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#### Enclosures with this issue

- BCA Membership Form
- World Directory of Crystallographers
- BCA Bristol Meeting Registration Form
- Small Molecules Feedback Form

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The striking pattern on the front cover of this Issue of Crystallography News is a prediction of the diffraction pattern from a crystal of the protein pea lectin illuminated by the continuous spectrum of synchrotron x-radiation from the newest source on the SRS, the superconducting wiggler magnet, which offers much shorter wavelength radiation than any other source at the SRS and is extremely intense.

The new instrument for protein crystallography on the wiggler beam line commenced operation this year after a design and construction period of 2 years. The instrument offers tunable, intense beams of x-radiation via monochromator/mirror beam line optics but in addition the possibility of illuminating samples with the full spectrum, modified only by the absorption of beryllium windows in the beam line (ie 0.2Å <λ< 4Å onto the sample). Experiments conducted by Dr J R Helliwell and his colleagues Drs M Papiz and R Liddington at Daresbury with a crystal of the protein pea lectin (space group P2₁2₁2₁, a = 50Å, b = 60Å, c = 136Å) revealed that in a series of six "snapshots" a complete sweep of the unique portion of reciprocal space could be achieved in less than a minute. The sample withstood a photon intensity level which we calculate to be ~ 10³-10⁴ photons/sec/mm². (A rotating anode emission line corresponds to ~10⁵ photons/sec/mm² at the sample).

In collaboration with Dr M Elder and P Machin of the Computer Applications Group at Daresbury the patterns are undergoing evaluation to assess the statistical quality of the data. Obviously the outcome of this will determine the applicability of the method in quantitative crystal structure analysis. The prediction, on the cover was made on the group's PERQ computer, taking especial advantage of the fine pixel resolution of the PERQ screen.

The pea lectin crystal used was kindly supplied by Dr H Knapbaur and Dr F L Suddath of the University of Birmingham, Alabama, USA and was of a size (= 0.3mm) that is usual in protein crystallography. The high intensity of the beam however can be used to study smaller samples. Dr H Harding of the University of Liverpool and her coworker Dr J Hails are taking advantage of the intense white beam to collect data on micro-crystals. In addition, the method has also been successfully exploited recently with the collection of good signal to noise data from micro-crystals of gramicidin A by Professor K O Hodgson and Dr S Hedman at Daresbury even with a protein micro-crystal mounted wet in a capillary.

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**CRYSTALLOGRAPHY NEWS** is published by the British Crystallographic Association. See page 36 for editorial information.

For details of advertisement rates please contact Mr S Sadler, Advertisement Manager, The Institute of Physics, Publishing Division, Techno House, Redcliffe Way, Bristol BS1 6NX. (Tel: 0272 397481).
It is 8 years since white beam experiments on protein crystals were attempted on the old NINA synchrotron (Helliwell and Bordas unpublished); unfortunately, the crystals used did not diffract at all. The present results, and those of the group led by Professor K Moffat, Cornell, USA, with "modified Laue" \( \frac{1}{3} \) = 0.2, diffract from protein crystals, necessitates the modification of presently available reviews on the subject!

**UNAUTHORISED "BCA" MEETINGS**

As a result of a meeting held in spring of this year being advertised unjustifiably as a "BCA" meeting, the Council has asked me to write a short item regarding procedures to be followed where ideas of new meetings arise outside of the Council or Group Committees.

The Association welcomes new initiatives in organizing meetings, whether on a particular topic of interest to crystallographers only, or on topics suitable for joint meetings with other societies. It is, however, essential that where the organizers wish to involve the BCA or use its name, it is done with the knowledge and consent of the Association. I need not spell out the potential confusion and mischief which might arise if this is not done.

Where the proposed meeting falls clearly within the ambit of a Group, and the organizers wish to work through the Group, the particular Group Secretary should be approached in the first instance. The Group Secretary would then make sure that the appropriate persons are informed.

Where the initiative is to hold a meeting under the aegis of the BCA as a whole, or to have the BCA associated in some way, the first approach should be to the Secretary of the BCA, who will inform the other Officers and Members of Council so that the proposal can be discussed.

I am already aware of several new initiatives for meetings with other organizations and of ideas for new types of meetings. I am glad that the existence of our Association helps to generate greater interest in meetings of various kind, as this is something which should benefit our members and scientists generally.

**ELECTIONS TO THE COUNCIL**

The terms of office of the following Officers or Members of the Council and with the 1985 BCA Spring Meeting:

- **Vice-President** - Professor D.W.J. Cruickshank FRS
- **Secretary** - Dr A.C. Skapski
- **Member** - Mr J.W. Harding

Dr Skapski and Mr Harding, having served two consecutive terms, are not eligible for re-election for a further term in the same office.

Elections will be held at the AGM on Tuesday, 26th March 1985, and nominations are invited for the above three vacancies. They should reach the Secretary by Friday, 22nd March 1985, at the Department of Chemistry, Imperial College, London SW7 2AY. The nominations should be signed by two members of the BCA, and be accompanied by the written consent of the candidate to serve if elected.
THE ANNUAL GENERAL MEETING
OF THE
BRITISH CRYSTALLOGRAPHIC ASSOCIATION

To be held in Lecture Theatre 2, School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TD, at 4.45pm on Tuesday, 26th March 1985.

AGENDA

1) Approval of the agenda.
2) Minutes of the Annual General Meeting held at Nottingham on Tuesday, 3rd April 1984.
3) Matters arising from the minutes.
5) Proposal to change the By-Laws of the Association:
   a) By-Law A.4 delete "(a) Ordinary" and the whole of subparagraph (b).
   b) By-Law B.2 delete 'Ordinary'.
   c) By-Law B.3 is deleted.
   d) By-Laws I.3, I.4, and I.5 are deleted.
6) Report of the Treasurer.
7) Consideration and approval of accounts.
8) Annual subscription for Ordinary Members - no change proposed.
9) Election of Officers - a) Vice-President
    b) Secretary.
10) Election of one other Member of Council.
11) Appointment of Auditors.
12) Any other business.

Changes to the By-Laws of BCA

The success and usefulness of 'Crystallography News' is bringing its own problems. Last year it cost just over £2 to get the four issues of Crystallography News to each member, but this is more than the finances of the Joint Groups can stand: indeed it exceeds their per capita income.

Council considered this problem at its September meeting. Everyone agreed that the distribution of Crystallography News is an essential part of our activities which must be maintained.

The Steering Committee, which drew up the BCA constitution, was determined to preserve the right of the Joint Groups to distribute their Newsletter, independently if they so wished. They included By-Law I3 which imposed a duty on the Joint Groups to meet the expenses of distributing the Newsletter. This is no longer practicable, so this By-Law must be deleted.

The By-Laws also give the Joint Groups the option to make their own arrangements for distributing notices of BCA meetings and (Annual) General Meetings. Because some of our members are members of BCA as well as members of a Joint Group, this leads to complications in membership records and makes it hard to avoid duplicate mailings to some individuals.

Other changes in the By-Laws are proposed to make the distribution of notices of BCA meetings the responsibility of the BCA and not of the Joint Groups. They do not affect the operation of the Joint Groups' own affairs.

Formal notice of the proposal to change the By-Laws appears in the Agenda of the Annual General Meeting, elsewhere in this newsletter.

D.M. Blow
President
MEMBERSHIP RENEWAL or APPLICATION for 1985

Subscriptions for existing or new members fall due on 1 January 1985. A membership renewal and application form is enclosed separately in this edition of Crystallography News. Please complete and return it with your subscription to the Treasurer at the address on the form. Brief details of the subscriptions payable for various categories of membership are given below.

ORDINARY AND REDUCED RATE MEMBERS

The 1985 subscription for ordinary members is £10 and that for Reduced Rate members £5. Reduced Rate members are those who either are no longer in full-time employment or are full-time students. The appropriate fee is due from all members in these categories except that those who joined the Association on or after 1 October 1984 are not required to pay a renewal subscription until 1 January 1986. The annual subscription includes membership of one of the four Groups. Further Groups may be joined by payment of £1 per additional Group.

JOINT MEMBERS

Those who in 1985 are members of the Royal Society of Chemistry Chemical Crystallography Group or of the Institute of Physics Crystallography Group are automatically members of the corresponding BCA Group. No subscription is required from Joint Members unless they wish to join additional Groups. The fee for additional Groups is £1 per group and should be returned to the Treasurer with a completed membership form. It would be immensely helpful for record purposes if Joint Members would return a membership form even if they are joining no additional Groups and consequently are not liable for a subscription.

WORLD DIRECTORY OF CRYSTALLOGRAPHERS

A new edition of the World Directory is being prepared and a separate form is enclosed in this edition of Crystallography News to enable the return of information for that revision. If members do not return that form their name, title and business address from the BCA membership renewal form will be used for the revision unless they state, by ticking the appropriate box, that they do not wish that.

R. Hine
Treasurer

World Directory of Crystallographers, Seventh Edition

The seventh edition of the World Directory of Crystallographers is now in preparation. All those whose names appeared in the Sixth Edition have been sent a form to allow them to update their entries. Any other scientist who wishes his name to be included in the Directory (as well as any who were in the Sixth Edition and have not received an updating form) should complete the form given in Crystallography News and return it as soon as possible to the UK Subeditor: Dr D W Penfold, UK Subeditor WD7, 5 Abbey Square, Chester CH1 2HU.

All UK members of the British Crystallographic Association should note that, unless they request otherwise on their Membership Renewal form (see elsewhere in this issue), their names, titles and business addresses will be included in the Seventh Edition whether or not they return a data entry form. All members are therefore urged to return a data entry form so that their entries can be as complete as possible. The data entry form can of course be copied. It should perhaps be noted that about half the present members of the BCA do not have their names in the Sixth Edition and, perhaps even more surprising, more than half of those whose names do appear in the Sixth Edition are not members of the BCA.

If you are one of those who belong to both the BCA and have their name in the Sixth Edition, please encourage your less fortunate colleagues to join you in this happy state.

D W Penfold
B.C.A. Annual Meeting March 25th-27th 1985 Bristol

Registration Details:

Deadline for papers*: January 14th 1985

Deadline for Registration: February 11th 1985

* Full scientific programs for each group were published in the previous B.C.A. newsletter. Titles and Authors of all presented papers will be published in the June Newsletter. This will enable all foreign members to follow our meetings more closely as well as those in the U.K. who are unable to attend.

Registration Fees:

The new shorter format of the meeting has led to the division of the scientific programs into two sessions: Session 1 will comprise of Monday afternoon and Tuesday: Session 2 will comprise of Tuesday afternoon and Wednesday.

Full registration fee (3 days: 2 sessions)
B.C.A. Member: £20.00 Student Member: £10.00

Session registration fee (Session 1 or Session 2)
B.C.A. Member: £15.00 Student Member: £7.50

ADDITIONAL fee for those Non-Members of the B.C.A. £10.00
ADDITIONAL fee for Student or Retired Non-Members £5.00

Registration:

Registration will take place from 11 a.m. in the School of Chemistry, Cantocks Close. For those participants wishing to check in at Goldney Hall, someone will be there to direct them to the Chemistry School. Lunch will be available from 12.15 p.m. in the School of Chemistry for those who have requested and paid for it.

Accommodation:

Delegates will be housed in Goldney Hall, Clifton in single rooms with hand-washing facilities. Six rooms share communal bathroom, kitchen and lounge areas. Continental breakfast is provided in each common area in the mornings. As there are no lifts, please indicate at the time of registration whether you will require ground floor accommodation and also if you would prefer to share a suite of rooms with other non-smokers.

Participants who prefer to make their own arrangements should request the hotel list on registration. There are several small hotels and guesthouses within walking distance of Chemistry. Bed and Breakfast, per night, in Goldney Hall is £10.75. Lunch, if ordered in advance, will be served in the School of Chemistry, cost £2.75.

Monday March 25th: Reception by the B.C.A. and University of Bristol, followed by an organ recital in the Great Hall and dinner immediately afterwards in Goldney Hall.

Tuesday March 26th: The B.C.A. Plenary Lecture will be given by Professor Dorothy Hodgkin O.M., F.R.S. The Conference Dinner will follow later in the Orangery at Goldney Hall, cost £9.75.

Transport:

Bristol is easily reached by the M4, M32 and M5 motorways and other major roads (see map below).

There are two British Rail Stations which serve the City (see map below), but be warned Parkway Station is out of town some 5 miles and requires a bus ride, an expensive taxi fare or a friend to enable you to reach Chemistry. Temple Meads is the City Centre Railway Station, a short bus ride or reasonable cab fare from the Hall and Chemistry.

National Coaches run an hourly (inexpensive) service to Bristol from London and regular services from many other major cities. The Coach Station is only 10 minutes walk from the Chemistry Department (but note it is uphill slightly if you are carrying luggage).

Further details (travel, maps, etc.) will be sent to each registered participant nearer the meeting.
Parking is rather limited at Goldney Hall itself, but there is local parking in Clifton close to the Hall for those delegates who arrive by car. We would discourage you from driving to Chemistry as the parking there is staff restricted.

There is an N.C.P. approximately halfway between the Residences and Chemistry. Also, we hope to run a minibus at strategic times for participants with a disability.

T-shirts with our B.C.A. logo are now available and will be on sale at the Meeting, or from the Organisers in advance. Cost £3.75. (Red or Black on White).

This will be held, throughout the meeting, in the Foyer of the School of Chemistry, common to the oral and poster sessions as well as the coffee/tea area. Exhibitors wishing to hire space for display of their products should contact:- JOHN HARDING, BRITISH RAIL RESEARCH, DERBY. Telephone 0332 - 42442 Exn. 3727, as soon as possible, with their anticipated requirements.

The poster exhibition will take place throughout the entire meeting. No space restriction is anticipated. The poster boards will be in position from Monday morning March 25th, to help those who have their oral session that afternoon.

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**B.C.A. BRISTOL 25th-27th March, 1985**

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**Invited Speakers include:** Professor Dorothy Hodgkin\(^\ddagger\), (Oxford); Professor Tom Blundell\(^\ddagger\), (London); Professor G.J. Davies\(^\ddagger\), (Sheffield); Dr. Ted Atkins\(^\ddagger\), (Bristol); Dr. G.S. Pawley\(^\ddagger\), (Edinburgh); Dr. F. Allen\(^\ddagger\), (Cambridge) and Professor D.W.J. Cruickshank (U.M.I.S.T.)\(^\ddagger\).

\(^\ddagger\) Given by the celebrated recitalist Jennifer Bate.
The Chemical Crystallography Session on Wednesday 27 March has as its theme the utilization and publication of crystallographic results.

The invited speakers are Dr F H Allen (University of Cambridge), "Crystallographic Data Bases: What's in them for You?"; Dr P Murray-Rust (GLAXO), "Chemical Applications of Crystallographic Data Files"; Dr M B Hursthouse (Queen Mary College), "Publication of Crystallographic Results". A panel-led discussion following the talks will provide an opportunity for lively debate. Those of us who joined the Chemical Crystallography Group through membership of the Royal Society of Chemistry will find this year's theme particularly relevant.

Poster contributions can be on any aspect of Chemical Crystallography.

Do come! Do bring a poster! (See elsewhere in Crystallography News for further details; our organiser is Dr A G Orpen, School of Chemistry, The University, Bristol BS8 1TS.)

Annual General Meeting Notice is given that the AGM of the Group will be held on Tuesday 26 March 1985 at 14.00hrs at the School of Chemistry, University of Bristol, during the BCA Spring Meeting. The business will include the election of members to fill posts falling vacant at the AGM. Officers due to retire at the coming AGM are the Chairman, Dr M B Hursthouse, the Vice-Chairman, Dr O Kennard, and two committee members, Dr C J Gilmore and Dr D R Russell; none are eligible for re-election to the same office. Nominations for the posts becoming vacant shall be proposed by not less than three members of the Group and shall be accompanied by the written consent of the nominee. Nominations for four Ordinary Members of the Committee, which shall be proposed by not less than three members of the Group and shall be accompanied by the written consent of the nominee, shall be sent to reach the Honorary Secretary of the Group not later than seven days before the Annual General Meeting.
CRUICKSHANK SYMPOSIUM : Manchester 11 - 13 September 1984

This highly successful symposium was organised by Dr Brian Beagley and other friends in the UMIST Chemistry Department to mark Professor Durward Cruickshank's retirement (fiscal but not scientific, as was evident throughout the proceedings). It was indeed a meeting of friends, old and new, with invited speakers (13) coming from as far afield as Oslo and Los Angeles and other participants (75) from Dundee, New Zealand and many Crystallographic establishments between.

The scientific sessions covered the main aspects of modern experimental and theoretical studies of crystal and molecular structure. The invited speakers gave clear accounts of their fields - to most of which Durward has contributed: crystallographic computing, considerations of accuracy, molecular dynamics (claimed by Dr Pawley as a thriving branch of physics), and ab initio calculations on small molecules compared with accurate crystal structures and the results of gas electron diffraction. Dr Hellitwell spoke about Durward's most recent interest, the use of synchrotron radiation, and presented him with a framed Laue diffraction pattern of great beauty from a pea lectin crystal recorded at the Daresbury 'Wiggler' Protein Crystallography Station. Professor Dorothy Hodgkin continued this theme with observations on the progress of biological structure determination.

The organisers are to be congratulated for arranging ample time, both between the scientific sessions and outside them, for informal contacts. On the first day, Durward invited participants and colleagues to a reception at the Whitworth Art Gallery, showing off Manchester University's remarkable collection of paintings, drawings and textiles. The conference dinner was also remarkable, for its triple toast to Professor D W J Cruickshank, F R S, as International Scientist (Professor Otto Bastiansen) and Crystallographer (Professor G A Jeffrey) in the Manchester Tradition (Professor Henry Lipson). In his reply, Durward gave further details of his progress from engineer to mathematician to mathematical chemist in Leeds, guided by Professor Cox (present, now Sir Gordon, at the Symposium). Constructing an electro-mechanical system for summing structure factors led naturally on to the use of electronic computers, encouraged by the world's first summer school in crystallographic computing at Cambridge in 1950.

In short, the symposium was a well-earned tribute to a charming and very approachable internationally minded crystallographer who has done much for his subject, both scientifically and organisationally.

C J E Kempster

X-RAY MICROSCOPY : 8 January 1985
A one-day workshop is to be held on Tuesday 8 January 1985 at King's College London to discuss the scanning transmission soft X-ray microscope : STXM.

The existence of very bright X-ray sources (e.g. at Daresbury) and the development of new X-ray focussing methods are now bringing X-ray microscopy to the threshold of a new era of application. The spatial resolution of the instrument initially would be about 70 nm, but it is hoped 10 - 20 nm would be reached eventually. Contrast would be provided by the natural differences in soft X-ray absorption, and specimens of thickness 1 - 2 μm could be examined. As the dwell time of the scanning spot would be 1 - 100 μs on one picture element, the study of some in vivo material could be contemplated. Using the natural divergence of the X-ray beam combined with specimen tilting, 3D images could be reconstructed.

Potential users should write immediately to Dr. Phil Duke, SERC Daresbury Laboratory, Daresbury, Warrington WA4 4AD, (giving name, address, telephone number and brief outline of interest in using the STXM).
Modern Crystallography
published in
Springer Series in Solid-State Sciences

Editors: M. Cardona, P. Fulde, H.-J. Queisser

Volume 15
B. K. Vainshtein
Modern Crystallography I
Symmetry of Crystals. Methods of Structural Crystallography
1981. 272 figures, some in color. XVII, 599 pages
Hard cover DM 98,–; approx. US $ 35.70
ISBN 3-540-10516-1


“This book is noteworthy for two reasons. Each subject is discussed in depth and with elegance. However, the discussion for each subject is extended into more areas than is generally found in crystallography texts. This will make it essential for everyone’s bookshelf.”

American Crystallographic Association

Volume 21
B. K. Vainshtein, V. M. Fridkin, V. L. Indenbom
Modern Crystallography II
Structure of Crystals
1982. 345 figures. XVII, 433 pages
Hard cover DM 114,–; approx. US $ 41.50
ISBN 3-540-16517-4

This second volume of Modern Crystallography describes the ideal atomic structure of crystals, the real structure of crystals with its various disturbances, and the electron structure and lattice dynamics. The fundamentals of the theory of chemical bonding between atoms are given, and the geometric representations in the theory of crystalline structure and crystal chemistry, as well as the lattice energy, are considered. The important classes of crystalline structures in inorganic and organic compounds and also the structure of polymers, liquid crystals, biological crystals, and macromolecules are described. The elements of the electron theory of crystal lattices, which help to classify crystals by their energy spectrum, are presented. Lattice dynamics and phase transitions are discussed. Concepts of the real structure of crystals with its various thermodynamic equilibrium and nonequilibrium disturbances are described. All types of defects are analyzed and described mathematically, with special emphasis on dislocation theory.

In preparation
Volume 36
A. A. Chernev
Modern Crystallography III
Crystal Growth
With contributions by E. I. Givargizov, K. S. Bagdasarov, V. A. Kuznetsov, L. N. Demianets, A. N. Lohachev 1984. 244 figures. XX, 517 pages
Hard cover DM 154,–; approx. US $ 56.10
ISBN 3-540-11516-X

The third in a four-part treatment of modern crystallography, this volume concentrates on the phenomena and techniques of crystal growth. The basic concepts are systematically presented and related to all facets of crystal growth. Recent results are reviewed and discussed by a team of experts. The first one-volume treatment of the main growth techniques used in industry today, this book is written on a level that affords the reader a basic understanding of the physical, chemical and technological principles involved.

Springer-Verlag
Berlin Heidelberg New York Tokyo

RADIATION SAFETY

New Draft Regulations

In July the Health and Safety Executive issued a new draft, the Ionising Radiation Regulations 1984. Unlike the previous draft, this consisted of Regulations only, with no accompanying Code of Practice. These regulations are intended to come into operation in 1985. The regulation whose details most concern us is Reg. 8, reproduced below. (Schedule 6, broadly, requires all places where the instantaneous dose rate exceeds 7.5μSv h⁻¹ to be in controlled areas.)

The BCA Radiation Safety Subcommittee submitted the following comment on this draft Regulation to the Health and Safety Executive.

"The regulation as written does not seem to cater for machines producing ionising radiation. There ought to be free access to the controlled area at certain times (when the machine is switched off, or a shutter is closed).

The regulation could mean that the controlled area only exists when the machine is switched on, etc., but if so 8 (5) concerning demarcation of the area should indicate that it is necessary to demark it in time also.

If the controlled area exists permanently, but access is only restricted at certain times (which has been our understanding until now) 8 (6) means that a written system of work is always required. It should be modified to allow access when there is no danger that the conditions of 8 (1) and (2) are fulfilled. We think that a written system of work for all such areas would be an excessive and unnecessary administrative burden, and that local rules should be adequate to cover a properly interlocked radiation enclosure."

New Draft Code of Practice

Early in November a new draft Code of Practice was received, comprising over 100 pages. Crystallographers will be most concerned by Part 2, Section 9, reproduced below. The BCA Radiation Safety Subcommittee has not yet formulated its comments, which are required by mid-December. Anyone wishing to make a comment or requiring further information should contact a member of the Radiation Safety Subcommittee.

Radiation Subcommittee: D.M. Blow – Imperial College
M. Hart – Manchester University
M.J. Whelan – Oxford University

From the draft "Health and Safety (Amtd.4) Ionizing Radiations Regulations 1985

Designation of controlled and supervised areas

8.-(1) Every employer shall designate as a controlled area any area under his control which employees can enter and which is required to be so designated by virtue of the provisions of Schedule 6.

(2) Every employer shall designate as a supervised area any area under his control, not being an area designated as a controlled area, in which any dose of ionising radiation received by persons in that area may exceed one-third of any dose which would require that area to be designated as a controlled area in accordance with paragraph (1).

(3) Notwithstanding the provisions of paragraphs (1) and (2), an employer may designate any area under his control as a controlled area or supervised area and any area so designated shall be treated for all purposes as an area designated under paragraphs (1) or (2) as the case may be.

(4) An employer shall not create in any area conditions which would require that area to be designated as a controlled area unless that area is for the time being under his control.

(5) Every employer shall ensure that each controlled area and supervised area that he has designated is suitably described in local rules and that, in the case of any controlled area—

(a) the area is physically demarcated wherever reasonably practicable; and

(b) access to the area is restricted by suitable means.

(6) The employer shall not permit any of his employees or other persons to enter or remain in a controlled area unless that employee or other person either—

(a) is a classified person; or

(b) enters or remains in the area under a written system of work such that—

(1) in the case of an employee aged 18 years or over, he does not receive in any calendar year a dose of ionising radiation exceeding three-tenths of any relevant annual dose limit, or

(11) in the case of any other person, he does not receive in any calendar year a dose of ionising radiation exceeding any relevant dose limit.

(7) An employer shall not permit an employee or other person to enter or remain in a controlled area in accordance with a written system of work under paragraph (6)(b), unless he can demonstrate, by personal dose assessment or other suitable measurements, that the doses are restricted in accordance with that paragraph.
SECTION 9  X-RAY OPTICS

Scope

1 This section of the code applies to any use or testing of a radiation generator for X-ray optics including crystallography, diffraction, emission and absorption spectrometry.

Segregation of the work

2 Dose restriction should be achieved by segregating all equipment in use either by:

(a) the provision of an enclosure, which may be a room or a purpose-made structure, or a photoelectric system the interruption of which curtails the emission of ionising radiations; or

(b) the provision of a close fitting enclosure of the beam and covers for any openings in the equipment through which X-rays could emerge.

Shielding

3 The material used for segregation should be capable of shielding the residual radiation from the useful beam and against scattered radiation so that an instantaneous dose rate of less than 7.5 μSv h⁻¹ is achieved at all accessible parts of the equipment. In many cases the shielding will form part of the equipment, i.e. covers, backstops, collimators, shutters etc, and these or similar provisions would need to be incorporated if photoelectric systems are used for segregation unless a sufficient distance can be used to provide the protection.

Effective devices

4 The shielding or barriers should be fitted with effective devices to ensure that the X-ray tube cannot be energised, or the shutter(s) of the tube opened, unless the shielding or barriers are in position. The device should also operate to de-energise the X-ray tube or close the shutter(s), thereby preventing access to the beam, whichever any cover or accessory is removed from an X-ray tube or if any barrier is moved. The devices should be designed to prevent unauthorised interference, or failure to a dangerous condition. Such an interlock can be either electrical or mechanical.

Automatic Indications

5 All persons in the immediate vicinity of the equipment should know when an X-ray tube is energised to produce X-rays; automatic means of indicating this should be provided as well as means to indicate clearly and, where reasonably practicable, automatically, whether any shutter is open or closed whilst an X-ray tube is energised.

6 Exceptionally it may be necessary to obtain access into the enclosure whilst the X-ray tube is energised and a shutter is open. An example would be where it is not practicable to use a recognised technique with all the safety features in place and it is not reasonably practicable to provide alternative safety features which could be used with the chosen technique.

7 In those cases covered by paragraph 6, where dose rates in the beam averaged over 1 cm² exceed 2.0 mSv h⁻¹ and where exposure to the beam is reasonably foreseeable, a permit to work system should be instituted and
followed. The system should specify precisely how the work should be undertaken and under what conditions, e.g., what safety features are to be retained. Such systems should be supervised to ensure that the work is being done as specified. Only a named person should have access to any facility provided to override the devices, which should be restored to normal operation as soon as the particular operation has been completed, or where the permit to work has expired or has been cancelled.

8 Where paragraph 6 applies and dose rates are so low, or exposure to the beam is so improbable, that an overexposure is most unlikely to occur, the employer may, in place of a permit to work, draw up a method of conducting the work that keeps doses to persons as low as reasonably practicable and which should be included in the local rules. Supervision should be exercised to ensure that the method set down is followed.

GRANTS IN AID

The JCPDS/International Centre for Diffraction Data invites proposals for grants for the preparation of diffraction powder data. A limited number of grants will be available for a one-year period starting 1 April 1985; these grants are intended to be modest supplements to existing projects in order to encourage the generation of powder data in accordance with the guidelines accepted by the International Union of Crystallography.

Proposals will be evaluated according to technical merit. Only proposals leading to the production of powder data for organic substances will be considered for the 1985 awards, and the maximum grant will be $3000 or the equivalent in other currency. The closing date for the receipt of proposals is 25 January 1985.

Guidelines for submitting proposals may be requested from:

The Secretary
JCPDS-ICDD
1601 Park Lane
SWARTHMORE PA 19801
United States of America

Preliminary enquiries may be addressed to A.J.C. Wilson, Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, CAMBRIDGE CB2 1EW.

FORENSIC FILE

A few copies of the Forensic Data File, containing the diffraction patterns and the relevant search indexes for about 3000 substances important in forensic applications, were exhibited at the meeting of the International Association for Forensic Sciences in Oxford in September. These copies are slightly 'shop-soiled', but in good condition; the selling price of new copies is $395. Offers or enquiries should be sent to A.J.C. Wilson at the address above. Fuller information about the Forensic File will be provided on request.
General Assembly expanded the scope of the Commission's responsibilities to include all small molecule research. Stezowski solicited suggestions for consultants to the commission in areas of small molecule research not represented by the members listed above.

Commission Newsletter

There must be communication in both directions between the Commission and the small molecule community. Bill Duax, as corresponding secretary, will publish a newsletter to be sent to 2-3 representative crystallographers per country (IUCr council members were asked to suggest names for this list). It would then be the responsibility of these individuals to disseminate the information contained in the newsletter within their own country. The newsletter will contain information about meetings, symposia and workshops both in crystallography and in related areas which overlap with crystallography. The main purpose of the newsletter will be to expand international communications. Efforts will be made to identify existing newsletters (such as those of the American and British Crystallographic Association) that may be willing to print articles concerning the Commission's activities. The newsletter will be prepared and distributed from Buffalo. Contributions should be mailed to Bill Duax in Buffalo.

Data Collection Service

Stezowski and Duax proposed that the commission organize an intensity data collection service soliciting laboratories in technologically advanced countries that would be willing to collect one or two data sets a year for crystallographers in need of such assistance. The Commission could establish a clearing house. Investigators willing to provide data collection service would be given a list of three to five candidates for data collection from which to choose. Investigators must be willing to collect the data without requiring co-authorship, the extent of collaboration being open to negotiation between the investigators in the laboratories concerned.

Olga Kennard stated that such a data collection service has been offered within the European Crystallographic Committees but that she thought it appropriate to have the Commission on Small Molecules take on the responsibility.

Interaction with other Scientific Societies

David Ducamp urged the Commission to establish stronger contacts with noncrystallographers. Stezowski requested suggestions for the names of other professional societies with whom the Commission should interact, developing joint symposia at national and international meetings. It was also proposed that the commission contact Editors of Journals to which contributions on small molecule crystallography are submitted and suggest the appointment of a subeditor on crystallography.

Minutes of an Open Meeting of IUCr Commission on Small Molecules Hamburg, Germany, August 16, 1984, over 50 people in attendance

The Commission on Small Molecules was created by the General Assembly of the Union on August 10, 1984 and its composition was expanded to include a chairman and ten delegates in actions taken at the general assembly meeting of August 14, 1994.

The charter members of the commission are John Stezowski, FRG, Chairman

- P. Codd (Canada)
- A. Kalman (Hungary)
- C. De Ruter (Belgium)
- S. Heidle (U.K.)
- W. Duax (USA)
- B. Oleksyn (Poland)
- S. Garcia Blanco (Spain)
- C. Tsitsenko (USSR)
- M. Hospital (France)
- N. Vijayan (India)

The following Terms of Reference define the responsibilities of the commission on small molecules.

I. Terms of Reference

a. To advise the IUCr in organizing or sponsoring sessions on small molecule structural analysis at congresses and conferences.

b. To promote and coordinate scientific exchange between countries in the field of small molecule structural analysis.

c. To cooperate with other commissions of the Union on matters dealing with small molecule structural analysis.

d. To cooperate with other international bodies interested in small molecule structural analysis.

e. Selection of commission members - in accordance with IUCr policy six to ten members.

Consultants to the Commission

Chairman John Stezowski stated that the IUCr will be watching the Commission carefully to see if it really serves a useful purpose. He feels that the early days are important - that we must establish ourselves now and not wait for the Australia meeting. Because the
Scope of the Commission

There was some discussion on the definition of a small molecule. Chairman said it is essentially an open point with a broad definition — we will include anyone who wants to work with us. Kennard wondered if there was an upper limit — again it was stressed that anyone interested is welcome. Richard Gilardi suggested that we worry less about size and more about being the areas of techniques and methods. Olga was still concerned about the number of amino acid residues a molecule must have before it crosses the line from small to large. John suggested keeping open lines of communication with the protein people — but once again we welcome all ye who enter here. A representative from Norway questioned whether electron diffraction studies of small molecules fall under the domain of the Commission. Stezowski welcomed their input.

Topics and Speakers for Commission Programs

Suggestions were solicited for topics and speakers for future IUCr meetings and other national and international meetings in which the advice of the Commission on Small Molecules may be required, requested or offered. Richard Gilardi noted that the USA Small Molecule Special Interest Group has organized a number of successful symposia focused on techniques of structure analysis, determination, and refinement and these proved to be of interest not only to most small molecule crystallographers, but to protein crystallographers as well. Gilardi noted that the sessions on Molecular Mechanics and Data Analysis drew crowds too large for the rooms they were assigned in Hamburg.

Gilardi proposed a microsymposium on rotation functions, translation functions and restrained refinement in joint sponsorship with the Commission on Macromolecules. Judy Flippen-Anderson proposed a session on Crystallographic Computing and Computers in joint sponsorship with the Commission on Computing. David Rae proposed a session on Assessment of Quality and Detection of Systematic Errors for small molecule determinations for which crystal quality and composition may limit accuracy. Penny Codding suggested that a special poster session for contributions closely aligned to microsymposia be promoted and identified. Flippen-Anderson suggested that a 2-3 minute tape demonstrating the talent of prospective invited speakers might be desirable.

Future Meetings


A request has been received from the organizers that the Commission officially sponsor the meeting and provide some financial support if possible. A. Kalman stated that there will be an emphasis on DNA structure and drug-DNA interactions. The organizers are encouraging participation by quantum chemists and NMR spectroscopists as well as X-ray crystallographers.

B. ECM 9, Torino, Italy Sept. 2-6, 1985

Stezowski attended a meeting of the program committee for the Torino Meeting and found them receptive to participation by the Commission. [A workshop tutorial entitled Molecular Systematics: Detection, Evaluation and Presentation will be held.] A chairman for the symposium is being sought.

C. Intercongress Symposium China, fall 1986

Dr. Huang stated that at the present time there is a great deal of activity in small molecule crystallography in China including studies of transition metal complexes, organometallics, natural products, and models for nitrogen fixation. He said that they would welcome the opportunity to host a meeting that would bring together leading investigators in small molecule crystallography in China and from abroad.

Olga Kennard said that such a meeting might best focus on methods of structure solution and data analysis. Stephen Neidle expressed the opinion that a meeting presenting the state of the art in correlation between molecular structure and biological function might prove more profitable to the Chinese in the long run. The Commission will send them recent programs from other meetings so they could choose what they want. Stezowski stated that a subcommittee may be needed to seek some financial support for the proposed Intercongress Symposium. Possible sources for support include UNESCO and WHO.

D. International School of Crystallography 11th Course: Static and Dynamic Implications of Precise Structural Information, Erice, May 26 - June 6, 1985. A. Dominions called attention to the fact that the topic of this 11th course is of special interest to the Commission.

E. Dr. García Bianco stated that the commission might be interested in the activities of the "Grupo IbéricoAmericanigle Cristalográfico", an organization of crystallographers from Spanish speaking countries in Europe and North and Central America that hold meetings every three years alternating between Europe and South America. The 1986 meeting is scheduled for Barcelona.

Other Topics

Hans Bürgi solicited input from those attending the Commission meeting concerning the "save the thermal parameters" movement.

William L. Dixon
Recording Secretary
Postdoctoral Research Associate in x-ray Interferometry at the Storage Ring Source

Applications are invited for the above post, funded by the SERC for two years from the date of appointment. The successful candidate will be expected to initiate and assist with research at the Daresbury synchrotron radiation source using existing facilities and commissioning a new station on the wiggler beamline.

Applicants are expected to hold a Ph.D. degree and should have an aptitude for pursuing research in experimental physics.

Salary will be on the Research Associate (IA) scale, with salary depending on age. For example, the salary appropriate to a Ph.D. graduate aged 27 is £8,330 per annum plus USS, corresponding to point 4 of the scale.

Applications, with full C.V. and names of two referees to

Professor M Hart FRS (Department of Physics, University of Manchester, MANCHESTER M13 9PL) from whom further details may be obtained.

University of Bristol
Department of Biochemistry
Bristol BS8 1TD

Postdoctoral Position to work on the Structure and Function of Ovotransferrin.

We have been awarded an SERC-funded postdoctoral position for 3 years and SRS beam-time at Daresbury to work on the crystallographic structure of duck ovotransferrin, investigate the nature of the iron binding sites and compare the structures of the two homologous domains. A great deal is known about the biochemistry and physiology of transferrin and detailed structural information is essential. Duck ovotransferrin crystallises from PEG 6000 in an orthorhombic space group with cell dimensions 51 x 86 x 179 Å. The R.A. will help with the preparation of transferrin and transferrin fragments, the search for heavy atom derivatives and data collection and processing.

Hilary Muirhead and John Williams.
UNIVERSITY OF MANCHESTER

Department of Physics

Postdoctoral Research Associate in X-ray Interferometry at the Storage Ring Source

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Hilary Muirhead and John Williams.
UNIVERSITY OF MANCHESTER
DEPARTMENT OF MEDICAL BIOPHYSICS
AND HANNAH RESEARCH INSTITUTE
CHEMIST/BIOCHEMIST

Required for a project on the precipitation of calcium phosphates in the presence of phosphoproteins. A substantial part of the project involves sample preparation and chemical analysis at the Hannah Research Institute, Ayr, Scotland with Dr C Holt. Phases will be characterised by EXAFS spectroscopy and X-ray diffraction at SERC Daresbury Laboratory and the University of Manchester in collaboration with Drs. S S Hasnain and D W L Hukins. This research post will be supported for 3 years by AFRC on the standard University salary scale. Further details from Dr D W L Hukins, Department of Medical Biophysics, University of Manchester, Stopford Building, Manchester, M13 9PT.

Good home required for Philips 1010 generator, not in working order, but useful for spares, together with counting chain etc. (valves) from a 1540 X-ray spectrometer.

Please contact: I.G.WOOD
Rothamsted Experimental Station
Harpenden
Herts AL5 2QD
Tel 05827 63133 (Ext. 311 or 278)

JOURNALS FOR SALE
Fifty-eight bound volumes of Acta Crystallographica in mint condition: from the first volume up to 1977.
Also Kristall und Technik, later Crystal Research and Technology, complete set of unbound numbers from the beginning to Vol.19, 1954, published by Akademie Verlag, Berlin.
Offers please to Dr Nora Wooster, 339 Cherry Hinton Road, Cambridge, CB1 4DH.

BRAGG LECTURES
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The Seventh Bragg Lecture will be given by Professor Sir David Phillips, FRS
on Monday, 28 October 1985 at 5.30 p.m.
at the University of Leeds,
and on Thursday, 31 October 1985 at 5.30 p.m.
at the Royal Institution,
21 Albemarle Street, London W1X 4LS.

The Eighth Bragg Lecture will be given by Professor Brian W Matthews
in August 1987
in Perth, Western Australia.
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(M. Moore: Hon. Sec. Bragg Lecture Fund Committee.)
FORTHCOMING MEETINGS & COURSES
additional to those listed in the September Issue (No. 10)

1985

7-8 Jan: Microscopy & Microcomputers: City University, London: The Administrator, Royal Microscopical Society, 37-38 St. Clements, Oxford OX4 1AJ.

25 Feb - 1 March: 36th Pittsburgh Conf. on Analytical Chemistry & Applied Spectroscopy: New Orleans, Louisiana: Mrs L. Briggs, Pittsburgh Conference, 437 Donald Road, Pittsburgh PA 15235, USA.


1-3 April: Molecular Crystals Discussion Group + Molecular Electronics Advisory Group: University of Kent at Canterbury: Dr J D Wright, University Chemistry Laboratory, Canterbury, Kent, CT2 7NH.

1-3 April: Polymer Liquid Crystals (Faraday Discussion Meeting): Cambridge: Mrs Y A Fish, Royal Soc. of Chemistry, Burlington House, London W1V OBN.

1-4 April: Progress in X-ray Studies by Synchrotron Radiation: Strasbourg: Conference on Synchrotron Radiation, Departement de Physique, 3 rue de l'Universite, F-67084 Strasbourg Cedex, France.


17-18 April: Small Angle Neutron Scattering from Organised Systems: London: Dr R W Richards, Dept of Pure & Applied Chemistry, Univ of Strathclyde, Glasgow G1 1XL.

24-29 June: Gordon Conference on Liquid Crystals: Wolfeboro, New Hampshire: Dr Alfred Sauge, Liquid Crystal Institute, Kent State University, Kent, Ohio 44242 USA.


28 July: 7th Bragg Lecture (5.30 p.m.): University of Leeds.

31 July: 7th Bragg Lecture (5.30 p.m.): The Royal Institution, Albemarle Street, London W1: Dr M Moore, Royal Holloway College, Egham, Surrey TW20 0EX.
1986

7-10 April:  B C A Spring Meeting: University of York:
Prof M M Woolfson, Dept of Physics, Univ of York,
Heslington, York YO1 5DD.

22-27 June:  A C A Summer Meeting: Hamilton, Ontario:
Prof Colin Lock, McMaster University, Hamilton,
Ontario, Canada.

8-11 July:  Molecules, Clusters & Networks in the Solid State:
Univ of Birmingham: Dr J F Gibson, Royal Society of
Chemistry, Burlington House, London W1V OBN.

17-22 August:  7th International Zeolite Conference: Tokyo:
Prof Hiro-o Tominaga, Dept of Synthetic Chemistry,
Faculty of Engineering, Univ of Tokyo, Bunkyo-
u, Tokyo 113, Japan.

* N.B. This list should be read in conjunction with the one
   given in the previous (September) issue.

CRYSTALLOGRAPHY NEWS

Camera-ready copy on A4 paper is welcome at any time, as well
as illustrations suitable for the cover. (Unfortunately half-
tones cannot be reproduced.) Please ensure items for inclusion
in the March issue are sent (preferably not crumpled!) to the
Editor by February 15: Dr Moreton Moore, Department of Physics,
Royal Holloway College, Egham, Surrey TW20 0EX. Telephone:
Egham 9734- (or from London 37-) 35351 extension 36. Telex:
335504.