine the relative proportion of the hydrates in a mixture and a graphical output comparing the observed intensity with that calculated is produced.

The role of infrared spectroscopy in mineralogy was described by Dr Jim Russell of the Macaulay Institute. He showed with numerous examples, how infrared spectroscopy can be used in the identification of minerals, particularly clay minerals. He showed that the technique would give information on such materials as whinstone where the presence of smectite, albite, chlorite and calcite could be detected in under five minutes by a skilled operator.

Dr David Blundell (ICI) presented the final paper of the meeting and dealt with the crystallinity in PEEK/carbon fibre composites. He showed that one could obtain a value for the crystallinity index of such a composite which correlates well with density. By using information obtained from low angle scattering and x-ray diffraction, values for the crystal thickness can be obtained. Techniques such as wide angle x-ray scattering and multiple internal reflection infra red are used to study these composites. Dr Blundell showed that cooling rate used in the fabrication process of the thermoplastics was related to the crystallinity of the final product.

W A Gutteridge  
7 December 1984



UNIVERSITY OF OXFORD

CLARENDON LABORATORY

Postdoctoral Fellowship in Powder Diffraction.

Applications are invited for a postdoctoral fellowship tenable for up to three years under the ICI Joint Research Scheme. The project involves the development of the use of x-ray and neutron powder diffraction for ab initio structure determination, with particular relevance to zeolites. Candidates should have experience in both x-ray crystallography and computing. Applicants should send their C.V. and should arrange for two references to be sent to Dr. A.M. Glazer, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU from whom further information can be obtained.

The post is available from 1 March 1985 on the Research IA scale (7,250-£12,150 p.a. with membership of USS).

Physical Crystallography Autumn Meeting  
on  
SURFACE CRYSTALLOGRAPHY  
28th November 1984, Imperial College

This one day meeting was held jointly with the Thin Films and Surfaces Group of the Institute of Physics. The individual groups organisers were Mary Halliwell and Jim Matthew. The meeting was attended by 70 delegates evenly distributed between the two groups and a total of 12 papers were presented.

ELECTRON DIFFRACTION TECHNIQUES

The opening paper was given by Prof. John Pendry (Imp.Coll) who reviewed the main techniques for the analysis of surfaces. He gave examples of studies of adsorbed molecules on surfaces by LEED (Low Energy Electron Diffraction) and how EELS (Electron Energy Loss Spectroscopy) can be used to determine the hydrogen positions. LEED has had success in determining the orientation of relatively complex molecules on surfaces and giving details of reconstruction of surfaces. Pendry also described the physics of SEXAFS (Surface Extended X-ray Absorption Fine Structure) but warned of the problems in the "data to determinable parameter" ratio. He also touched on RHEED (Reflection High Energy Electron Diffraction) in determining monolayer deposition by MBE; photoemission he considered to have lost its way (using up SERC money!) except for the work on semiconductors. 2-D X-ray diffraction also shows promise if surface d-spacings can be determined, but measuring diffracted rays perpendicular to the surface with large momentum transfers imposes serious intensity problems. The more familiar geometry with the diffraction vector parallel to the surface will only give a projection. He completed his talk by saying there was too much chasing of pet theories in surface structure analysis.

Prof. Martin Prutton followed this with a review of LEED and RHEED, although he concentrated on the former. LEED essentially gives the bulk back-diffraction pattern and subsidiary reflections from a reconstructed surface. The results from LEED studies were shown to be very sensitive to apparatus and operators (after Müller). The computing time also appeared horrific; for a structure he quoted it took 11m cpu time/trial model on a CRAY (3h on a conventional mainframe). The data collection time is > 2 weeks/dataset, although this can be improved with TV techniques. I was left with the impression that LEED had little going for it, except that it is not as sensitive to surface topography as RHEED.

Prof. John Beeby presented the case for RHEED where he showed that there was good agreement between calculations and experiment. An important advantage of RHEED is that the surface rumpling parameter and perpendicular contraction of the surface can be separated by choosing different azimuths. The calculations for elastic scattering are rapid and can also be done for the inelastic case.

Dr. Tear gave an account of a new computer controlled LEED

machine, the size and technology involved appeared daunting. The diffraction pattern is collected by a TV camera that scans the surface of a glass phosphor-coated sphere. This requires its own algorithm to correct the data, which can now be collected in 30m.

Dr. Bob Pond (Liverpool Univ.) gave a very good presentation on theoretical predictions of interfaces by simply considering the symmetry and orientation of the two materials in contact. With this approach he has predicted antiphase domains and other interphase discontinuities which have been observed experimentally.

#### X-RAY TECHNIQUES

Dr. Thomas (Oxford Univ.) described his X-ray techniques for studying physisorbrates on surfaces. To increase the surface area, the samples are in powdered form which allows kinematic theory to be used. This method allowed him to derive the vibrational and rotational energy states and to determine the degree of wetting and whether adsorbates were commensurate. He also described some preliminary work on neutron and X-ray 2D diffraction. Dr. Peter Maksym (Leicester Univ.) described his calculations on 2D X-ray diffraction and showed that the kinematic and the dynamical calculations are in close agreement even for the case when one would expect kinematic calculations to break-down. This will greatly assist information retrieval from diffraction profiles. Dr. Phil Woodruff (Warwick Univ.) described his EXAFS work and concluded that to obtain surface structure information is a slow process requiring a slow "chipping away" to obtain structural variables. Dr. Andrews (GEC) gave an account of measuring surface roughness by examining diffuse scattering and Dr. Duke (Daresbury) described the progress on the construction of Fresnel zone-plates to produce a focused X-ray source for a scanning X-ray microscope.

#### NON-DIFFRACTION TECHNIQUES

Dr. Roy Willis (Cambridge Univ.) described vacuum tunnelling microscopy to obtain surface atomic structure by mapping the surface potential, and LEED spot profile analysis to study surface structural phase transformations. The final paper of the meeting was by Dr. Richard Forbes (Surrey Univ.) who informed us that the understanding of Field Ion Microscopy has only recently (1982) been agreed upon.

This meeting was a great success and showed that surface studies requires many techniques to obtain a coherent picture and then still requires a lot of critical interpretation. The subject is also thick with acronyms, fortunately all delegates were presented with a booklet of their meanings, compiled by Matthew and Prutton.

Paul F. Fewster

#### CHEMICAL CRYSTALLOGRAPHY GROUP

#### Spring Meeting, 25-27 March, 1985

At the time of writing it is still six weeks to go before the BCA Spring Meeting at Bristol. The Chemical Crystallography Group's session on the theme of utilisation and publication of crystallographic results promises to be a most interesting and lively occasion. The AGM of the Group will be held at Bristol on Tuesday, 26th March, at 14.00 hours. Any last minute arrangements relating to the Spring Meeting can be made through Dr. J.A.K. Howard or Dr. A.G. Orpen, School of Chemistry, Cantocks Close, Bristol, BS8 1TS.

#### Autumn Meeting

A one-day meeting of the Group will be held on Tuesday, 19th November, 1985, at the Chemistry Department of Birkbeck College, London, which is not far from Euston Station. The provisional title for the meeting is "Systematics in Structural Chemistry". There will probably be two invited speakers, with the remaining time allocated to contributions offered by members. All contributions will be presented orally. This meeting is an excellent opportunity for members to exchange information about their work. More details will be available in the next Crystallography News.

#### Spring Meeting, 1986, York

The committee is currently considering the Group's programme for the 1986 meeting. We would be very pleased to receive members' suggestions regarding the programme for this and other future meetings. It is always most helpful to have guidance from members as to topics of interest and to receive comments concerning general arrangements for Group meetings.

Secretary/Treasurer: Dr. B. Beagley, Department of Chemistry, UMIST,  
P.O. Box 88, Manchester, M60 1QD.





BRITISH CRYSTALLOGRAPHIC ASSOCIATION  
INDUSTRIAL GROUP

Secretary/ Treasurer:  
Dr. J. I. Langford,

Department of Physics,  
University of Birmingham,  
Birmingham B15 2TT.  
Tel. (021-) 472 1301  
ext. 3498/3471

BCA Annual Meeting 1985

University of Bristol  
March 25th to 27th  
Industrial Symposium March 26th

The Chairman and Committee look forward to a good attendance of group members at the above meeting with the reminder that even at this late stage it is still not too late to submit a poster. Titles preferably direct to the local organiser Dr Judith Howard, School of Chemistry (0272-24161 ext 424/539), or Brian Bellamy, AERE Harwell (0235-24141 ext 4524).



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Tel. (021-) 472 1301  
ext. 3498/3471

ANNUAL GENERAL MEETING 1985

The 2nd Annual General Meeting of the Industrial Group will be held at the School of Chemistry, University of Bristol at 3.00 p.m. on Tuesday, 26 March 1985.

AGENDA

1. MINUTES OF 1ST ANNUAL GENERAL MEETING held at the University of Nottingham on Tuesday, 3 April 1984.
2. MATTERS ARISING.
3. CHAIRMAN'S REPORT.
4. TREASURER'S REPORT.
5. ELECTION OF OFFICERS AND COMMITTEE.
6. OTHER BUSINESS  
To deal with any other business admitted by the Chairman.

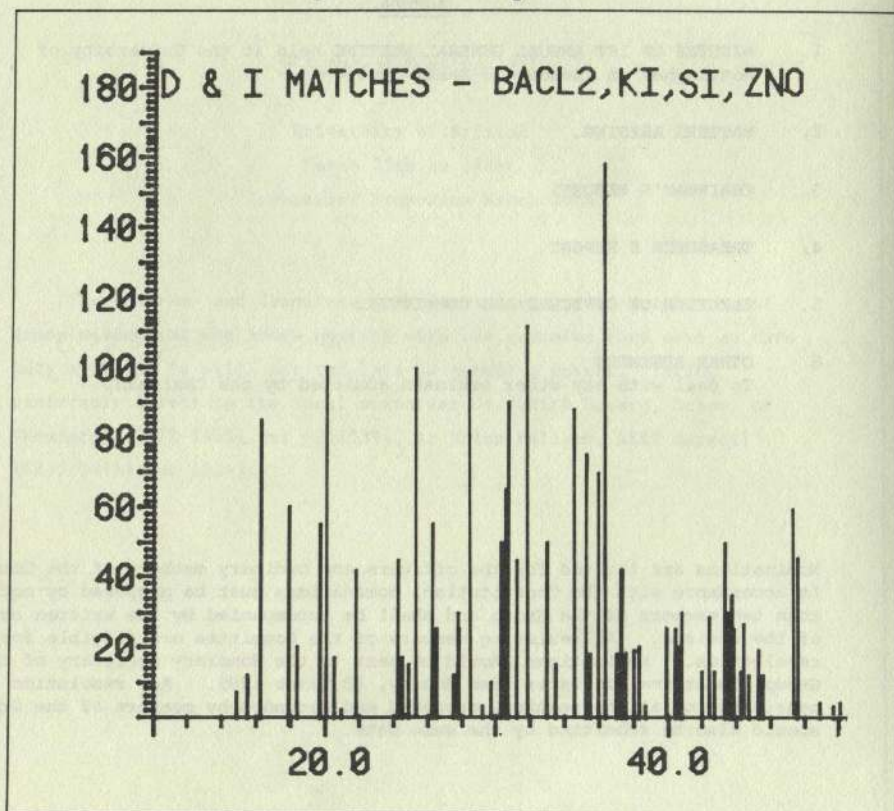
Nominations are invited for the officers and ordinary members of the Committee. In accordance with the Constitution, nominations must be proposed by not less than two members of the Group and shall be accompanied by the written consent of the nominee. All existing members of the Committee are eligible for re-election. Nominations should be sent to the Honorary Secretary of the Group, to arrive not later than Monday, 18 March 1985. Any resolution for consideration at the meeting, proposed and seconded by members of the Group, should also be submitted by the same date.

January 1985

J. I. Langford,  
Hon. Secretary.

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BRISTOL UNIVERSITY 25th - 27th MARCH 1985

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**BRITISH CRYSTALLOGRAPHIC ASSOCIATION  
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*Secretary/ Treasurer:*  
Dr. J. I. Langford,

Department of Physics,  
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Tel. (021-) 472 1301  
ext. 3498/3471

**AUTUMN MEETING 1985**

**Preliminary Notice**

This meeting is to be held on Thursday 14 November at AERE Harwell and will be entitled:

**CRYSTALLOGRAPHY IN INDUSTRY**

The aim of the Autumn Meeting is to provide participants with the opportunity to discuss the use of crystallographic techniques in industrial and technical applications. No specific topic has, therefore, been selected for this meeting and it is expected that contributions will span a range of techniques. The formal call for contributed papers will be contained in the next Crystallography News. However, you should note that:

The number of participants must be limited 60.

It is not too early to submit a contribution - some have already been received. These and any requests for further information should be addressed to:

Mr B A Bellamy  
Materials Dev Division  
Building 393  
AERE Harwell  
DIDCOT  
OXON OX11 0RA

Tel: 0235-24141  
Ext: 4524/4041

**MAKE A NOTE IN YOUR DIARY NOW**



**BRITISH CRYSTALLOGRAPHIC ASSOCIATION  
INDUSTRIAL GROUP**

*Secretary/ Treasurer:*  
Dr. J. I. Langford,

Department of Physics,  
University of Birmingham,  
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ext. 3498/3471

**SPECIALIST INTEREST WORKSHOPS**

The concept for these meetings is one of maximum interest - minimum breadth, with the aim to cater for a minority with a specific interest in common. Participants at such a meeting would be expected to range from experts to those whose entry into the particular topic is imminent.

It is planned that Workshops on the following topics will take place during the early Summer-Autumn 1985.

- |   |   |
|---|---|
| Position Sensitive Detectors:<br>(early Autumn)                   | Organiser: Mr P B McAllister<br>Analytical Services<br>BICC Res and Eng Ltd<br>38 Wood Lane<br>LONDON W12 7DX<br>01 743 1212                |
| Stress Analysis by XRD:<br>(April/May)                            | Organiser: Dr C Baxter<br>Aero Division<br>R and D Group Labs<br>Rolls-Royce (1971) Ltd<br>PO BOX 31<br>Derby DE2 8BJ<br>0332-42424 Ext 711 |
| Interpretation of Double-<br>Crystal Rocking Curves<br>(May/June) | Organiser: Mr C Dineen<br>Hirst Research Centre<br>GEC plc<br>East Lane<br>WEMBLEY<br>Middlesex HA9 7PP<br>01 904 1262 Ext 281              |

Please contact the relevant Organiser if you wish to take part in any of these Workshops.



BRITISH CRYSTALLOGRAPHIC ASSOCIATION  
INDUSTRIAL GROUP

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ext. 3498/3471

FINANCIAL ASSISTANCE TO STUDENTS ATTENDING MEETINGS

To encourage the participation of students in Industrial Group activities the Committee has resolved to provide bursaries to help defray travel and/or registration costs incurred by students attending Industrial Group meetings. Such bursaries are, in general, not intended to cover the total cost of attendance at a meeting, but to supplement financial assistance from other sources. Financial constraints dictate that only a limited number of awards can be made available per year. Applications for bursaries will be considered on their merits.

Terms and Conditions

- 1 Applicants must be studying at an institution of higher education in the UK.
- 2 Applications must be supported by a recommendation from the Head of Department. Awards will not normally be made to more than one applicant from any one Department in respect of the same conference.
- 3 It is a requirement that the applicant must be contributing to the conference ie verbal presentation or poster paper.
- 4 Applicants must provide the following information:
  - (a) Title of paper/poster accepted as part of the conference programme.
  - (b) A brief description of the applicant's own research.
  - (c) An estimate of the total cost to the applicant of attendance at the conference.
  - (d) A statement of actions the applicant has taken to obtain support from other sources.

Applications by letter, together with supporting letter from Head of Department, should be sent to the Secretary of the Industrial Group (see above for address).

FIRST ANNOUNCEMENT

A joint meeting of the British Radio Frequency Spectroscopy Group and the British Liquid Crystal Group

BIOLOGICAL MEMBRANES AND OTHER LIQUID CRYSTALS  
The use of Probes in their Investigation

University of Southampton  
23rd - 25th September, 1985

The object of the meeting is to discuss the use of probe techniques in the study of the static and dynamic properties of biological membranes as well as other liquid crystals. This would encompass the application of such techniques together with their advantages and disadvantages. The range of spectroscopies is intended to be wide and will include N.M.R., E.S.R., fluorescence and Raman.

Invited Speakers

N. Boden (University of Leeds)  
R.J. Cherry (University of Essex)  
M.A. Hemminga (Agricultural University, Wageningen)  
G. Kothe (University of Stuttgart)  
Y. Levine (Biophysics Research Group, Utrecht)  
D. Marsh (Max-Planck-Institut, Gottingen)  
E. Meirovitch (Weizmann Institute of Science)  
A. Watts (University of Oxford)  
C. Zannoni (University of Bologna)

Other Contributions

Time will be available for participants to present their latest work either as oral contributions or as posters.

Organizing Committee

J.W. Emsley G.R. Luckhurst  
A.G. Lee J.M. Seddon

Further details and registration forms may be obtained by writing to:

Dr. J.M. Seddon  
Department of Chemistry  
The University  
Southampton, SO9 5NH  
United Kingdom

Conference on

**CRYSTAL DEPOSITION AND DISSOLUTION IN TISSUES**

Lugrin near Evian-les-Bains, September 26-28, 1985

**Topics:**

**A. EXTRACELLULAR AND INTRACELLULAR SOLID PHASES**

Chairman: Prof. K. Simkiss, Department of Zoology, University of Reading, Reading, England

**B. OCCURRENCE OF BIOMINERALS**

Chairman: Dr. K. P. H. Pritzker, Mount Sinai Hospital, Toronto, Canada

**C. MINERALIZATION PROCESSES**

Chairman: Dr. E. C. Moreno, Forsyth Dental Center, Boston, USA

**D. MINERALIZATION THEORIES (with panel discussion)**

Chairman: Prof. W. Fleisch, Pathophysiological Institute, University of Bern, Bern, Switzerland

**E. DEMINERALIZATION**

Chairman: Dr. J. C. Elliott, The London Hospital Medical College, London, England

**Program:** Each session consists of one main lecture and three additional lectures with ample time for discussion. Facilities for the presentation of posters will be provided.

**Organizing Committee:** C. A. Baud (Genève), L. Blomen (Zoetermeer), J. C. Elliott (London), C.-Y. Gerbaulet (Evian), W. E. Klee (Karlsruhe), E. C. Moreno (Boston), K. P. H. Pritzker (Toronto), H. Schäfer (Hamburg)

**Location:** CENTRE DE VACANCES - C. E. SNIAS, F-74500 Lugrin (near Evian-les-Bains, France)

**Access**

by car: Via Evian. There is ample parking space at the vacation center.  
by plane: To Geneva (a bus service to Lugrin will be arranged)  
by train from France or via France: To Evian  
by train from Switzerland or via Switzerland: To Lausanne and then by boat across the lake to Evian

**Fee:** FF 1500.- or \$ 150.- for conference, accomodation (from Wednesday evening, September 25, until Sunday morning, September 29) and for all meals.

9th European Crystallography Meeting - ECM9 - Turin, Italy

A One-Day Pre-Meeting Tutorial : Sunday 1st September 1985

MOLECULAR SYSTEMATICS - DETECTION, EVALUATION, PRESENTATION.

Organized by the IUCr Commission on Small Molecules in collaboration with the Programme and Organizing Committees of ECM9, and with co-sponsorship from the IUCr Commission on Crystallographic Teaching.

Chairman : Dr Frank H. Allen (Cambridge, UK)  
Co-Chairman : Prof. Aldo Domenicano (Rome, Italy)

The role of small-molecule crystallography has undergone significant changes in the past two decades. Automated methods have reduced the time scale for most analyses to days and weeks, rather than months or years. For many chemists X-ray crystallography is a method of choice rather than the method of last resort. As a result the literature now contains reports of some 80,000 crystal structures. Auto-crystallography should, however, bring its own benefits - not least, perhaps, some extra time to consider the broader implications of the work, whether these are crystallographic, chemical, biological or physical in nature. Indeed there is already a trend towards the use of both new and existing structural results in systematic studies of bonding theories, conformational analysis, chemical reactivity and reaction pathways, structure activity studies, hydrogen bonding, solid-state effects, etc.

The International Union of Crystallography has recently recognized the broadening scope of the field by the establishment of a specialist Commission on Small Molecules (CSM); the Tutorial on MOLECULAR SYSTEMATICS represents the first scientific venture of the new Commission. The Tutorial will be held in the Department of Chemistry, University of Turin, on Sunday 1st September 1985, from 9.30 to 17.30. There is no additional registration fee for this one-day session.

The following have been invited to speak on the topics indicated (only one acceptance remains outstanding) :

- Prof. H.J.Geise (Belgium) : Lengths, angles and geometric descriptors - their utility and limitations in comparative stereochemistry.  
Dr R.Taylor (UK) : Statistical techniques for systematic analyses of conformation.  
Prof. H.-B.Bürgi (Switzerland) : Molecular motion, inferences from anisotropic displacement parameters.  
Prof. G.Gilli (Italy) : Reaction pathways and transition-state geometries - the structure correlation principle.  
Dr F.H.Allen (UK) : Crystallographic databases as research tools in systematic studies of molecular structure.  
Dr M.N.Liebman (USA) : Structural comparisons by use of distance-matrix partitioning methods.  
Dr A.J.Kirby (UK) : The use of crystallographic results in structure-reactivity studies.  
Dr J.Bernstein (Israel) : Conformational polymorphism - the interplay between crystal forces and conformation.  
Dr J.J.Stezowski (FRG) : The Commission on Small Molecules of the IUCr - its role and future plans.

Speakers have been asked to provide summaries of their lectures together with a list of important leading references to their topic. These will be distributed at the Meeting.

A finalized program, with timings, directions, etc., should be available in late June. Those interested in attending the Tutorial should register with :

Dr Frank H. Allen,  
University Chemical Laboratory,  
Lensfield Road,  
CAMBRIDGE CB2 1EW,  
England.

An early indication of interest would be appreciated, so that suitable arrangements can be made in Turin.

UNIVERSITY OF EDINBURGH  
DEPARTMENT OF BIOCHEMISTRY

COMPUTING OFFICER (GRADE 2)

Applications are invited for the post of Computing Officer Grade 2 (CO2). The duties of the CO2 will be to assume responsibility for the operation of molecular graphics equipment and for computing facilities within the Department of Biochemistry. It is also expected that the CO2 will engage in research on biomolecular structure. Present interests in the Department in this area concern globular and fibrous protein structure by X-ray diffraction and associated techniques. Informal enquiries about the post would be welcome and should be addressed to Professor A Miller (031-667-1011 ext 2336). Subject to a probationary period, the appointment will be tenable until normal retirement age. Salary will be within the range £7,520-£12,150 per annum.

Further particulars may be obtained from the Secretary to the University, University of Edinburgh, Old College, South Bridge, Edinburgh EH8 9YL, with whom applications (3 copies) including curriculum vitae and names and addresses of two referees, should be lodged not later than 29th March 1985.

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RESEARCH STUDENTSHIP IN

X-RAY STRUCTURE ANALYSIS AND COMPUTER GRAPHICS

Applications are invited for an SERC Earmarked Studentship (for appointment by April 23rd, 1985) to work with Dr. Kim Henrick and Dr. Mary McPartlin on a project entitled "Structural Studies of Hydrocarbon Derivatives of Polynuclear Metal Carbonyl Compounds". The research will be in collaboration with the University of Cambridge, and will involve use of X-ray diffraction to determine the structures of new hydrocarbon derivatives of metal cluster compounds of ruthenium and osmium. Computer graphics will be used to investigate the role of the surface ligands in determining polynuclear structure.

Standard SERC conditions apply to this grant which will run for three years.

Applications with the names of two academic referees and curriculum vitae should be sent as soon as possible to:

Dr. P.G. Owston,  
School of Chemistry,  
Department of Applied Physical Science,  
The Polytechnic of North London,  
London N7 8DB.

METHODS AND APPLICATIONS IN CRYSTALLOGRAPHIC COMPUTING,  
Edited by S R Hall (Univ. of W. Australia) and T Ashida (Nagoya  
University). Clarendon Press, Oxford, 1984 ISBN 0-19-855190-8  
£25 506 pp + ix

This volume is a collection of papers presented at the International  
Summer School on Crystallographic Computing held at Kyoto, Japan,  
18-27 August 1983. It opens with five papers on data measurement  
and processing: film measurement and area detectors for single-  
crystal diffraction patterns (Arndt), diffractometer control  
techniques (Clegg), intensity measurement by diffractometry (Clegg),  
correcting intensity data for systematic effects (Flack) and  
'photon factory' data collection systems (Satow).

Solution techniques are treated in the following papers:  
Patterson methods and protein applications (J E Johnson), three  
papers on structure invariants and seminvariants (Schenk, Overbeek  
and Kiers), a review of multiresolution methods (Woolfson), and  
papers on direct methods for macromolecules (J. Karle), isomorphous  
replacement and anomalous dispersion for proteins (Bricogne) and  
Crystallographic inversion using information theory (Varghese and  
S W Wilkins).

The section on refinement techniques comprises papers on least  
squares and weights (Rollett), least squares and optimization  
(Diamond), fast Fourier transform least squares (Isaacs),  
refinement constraints in proteins and nucleic acids (Sussman),  
phase extension techniques for proteins (Bricogne), and the  
refinement of myoglobin and cytochrome C (Takano) and of 22n insulin  
(Sakabe, Sasaki and Sakabe).

There are four useful papers on accurate electron density analysis:  
on diffraction theory and practice (Kato), electrostatic properties  
(Spackman and Stewart), d-electron distributions in transition  
metal compounds (Marumo), and high precision problems (Maslen).

Next are papers on computer software (Hall), array processors  
(Furey), the design of crystallographic databases (I.D. Brown)  
and on automatic analysis of crystal and molecular geometry on  
data files (Murray-Rust). The computer theme continues with  
interactive vector graphics (Diamond) and graphics for molecular  
modelling (Pflugrath, Saper and Quiocho).

The book is completed by papers on powder methods (Shirley),  
gas electron diffraction (Kuchitsu), electron microscopy at atomic  
level (Uyeda) and on lattice imaging (Iijima), as well as  
reproducing eighteen brief communications. It is illustrated  
by numerous line diagrams of good quality. Despite the lack of  
an index, this useful volume should be on the bookshelf of every  
crystallographer making use of computing, (i.e. almost all of us!)

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FORTHCOMING MEETINGS

- 1985
- 25-27 March BCA Spring Meeting, Bristol : Dr Judith Howard,  
Dept of Inorganic Chemistry, Univ of Bristol,  
Cantock's Close, Bristol BS8 1TS
- 26-28 March Solid State Chemistry Annual Conference,  
St. Andrews : Dr J F Gibson, Royal Society of  
Chemistry, Burlington House, London W1V 0BN
- 1-3 April Molecular Crystals Discussion Group, Canterbury:  
Dr J D Wright, Univ Chemistry Lab, Canterbury,  
Kent, CT2 7NH
- 1-3 April Polymer Liquid Crystals, Cambridge : Mrs Y A Fish,  
Royal Society of Chemistry, Burlington House,  
London W1V 0BN
- 1-4 April Progress in X-ray Studies by Synchrotron  
Radiation, Strasbourg : Departement de Physique,  
3 rue de l'Université, F-67084 Strasbourg Cedex,  
France
- 15-17 April Molecular Graphics Society Annual Meeting,  
Oxford : Dr R Hubbard, Dept of Chemistry, Univ of  
York, Heslington, York YO1 5DD
- 15-19 April Principles of Electron Microscopy + TEM, Leeds:  
The Administrator, Royal Microscopical Society,  
37/38 St Clements, Oxford OX4 1AJ
- 17-18 April Small Angle Neutron Scattering from Organized  
Systems, London : Dr R W Richards, Dept of Pure  
& Applied Chemistry, Univ of Strathclyde,  
Glasgow G1 1XL
- 22-24 May Metals Structures Conference, Melbourne :  
The Institute of Engineers Australia, 11 National  
Circuit, Barton ACT 2600 Australia
- 24 May - 6 June Static & Dynamic Implications of Precise  
Structural Information (Course), Erice, Sicily :  
Dr P Murray-Rust, Glaxo Group Research Ltd.,  
Greenford, Middx. UB6 0HE
- 24-28 June Gordon Conference on Liquid Crystals, Wolfeboro,  
New Hampshire : Dr Alfred Saupe, Liquid Crystal  
Institute, Kent State University, Kent, Ohio  
44242 USA
- 7-12 July 7th Internat Conf on the Chemistry of the  
Organic Solid State, Iraklion, Crete : Dr E  
Hadjoudis, Chemistry Dept Nuclear Research  
Centre, "Demokritos", Aghia Paraskevi, Attiki,  
Greece
- 28 July - 3 August Sagamore VIII on Charge, Spin and  
momentum densities. Sångå-Såby, Sweden  
Prof. Ivar Olovsson, Dept of Chemistry,  
University of Uppsala, Box 531, S-751 21  
Uppsala, Sweden.
- 29 July - 2 August 2nd International Synchrotron Radiation  
Instrumentation Conf. Stanford University  
K M Cantwell, Administrative Coordinator  
SSRL Bin 69, P O Box 4349, Stanford CA 94305 USA
- 12 - 16 August Zeolite 85: Occurrence, properties  
and Utilization of Natural Zeolites.  
Budapest: Dr J Engelhardt, Central Research  
Institute for Chem, Hungarian Academy of Sciences,  
H-1525 Budapest, P O Box 17 Hungary.
- 14-16 August 1985 Protein Crystal Growth, Stanford,  
Dr R C DeMattei, Center for Materials Research,  
Stanford Univ., Stanford CA 94305 USA
- 18-23 August 1985 Structural Studies of Synchrotron Radiation:  
ACA Meeting, Stanford University.  
K M Cantwell, SSRL, Stanford Univ. P O Box 4349,  
Bin 69, Stanford CA 94305, USA
- 19-24 August Int. Conf. on Neutron Scattering, Santa Fe,  
New Mexico.  
Dr J Eckert, Los Alamos National Lab., Mailstop H805,  
Los Alamos, New Mexico 87545 USA.
- 20-24 August 12th Hungarian Diffraction Conf. Sopron, Hungary,  
Roland Eötvös Physical Society, H-1368 Budapest,  
P O Box 240, Hungary.
- 1 September Molecular Systematics - Detection, Evaluation,  
Presentation, Turin.  
Dr Frank J Allen, Univ. Chem. Lab., Lensfield Road  
Cambridge, CB2 1EW  
(see this issue)
- 2-5 September EMAG 85, Newcastle-on-Tyne  
The Meetings Officer, The Institute of Physics,  
47 Belgrave Square, London, SW1X 8QX.
- 2-6 September 9th European Crystallographic Meeting (ECM-9)  
Turin, Prof. G Ferraris, Istituto di Mineralogia,  
Cristallografia e Geochimica, Università di Torino,  
via san Massimo 22, 10123 Torino, Italy.
- 9-10 September Microscopy of Polymers & Composites, Brunel  
University, Uxbridge.  
The Administrator, Royal Microscopical Society,  
37/38 St Clements, Oxford, OX4 1AJ.
- 14 Sept - 1 Oct 1985  
Summer School on Synchrotron Radiation Sources  
and their Applications.  
Univ. of Aberdeen (14-28 Sept)  
+ Daresbury Laboratory (28 Sept - 1 Oct)  
Prof G V Marr, Dent of Natural Philosophy,  
Aberdeen Univ, Aberdeen, AB9 2UE.



- 16-18 September Strength and Structure in Carbons and Graphites  
Univ. of Liverpool.  
The Meetings Officer, IoP, 47 Belgrave Sq.,  
London, SW1X 8QX.
- 17-19 September Image Simulation & Processing for High Resolution EM  
Cambridge Univ.  
The Administrator, Royal Microscopical Society,  
37/38 St Clements, Oxford, OX4 1AJ.
- 19-21 September 6th Meeting of the Geological Societies of  
the British Isles.  
Birmingham  
Professor P A Garrett, Dept of Geological Sciences,  
The University, Birmingham B15 2TT
- 23-25 September Biological Membranes and other Liquid Crystals  
Southampton  
Dr J M Seddon, Dept of Chem., The University,  
Southampton, SO9 5NH (see this issue)
- 26-28 September Crystal Deposition and Dissolution in Tissues  
Evian-les-Bains  
Prof W E Klee, Institut für Kristallographie  
der Universität, Kaiserstrasse 12, D-7500 Karlsruhe  
Fed. Rep. Germany, (See this issue).
- 30 Sept - 4 Oct 11th Molecular Crystal Symp. Lugano, Switzerland.  
Mr D Kojler, Dept of Physics, Univ. of Basel,  
Klingelbergstrasse 82, CH-4056 Basel, Switz.
- 28 October '85 7th Bragg Lecture : 5.30 pm Univ. of Leeds  
Dr M Moore, Dept of Phys, Royal Holloway College  
Egham Hill, Egham, Surrey, TW20 OEX.
- 31 October '85 7th Bragg Lecture : 5.30 pm Royal Institution,  
London, W1.  
Dr M Moore, Dept of Physics, Royal Holloway College  
Egham Hill, Egham, Surrey, TW20 OEX.
- 7 November '85 Mineralogical Society General Meeting,  
Burlington House, London, W1  
Min. Soc., 41 Queen's Gate, London SW7 5HR
- 14 November '85 Crystallography in Industry (BCA Industrial Group)  
AERE Harwell  
Mr B A Bellamy, Materials Division, Bldg 393,  
AERE Harwell, Didcot, Oxon OX11 0RA
- 19 November '85 Systematics in Structural Chemistry,  
(Chem Cryst. Gp: BCA) Birkbeck College, London.  
Dr B Beagley, Dept of Chem., UMIST, P O Box 88  
Manchester M60 1QD
- 18-20 December Annual Solid State Physics Conf. Reading  
Dr J A Blackman, Dept of Physics, Univ of Reading  
Whiteknights, Reading, Berks, RG6 2AF

1986

- 7-10 April 1986 BCA Spring Meeting, Univ. of York  
Prof. M M Woolfson, Dept of Physics,  
Univ. of York, Heslington, York, YO1 5DD
- 8-11 April 1986 RSC Annual Meeting, University of Warwick,  
Coventry  
Dr J F Gibson, Royal Society of Chemistry,  
Burlington House, London, W1V 0BN
- 10-19 June 1986 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.
- 22-27 June 1986 ACA Summer Meeting, Hamilton, Ontario  
Dr I D Brown, Inst for Materials Research,  
McMaster Univ., Hamilton, Ontario, Canada  
L8S 4M1
- 5-12 July 1986 Internat. Summer School on Crystal Growth  
Edinburgh  
Dr P M Dryburgh, School of Engineering,  
King's Buildings, Univ of Edinburgh, EH9 3JL.
- 8-11 July 1986 Molecules, Clusters and Networks in the Solid  
State, Univ of Birmingham,  
Dr J F Gibson, Royal Soc. of Chem., Burlington  
House, London, W1V 0BN
- 13-18 July 1986 14th General Meeting of the International  
Mineralogical Association Stanford Univ  
California.  
Prof C T Prewitt, S.U.N.Y., Dept of Earth and  
Space Sciences, Stony brook, N Y 11794, USA
- 14-18 July 1986 International Conf. on Crystal Growth ICCG-8  
York  
F W Ainger, Allen Clark Research Centre,  
Plessey Research (Caswell) Ltd, Caswell,  
Towcester, Northants NN12 8EQ
- 17-22 August 1986 7th International Zeolite Conf. Tokyo  
Prof. Hiro-o Tominaga, Dept of Synth. Chemistry,  
Faculty of Engineering, Univ of Tokyo, Hongo,  
Bunkyo-ku, Tokyo 113, Japan.
- 8-11 September 16th European Solid State Device Research  
Conference (ESSDERC '86) Cambridge  
The Meetings Officer, IoP, 47 Belgrave Sq.,  
London SW1X 8QX
- 8-12 September Lattice Defects in Ionic Crystals, Madrid  
Mr F J Lopez, Dept. Optica y Estructura Materia,  
Universidad Autonoma de Madrid, Cantoblanco,  
E-28049 Madrid, Spain.

- 17-19 December 1986 Annual Solid State Physics Conf  
Imperial College, London  
The Meetings Officer, Institute of Physics  
47 Belgrave Square, London SW1X 8QX
- 1987
- 7-9 April 1987 BCA Spring Meeting  
Heriot-Watt Univ. Edinburgh  
Dr J C Halfpenny, Dept of Chem  
Napier College, Colinton Road  
Edinburgh, EH10 5DT
- 13-16 April 1987 RSC Annual Congress Swansea  
Dr J F Gibson, Royal Society of Chemistry  
Burlington House, London W1V 0BN
- 12-20 August 1987 14th General Assembly and International  
Congress of Crystallography, Perth, W.A.  
Dr E N Maslen, Crystallography Centre,  
Univ. of Western Australia, Nedlands 6009  
Western Australia.
- 27 Aug - 6 Sept Crystal Growth in Science & Technology  
Erice, Trapani, Sicily  
Dr Lodovico 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 de Sanseverino, International  
School of Crsytallography, Piazza Porta  
San Donato 1, 40127 Bologna, Italy.
- 1989
- 1 - 11 June 1989 X-ray Crystallography & Drug Action,  
Erice, Sicily  
Prof L Riva di Sanseverino, International  
School of Crystallography, Piazza Porta  
San Donato 1, 40127 Bologna, Italy.
- 1990
- ? August 1990 15th General Assembly I.U.Cr. Bordeaux  
Exec. Sec. I.U.Cr, 5 Abbey Square,  
Chester CH1 2HU.

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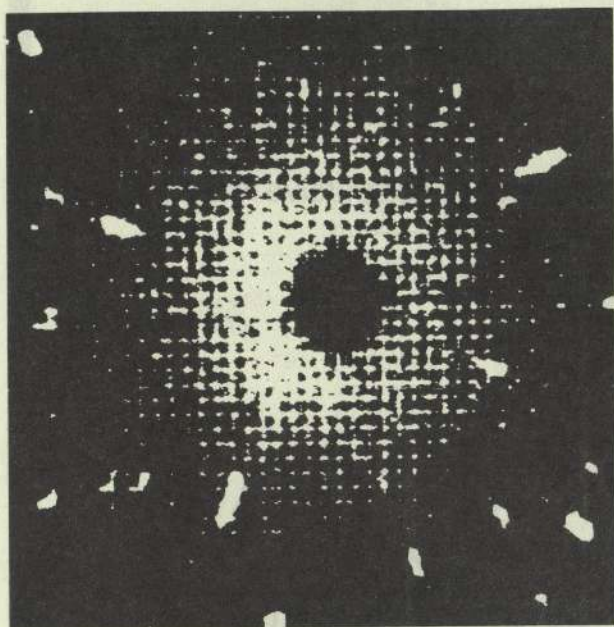
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