

# CRYSTALLOGRAPHY NEWS



BRITISH  
CRYSTALLOGRAPHIC  
ASSOCIATION

No. 2      SEPTEMBER 1982

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and reply form.

THE SIXTH BRAGG LECTURE

Professor M.M. Woolfson

*University of York*

will lecture on

STRUCTURAL  
CRYSTALLOGRAPHY  
IN THE 1980'S

at 5.30 p.m. on

Wednesday, 27 October

at the University of Manchester  
Institute of Science & Technology  
(UMIST) in the Renold Theatre

and at 5.30 p.m. on

Thursday, 28 October

at the University of Cambridge  
Chemical Laboratories, Lensfield Road.

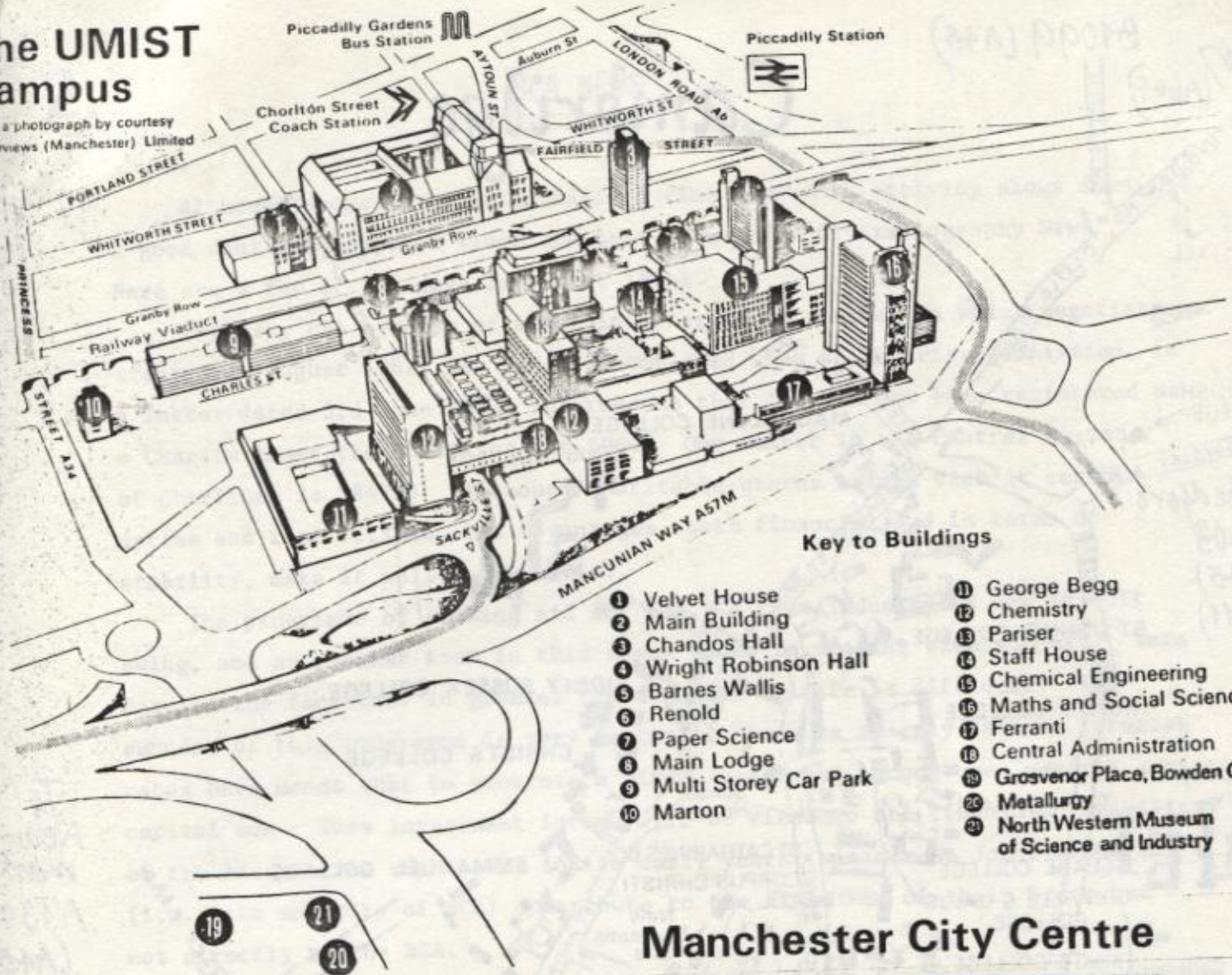
*The Bragg Lectures, founded in 1962, are given at intervals to commemorate the work of Sir William Bragg and his son, Sir Lawrence Bragg. Eminent crystallographers lecture on subjects of their own choice in the towns where the Braggs worked.*

ADMISSION FREE WITHOUT TICKET

*M. Moore, Royal Holloway College, Egham, Surrey*

# The UMIST Campus

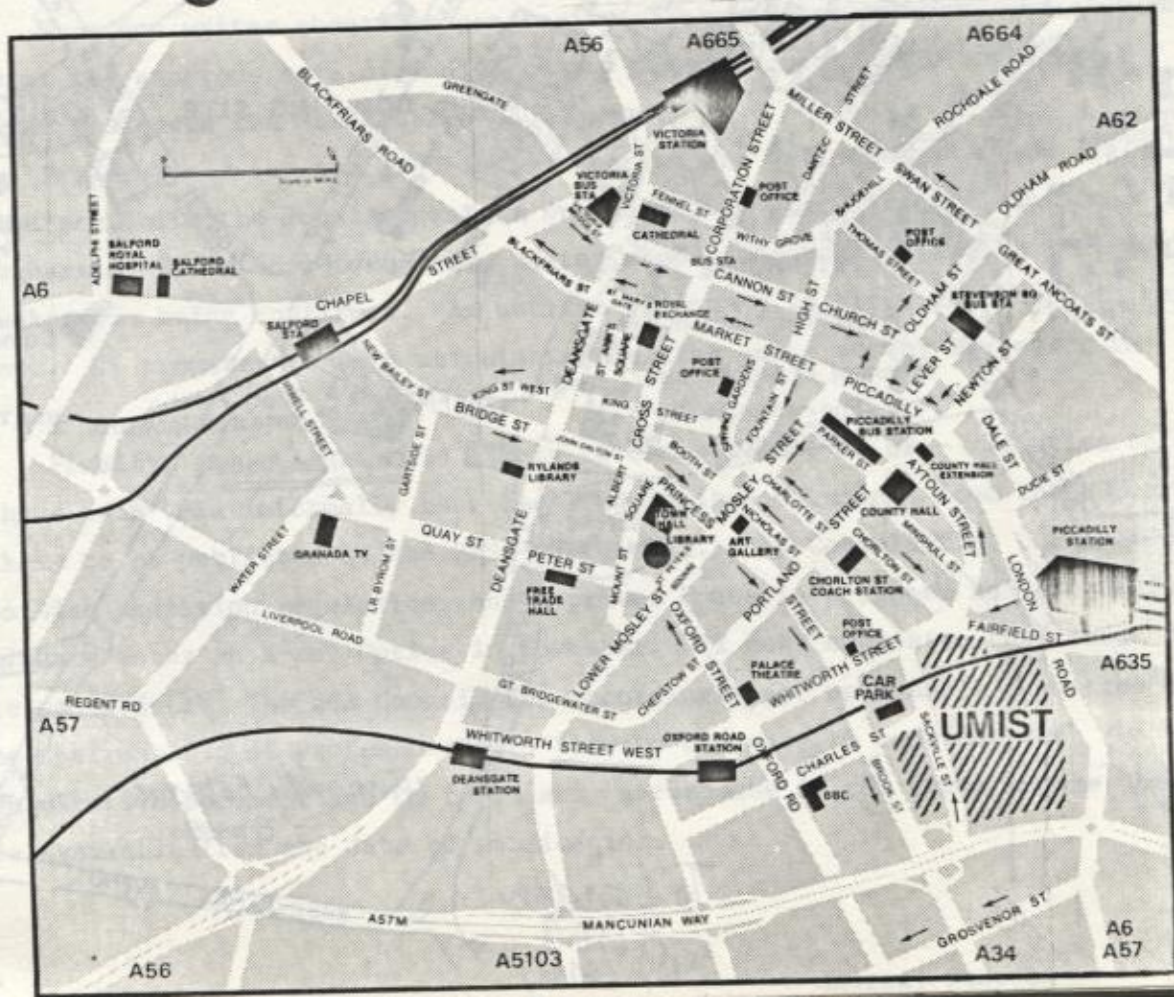
From a photograph by courtesy of Airways (Manchester) Limited



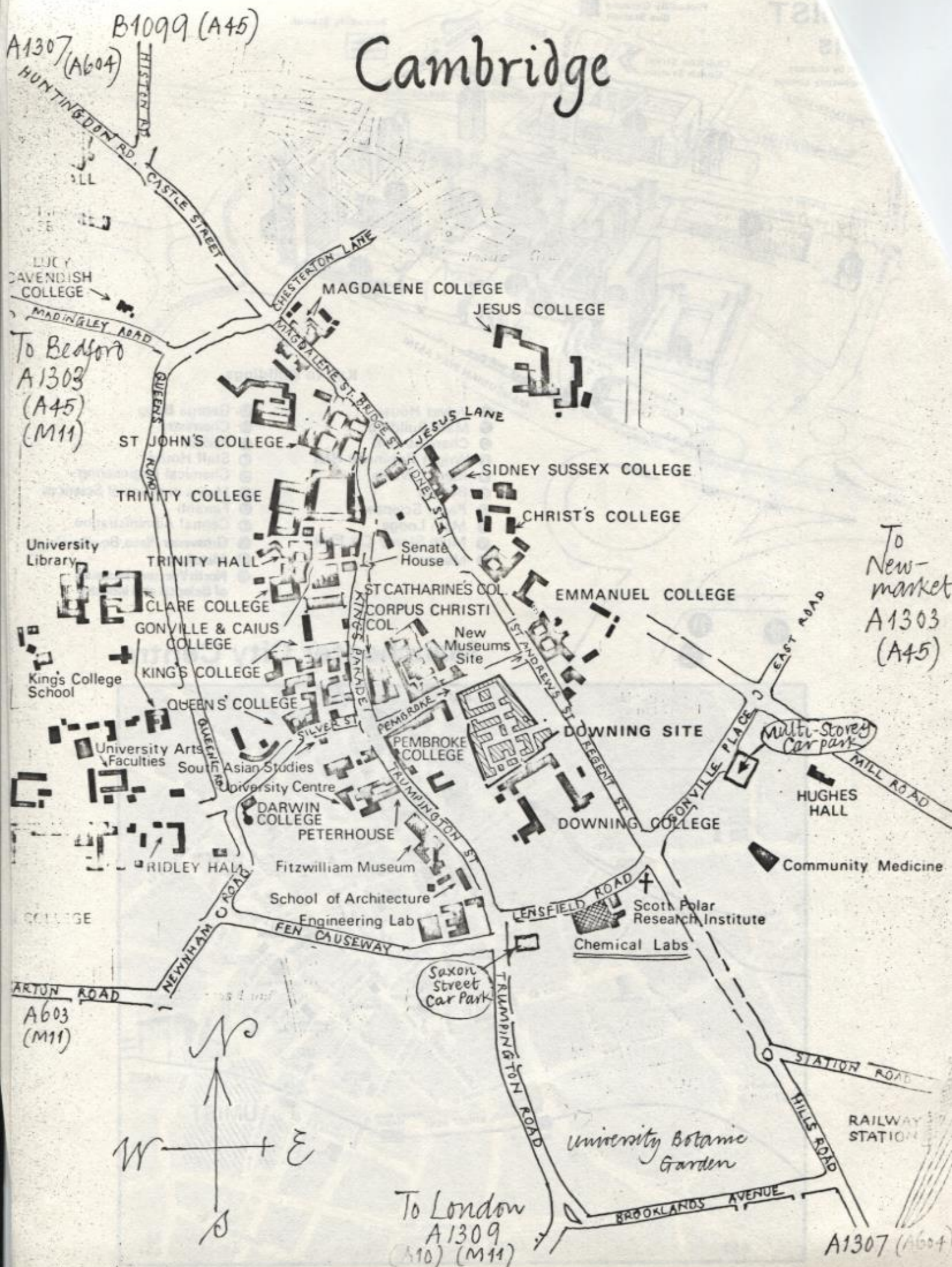
### Key to Buildings

- |                         |   |
|-------------------------|---|
| 1 Velvet House          | 11 George Begg                                  |
| 2 Main Building         | 12 Chemistry                                    |
| 3 Chandos Hall          | 13 Pariser                                      |
| 4 Wright Robinson Hall  | 14 Staff House                                  |
| 5 Barnes Wallis         | 15 Chemical Engineering                         |
| 6 Renold                | 16 Maths and Social Sciences                    |
| 7 Paper Science         | 17 Ferranti                                     |
| 8 Main Lodge            | 18 Central Administration                       |
| 9 Multi Storey Car Park | 19 Grosvenor Place, Bowden Court                |
| 10 Marton               | 20 Metallurgy                                   |
|                         | 21 North Western Museum of Science and Industry |

## Manchester City Centre



# Cambridge



Although summer is traditionally a time when work activity slows down, a good deal has happened since the last issue of "Crystallography News". Here are a few of the more important items.

Firstly, the process of attaining charitable status, on which negotiations started in August 1981, was finally completed when the Charity Commission, in a letter dated 3rd June 1982, informed me that the BCA has been registered as a Charity under the Charities Act 1960. Our number in the Central Register of Charities is 284718. Although charitable status brings with it certain duties and restrictions, the advantages, both financial and in terms of stability, make it well worth while.

The programme of seeking aid for the BCA from Industry is now in full swing, and as another item in this issue shows is meeting with success. This despite the fact that in general the economic climate is difficult. The success of this programme is very fortunate, because sharply falling interest rates have meant that to generate a given investment income one needs a greater capital sum. This investment income will be vital to the financial stability of the Association especially in its early years, since most Joint Members (i.e., the majority of BCA) contribute to the finances of their Group but not directly to the BCA.

When one writes about the generosity of companies, however, one should not forget the generous acts of individuals. In particular, that one Founder Member has given the Association £500!

Preparations for the 1983 Spring Meeting are well in hand. The organising committee, with the local organiser Dr. Moreton Moore, first met in June. Programmes of the four Groups are taking shape, and the availability of invited speakers is being confirmed. An outline programme is given elsewhere in this issue. It promises to be a stimulating meeting and a worthy successor to Durham.

Finally, an item which is likely to concern most of us - radiation safety. I have been told informally that the long-awaited documents from the HSE are likely to be published by the HMSO quite soon. The Consultative Document on Ionising Radiation Regulations and Approved Codes in October, and the draft Guidance Notes on X-ray Optics in November. (I must emphasise that these dates are tentative). The BCA Council has accordingly set up a small committee under the chairmanship of Professor David Blow to be ready to consider the consultative document and to formulate a response in the three months which are available from the date of publication.

3.

Cambridge  
NOTICE TO FOUNDER MEMBERS

At the Durham Meeting an idea was put forward that the first page of the Association's Minute Book be reserved for the signatures of Founder Members. A number of those who became Founder Members at Durham have already signed this page, and all Founder Members who have not yet done so are invited to add their signatures.

The Minute Book will, of course, be available at our Spring Meeting at Royal Holloway College, and at all subsequent annual meetings. Alternatively, if you happen to be in the vicinity of Imperial College, you can get in touch with me and sign the book there. For the sake of historical record it would be good to inscribe all the signatures in due course.

May I also remind those of you who are thinking of becoming Founder Members that the time-limit for joining this category is the end of this year.

Andrzej Skapski

4.

DONATIONS TO THE BCA

The following generous donations from Industry are gratefully acknowledged.

Imperial Chemical Industries p.l.c.	£1000	British Petroleum Co.Ltd.	£500
Marconi Avionics Ltd	£500	Philips Research Laboratories	£500
Roche Products Ltd	£500	Smith, Kline & French Research Ltd.	£500
Unilever UK Central Resources Ltd.	£500	The Wellcome Foundation Ltd.	£500
Esso Group of Companies	£400	Siemens Ltd.	£300
Glaxo Group of Companies	£250	Perkin-Elmer Ltd	£250
G.D.Searle & Co.Ltd.	£250	Oxford Instruments Ltd	£100
W & C.Spicer Ltd.	£100	Wyeth Laboratories	£100

This second list records donations received in the period June-August 1982.

In addition the number of Founder Members has increased by 18, one of whom has most generously subscribed £500.

5.

BCA MEETING, ROYAL HOLLOWAY COLLEGE28 - 31 March 1983

The Easter meeting of the BCA will be held in William Crosland's magnificent château-like building of the Royal Holloway College, situated at Egham in Surrey: half an hour's journey by rail from Waterloo Station, and close to Heathrow Airport and the M3, M4 and M25 Motorways. The poster sessions will take place in the recently restored Picture Gallery, on the afternoons of Tuesday 29th and Wednesday 30th March.

The Conference will start with registration and buffet lunch on Monday 28th March. The first afternoon will be devoted to the Biological Structures Group, Tuesday morning to the Physical Crystallography Group, Wednesday morning to the Industrial Group and Thursday morning to the Chemical Crystallography Group. The Conference will end for most delegates after lunch on Maundy Thursday but some will want to stay on for the CAD-4 Users Meeting being organized by Michael Hursthouse. There will also be a reception, a plenary lecture and a conference dinner. Full details and registration forms will be included in the December issue of Crystallography News.

6.

CALL FOR CONTRIBUTIONS

for the

INDUSTRIAL SYMPOSIUM

to be held during the

B.C.A. MEETING: ROYAL HOLLOWAY COLLEGE: 28-31 MARCH 1983

Contributions are requested on all aspects of Industrial/Applied Crystallography for ;

- (a) verbal presentation (20 mins) in the morning session, and/or
- (b) in a form suitable for poster display

The invited speakers in the morning session will be :

Mr C Baxter : Rolls Royce Limited, Derby

Mr W A Gutteridge : Cement and Concrete Association, Slough

Provisional titles for both verbal and poster contributions are required by 22 October 1982, and abstracts by 21 January 1983.

These should be sent to :

Mr G W Smith : B P Research Centre  
Chertsey Road  
Sunbury-on-Thames  
Middlesex  
TW16 7LN



When, just before the Durham Meeting, I had to order BCA notepaper, the problem arose of some identifying mark for the BCA. My first reaction was to have a simple **BCA**, at least in the interim. But, alas, we are not alone! A quick glance through the relevant compendia reveals that we jostle with the British Casino Association, British Car Auctions, British Chiropractors Association, to name but a few. So something more specific would be needed.

A coat of arms is rather splendid, but mightily expensive, and perhaps could be considered by our successors on the occasion of the BCA's 50th anniversary. But a logo is modern, neat and free!

A few words with some colleagues produced quite a number of very plausible logos (some of which are shown below), but rather than have the Secretary make this invidious decision we decided to do the thing more democratically and also to give crystallographers the chance to release their hidden artistic (?) talents.

So as a light-hearted aside from the serious business of the Spring Meeting, there will be a Logo Competition to choose a suitable sign for the BCA. There are still over 6 months to go, and further details will be released later, but in the meantime please start thinking and doodling.

[And if you have been patiently waiting for what Lagavulin had to do with Logo, here is the answer. As a prize to the winner the Secretary offers a bottle of Lagavulin 12-year old malt whisky {and if you do not like whisky, I am sure some kind of a barter deal can be arranged}].

Andrzej Skapski



8a.

JOINT INSTITUTE OF PHYSICS/BRITISH CRYSTALLOGRAPHIC ASSOCIATION  
CRYSTALLOGRAPHY GROUP

At the Annual General Meeting of the above group, which was held at Durham on April 7th, consideration was given to an alternative name for the group. It was felt that the present name was inappropriate for a joint group of the BCA. Many suggestions were made but that receiving majority support from the members present was "Physical Crystallography Group". This change of name has been agreed by the Council of the Institute of Physics. The final stage in effecting the change is for the members to authorise the appropriate changes in the constitution and rules of the group. An Extra-ordinary General Meeting will be held for this purpose on 25th November, 1982 at 2.00 pm in the Lecture Theatre, Geological Society, Burlington House, Piccadilly, London.

8b.

JOINT INSTITUTE OF PHYSICS/BRITISH CRYSTALLOGRAPHIC ASSOCIATION  
CRYSTALLOGRAPHY GROUP

The committee for the period 1st October 1982 to 30th September 1983 will be as follows with the year in which membership ceases given in brackets.

Chairman	Professor M.M. Woolfson (1984)
Vice-Chairman	Dr. B.T.M. Willis (1984)
Hon. Secretary and Treasurer	Dr. R.H. Fenn (1983)
Committee:-	Dr. A.A. Balchin (1983) Dr. C. Dineen (1983) Dr. I.F. Ferguson (1985) Dr. A.M. Glazer (Coopted) Dr. J.C. Halfpenny (1985) Professor M. Hart (Coopted) Dr. J.R. Helliwell (1985) Professor A.J. Leadbetter (1985) Mr. P.B. McAllister (1985) Dr. R.W.H. Small (Coopted) Dr. A.J. Smith (1984)



9.

INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY

Volume A: Space-Group Symmetry edited by Th. Hahn, Institut für Kristallographie, RWTH, Aachen, F.R.G.

1982, approx. 832 pp.

Cloth Dfl. 385,-/US \$165.00/£ 80.00 ISBN 90-277-1445-2

Individuals are entitled to purchase this volume at the reduced price of Dfl. 215,-/US \$90.00/£ 45.00. They should declare that the copy is for their personal use only and will not be put at the disposal of any library.

The Commission on International Tables of the International Union of Crystallography has, since 1973, been preparing the material for a totally revised and extended edition of the tables of symmetry groups. The results of these years of collaborative effort have led to the production of completely new tables on the 17 plane groups and 230 space groups, comprising about 630 printed pages. This work is complemented by a comprehensive introduction in which symmetry is discussed and the theory and use of the tables is described in detail.

Compiled by the foremost experts in the field of crystallographic symmetry, this book represents the only standard work on the subject and should be regarded as a yardstick by which all other publications may be judged. It is a vital work for all those concerned with the determination of crystal structures, and taking into account the clear and explanatory nature of the introduction, will provide an invaluable aid in the teaching of the subject.

Editorial Committee and Contributing Authors:

H. Arnold, E. F. Bertaut, Y. Billiet, M. J. Buerger, H. Burzlaff, P. M. de Wolff, J. D. H. Donnay, W. Fischer, D. S. Fokkema, Th. Hahn, H. Klapper, E. Koch, G. A. Langlet, A. Vos, H. Wondratschek, and H. Zimmermann.

Table of Contents: Foreword. Preface. Part I: Tables for Plane Groups and Space Groups. 1. Symbols and Terms Used in this Volume. 2. Guide to the Use of the Space-Group Tables. 3. Space-Group Determination and Diffraction Symbols. 4. Synoptic Tables of Space-Group Symbols. Group-Subgroup Relations. 5. Transformations in Crystallography. 6. The 17 Plane Groups (Two-dimensional Space Groups). 7. The 230 Space Groups. Part II: Symmetry in Crystallography. 8. Introduction to Space-Group Symmetry. 9. Crystal Lattices. 10. Point Groups and Crystal Classes. 11. Symmetry Operations. 12. Space-Group Symbols and Their Use. 13. Isomorphic Subgroups of Space Groups. 14. Lattice Complexes. Subject Index.

Copies are available from: D. Reidel Publishing Company

P. O. Box 17

3300 AA Dordrecht

Holland

or

190 Old Derby Street

Hingham, MA 02043

U.S.A.

All individual orders must be prepaid.

## The NETWORK, the MICROFILM RECORDER, and GRAPHICS PACKAGES

## The SERC Network

In the 1960s crystallographers needing large computational power had to travel to the Atlas Computer and spend days away from home calculating their results with the aid of decks of punched cards or reels of paper tape.

During the 1970s, computer power increased, and remote workstations were set up, so that the scientists could analyse their data without having to waste time in travelling to the computer site.

In July 1982 the SERC maintains two large computing facilities. At the Rutherford Appleton Laboratory (RAL), there are now an IBM 360/195, 3032, and 3081 used mainly for Nuclear Physics and Astronomy Board work. At the Daresbury Laboratory (DL), there is a NAS 7000 and a Cray 1 for Science Board work. Originally workstations were merely remote card readers and lineprinters; terminals were added to enable users to edit their files interactively.

During the 1980s these workstations are being upgraded and the central computers linked to the packet-switching minicomputer network set up by the Engineering Board. Better display terminals allow users to complete many of their data processing tasks locally, with only the largest 'number crunching' jobs submitted via the network to the central sites.

There are now about 100 U.K. institutions linked to our central computers as well as overseas laboratories in Geneva (CERN) and Hamburg (DESY).

The network provides better facilities for

- (a) Data capture
- (b) Pre/post processing
- (c) Batch job submission to central number crunchers
- (d) Information retrieval from databases
- (e) File transfer, for easier sharing of programs and data
- (f) Access to the FR80 microfilm recorder

## Databases

Several databases are available on the network. Some of interest to crystallographers are CSSR (Crystal Structure Search and Retrieval) the Brookhaven Protein Databank, and JCPDS (Joint Committee for Powder Diffraction Standards). CSSR is mounted at Edinburgh and gives access to the more than 40,000 Organic and Organometallic Crystal Structures database collected by the Cambridge Crystallographic Data Centre. The atomic co-ordinate holdings of the Brookhaven

databank have been available at DL for several years, recently some of the structure factor data has been added.

JCPDS is also mounted at DL, where a 'minifile' containing just the data of interest to a particular user can be extracted and stored for future reference. One convenient way to do this is to make a microfiche using the FR80 microfilm recorder at RAL. (See Fig. 3)

## FR80 Microfilm Recorder

This recorder makes computer output directly on microfilm. It consists of a controlling computer, several magnetic tape drives for input, and a high precision cathode ray tube for output. The tube has an optically flat surface coated with a white phosphor. Diagrams drawn on the surface are recorded on film by means of lens systems and cameras.

The four cameras are 16mm film, 35mm film, 12inch wide hardcopy paper and 105mm film for microfiche, normally run at 48X reduction. A colour filter system allows direct production of colour film. The electron beam intensity is variable to make grey scale images with 256 density levels. The plotting area is divided into a square raster of 16384 addressable points.

Special circuitry draws long vectors and outputs text using 'hardware characters' at high speeds (up to 10,000 a second)

## Data Compilation work at RAL

Early in 1976 we were asked by the Data Compilation Committee of the Science Board to undertake a feasibility study to find out whether the FR80 could be used to solve the printing problems associated with the publications of the Cambridge Crystallographic Data Centre. They had just published volume A1 of the series 'Molecular Structures and Dimensions'. Its pages contain several parts which are difficult for conventional phototypesetters to handle. There are Greek letters, chemical formulae, (e.g.  $\alpha$  hydroxymalonic acid  $C_3H_4O_5$ ), stereo pair diagrams and chemical structure diagrams.

The ever-increasing numbers of measured structures made the previously used manual methods of pasting together the separate pieces no longer practical. After more than a year of programming, the first book was made in 1977. We have now prepared the camera-ready copy for their last 6 annual volumes, and the Index Volume (II). Fig 1 shows part of 3 of the 7 different types of index printed in the latest volume. There is a

simple typeface for the Compound Name Index, a more complex one using **bold** and *italic* for the main bibliography and an index of diagrams.

### Diagrams from PLUTO78

We also worked on the problems associated with other parts of their publications such as the A1 volume. The stereo pairs were previously been drawn by the Cambridge program PLUTO78, so it was adapted to use the FR80. (see Fig 2 for examples ). It was also mounted on the GEC minicomputers of the SERC Interactive Computing Facility, so that staff at Cambridge can use it to decide from which direction the structures should be drawn, and the file of drawing instructions later sent over the network to the FR80.

**Stereo Viewer.** The diagrams can either be drawn on hardcopy paper ( as in Fig. 2) or sent directly to 35mm film in the format which fits the cheap 'Open University' stereo viewer. These facilities are available to all our users on the network, not just to Cambridge.

### Structure Diagrams

These were a more difficult problem, since they had been hand drawn for the A1 volume, and we had not previously attempted to mix diagrams and technical text in one page by computer program. We defined a format to transfer diagrams from Cambridge to RAL on magnetic tape. Various different ways of combining the text and diagrams were evaluated, and one finally chosen for volume 13 (see Fig 1) The 220 pages containing 3500 diagrams were sent to the printer in April, and the book published in July 82.

### Simulation of Images

We have also attempted to simulate photographic images using our computers and the FR80. Fig 3 shows a simulated electron microscope image of Wollastonite and some powder diffraction patterns. Fig 4 shows a shaded molecule. Such images can be made quickly by overprinting on a conventional lineprinter, but then they need thick paper, and are often large and cumbersome to handle. The FR80 produces much higher quality suitable for publications. There are probably many other uses of this technique which we have not tried so far, e.g. simulation of surface defects of crystalline materials.

### Graphics Kernel System (GKS)

After several years of international discussions (aided by RAL staff) this graphics system has recently been adopted as a Draft International Standard by ISO TC97/SC5. GKS is intended to be a portable low-level system, on top of which the user builds a particular application. It is *not* a molecular graphics system like FRODO, or BILDER. It is more like the GINO-F system currently used on the SERC minicomputer network.

There is an associated international effort trying to define a standard metafile format. Pictures written on magnetic media in this format would be easily recreated by any site running a G.K.S.system, even if they did not have the particular application program which originally created it. The format should enable SERC users to send completed pictures more easily around the network and to the FR80.

Version 6.2 of G.K.S. was implemented on the VAX computers of the SERC's Astronomy Board STARLINK network. Work is in progress to implement version 7.2 on the RAL computers.

### The Future

We are trying to bring simple-to-use molecular drawing packages within reach of most of the UK research community by mounting them on the SERC network. We already have PLUTO78: A.M.Lesk's program CPKLOT (See Fig 4 ) is being adapted for the FR80 and the GEC minicomputers. We will try to mount the programs on the single-user computers (e.g.PERQs) as they become available, if there is enough user demand. Donations of further programs, and suggestions for improvements or additional programs are always welcome.

We are also eager to find new uses for our graphical equipment, and happy to discuss possible projects with our users at any time.

For further information on any of these topics contact

K.M.Crennell, Computing Division, Atlas Centre,  
Rutherford Appleton Laboratory, Chilton, Didcot,  
Oxon OX110QX

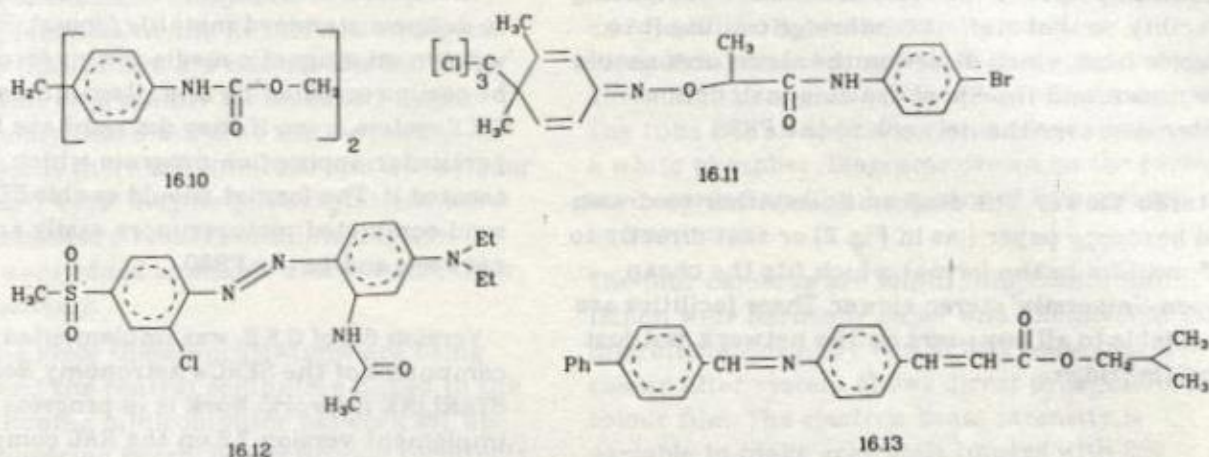
Telephone (0235) Abingdon 21900 ext. 6397

31 July 1982

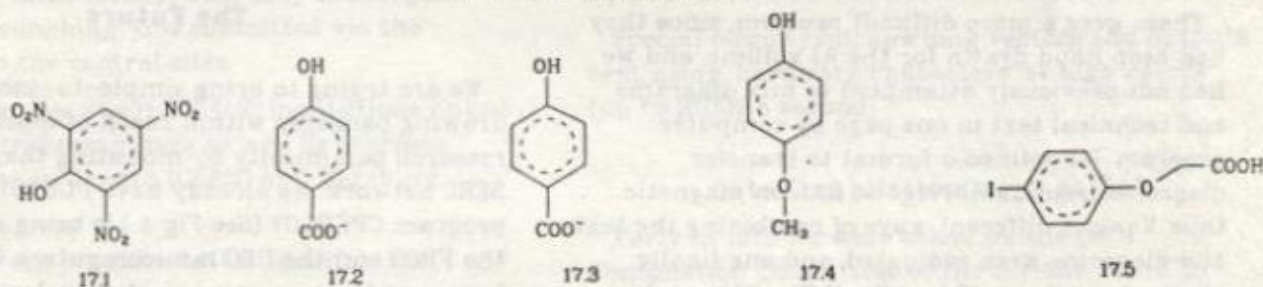
Aluminium

minium acetonitrile solvate]	pentakis(Acetonitrile)-chloro-aluminium tetrachloro-alu	68
niun)-hexakis(methyl-aluminium))	bis- $\mu$ -methyl*Amido-hexa- $\mu$ (3)-methylimido-bis(dimethyl-alumi	68
enyl-dicarbonyl-iron))	bis(dimethyl Amine)-trichloro-aluminium	68
4,4-dichloro-1,3-bis(trimethylsilyl)-1,3-di	tetraethyl Ammonium triphenyl-aluminium-( $\eta$ (5)-cyclopentad	73
minium) benzene solvate]	Aza-2-phosphonia-4-aluminata-cyclobutane	64
	( $\eta$ (6)-hexamethyl*Benzene)-titanium-bis(di- $\mu$ -chloro-dichloro-alu	74
	di- $\mu$ -chloro-bis( $\eta$ (6)-*Benzene-tin) tetrachloro-aluminium	69
	dimethyl-bis(2,2'- Bipyridyl)-cobalt(iii) tetraethyl-aluminium...	71.108
	dimethyl-bis(2,2'-bipyridyl)- Cobalt(iii) tetraethyl-aluminium	71.108
thylsilyl)-1,3-diaza-2-phosphonia-4-aluminata-	Cyclobutane.....[4,4-dichloro-1,3-bis(trimet	64
hyl-aluminium))	bis( $\eta$ -*Cyclopentadienyl)-ytterbium-di- $\mu$ -methyl-(dimet	71

ANILINES

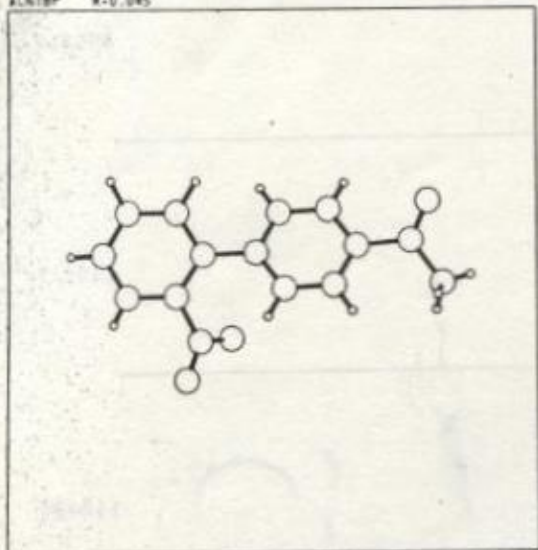


17 Phenols and Ethers

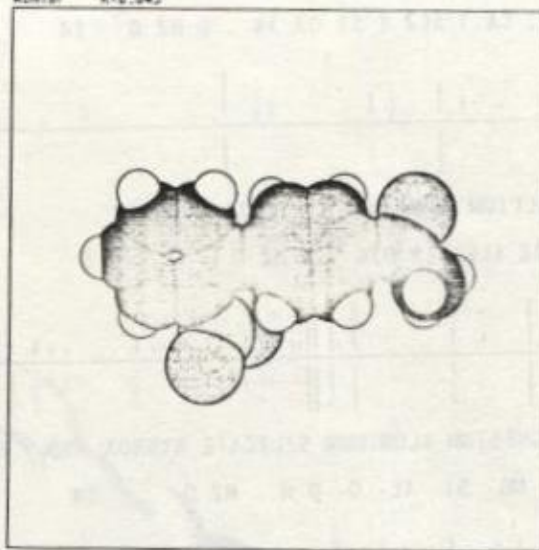


<p>171.17 (1979) - enno - tricarbonyl - iron  <math>C_{12}H_{10}ClFeO_4</math>                  J.Wenger, N.H.Thuy, T.Boschi, R.Roulet, A.Chollet, P.Vogel,                  A.A.Pinkerton, D.Schwarzenbach  <i>J Organomet Chem.</i>, 174, 89, 1979</p>	<p>72.C (<math>\mu^4</math> - Acetylene) - dodecacarbonyl - tetra - osmium  <math>C_{14}H_2O_{12}Os_4</math> Main entry is 71.57</p>
<p>72.16 Tricarbonyl - (6.7 - methylene - exo - 3 -                  oxatricyclo(3.2.1.0<sup>2,4</sup>)octane) - exo - iron  <math>C_{12}H_{10}FeO_4</math>                  J.Wenger, N.H.Thuy, T.Boschi, R.Roulet, A.Chollet, P.Vogel,                  A.A.Pinkerton, D.Schwarzenbach  <i>J Organomet Chem.</i>, 174, 89, 1979</p>	<p>72.C Tetracarbonyl - tungsten - (<math>\mu</math> - 1 - methyl - 2 -                  but - 2 - ene - di - ylidene) - pentacarbonyl -                  tungsten  <math>C_{14}H_8O_6W_2</math> Main entry is 71.61</p>
<p>72.17 bis(<math>\eta^2</math> - Methylacrylate) - tetracarbonyl - tungsten  <math>C_{12}H_{12}O_8W</math>                  F - W.Grevels, M.Lindemann, R.Benn, R.Goddard, C.Kruger  <i>Z Naturforsch., Teil B</i>, 35, 1298, 1980</p>	<p>72.C 1.4 - Dihydroxy - 2.3 - diethyl - butane - 1.1.4.4 -                  tetrayl - bis(tricarbonyl) - iron  <math>C_{14}H_{12}Fe_2O_8</math> Main entry is 71.64</p>
<p>72.C Dicarbonyl - (4 - 5 - <math>\eta</math> - 1.2 - difluoro - 1.2 -                  bis(trifluoromethyl) - pent - 4 - enyl) -                  (trimethylphosphite) - cobalt (at 183°K)  <math>C_{12}H_{14}CoF_2O_3P</math> Main entry is 71.38</p>	<p>72.C (<math>\mu^2</math> - Acetylene) - (<math>\sigma,\sigma,\eta^2,\eta^2</math> - glyoxal -                  bis(isopropylamine)) - tetracarbonyl - di -                  ruthenium  <math>C_{14}H_{18}N_2O_4Ru_2</math> Main entry is 71.68</p>
	<p>72.C <math>\mu</math> - 2 - sigma2 - 3 - <math>\eta</math> - (4.5 - Dihydro - 2 -                  furyl) - (bis(trimethylphosphine) - platinum) -                  tetracarbonyl - manganese (red format 200°K)  <math>C_{14}H_{22}MnO_4P_2Pt</math> Main entry is 71.75</p>

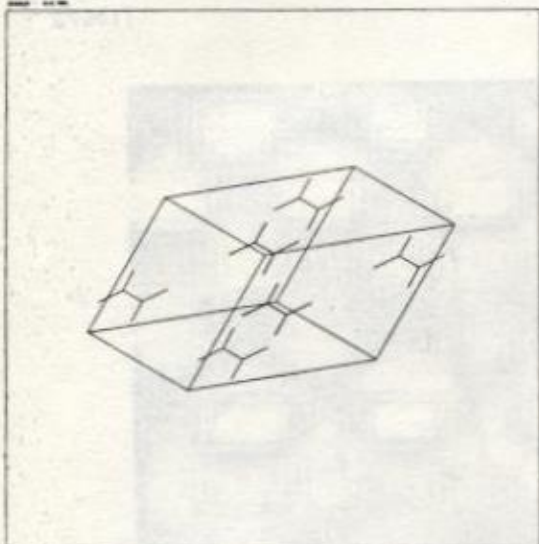
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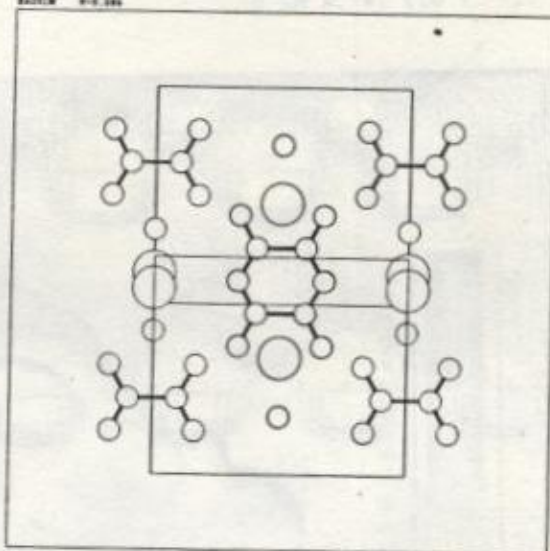
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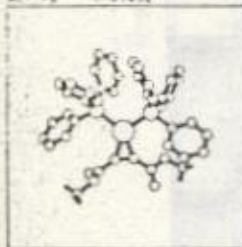
ADAM



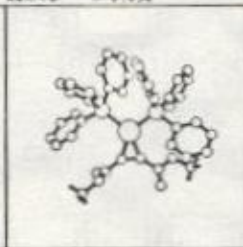
ADAM R=0.045



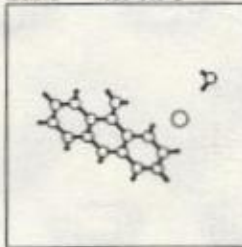
ACRFD R=0.052



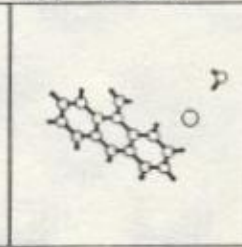
ACRFD R=0.052



AMACRO ROBS=0.042



AMACRO ROBS=0.042

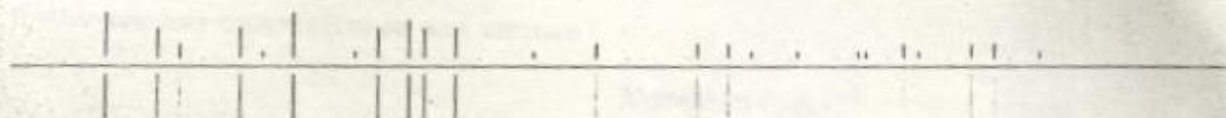


Some of the diagrams obtainable from the FR80 using PLUTO78  
 [Max no of atoms 400]

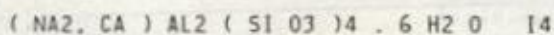
Fig.2

ZEOLITE GROUP

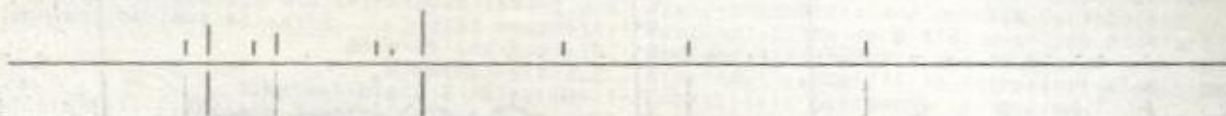
Wlat



SODIUM CALCIUM ALUMINUM SILICATE HYDRATE / GMELINITE



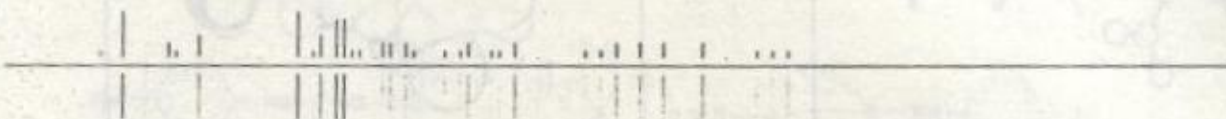
090419



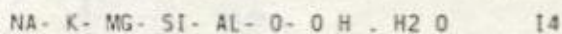
SODIUM CALCIUM ALUMINUM SILICATE HYDRATE



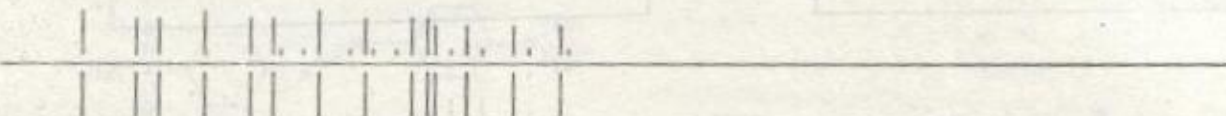
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SODIUM MAGNESIUM ALUMINUM SILICATE HYDROX HYD / FERRIERITE



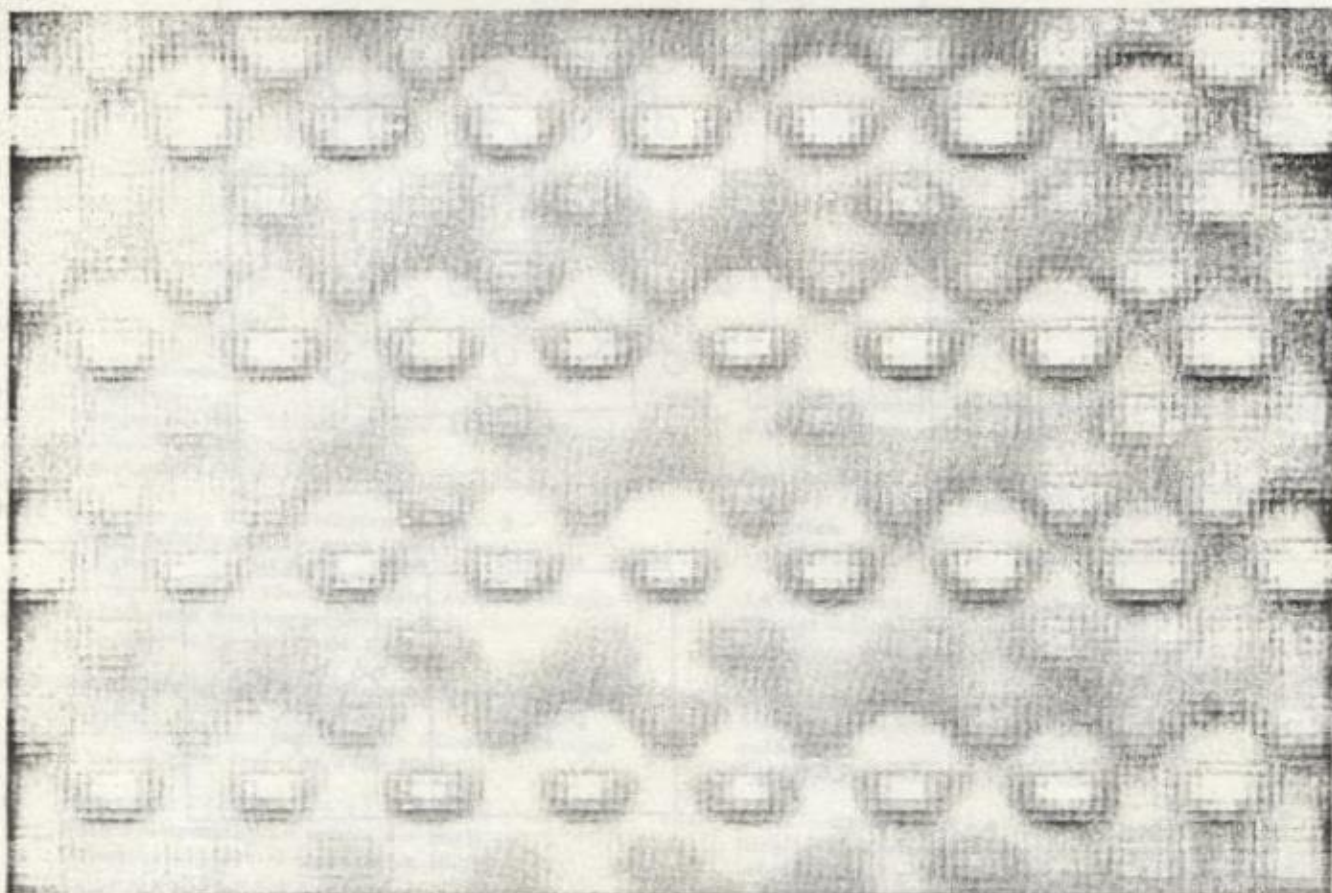
110429



SODIUM ALUMINUM SILICATE HYDRATE / FAUJASITE



110672



Examples of simulated images made with the FRSO. The lower one is an electron microscope image, the upper one, two attempts for each line to diffraction lines. Fig.



The International Union of Crystallography and the Cambridge Crystallographic Data Centre announce the publication of the latest volume in their series, Volume 1, entitled Crystallography Today, Organic and Organometallic Crystallography. This volume contains references to 1000 structure determinations published during this period.

Volume 13 sees the introduction of the new Chemical Index. Chemical diagrams, virtually all contained in the book are included in the new 218 page Index.

The price of the new volume is £12.00 (US \$24.00) and is available from the publishers, Cambridge University Press, 32 Avenue of the Americas, New York, N.Y. 10013.

Volume 13 also contains a new section on Organic and Organometallic Crystallography, which is a new section in the series. This section contains references to 1000 structure determinations published during this period. The price of the new volume is £12.00 (US \$24.00) and is available from the publishers, Cambridge University Press, 32 Avenue of the Americas, New York, N.Y. 10013.

The Laboratory of Dr. P. Pauling, University of California, San Francisco, California, U.S.A. is pleased to announce the publication of this volume.



Dr. P. Pauling, University of California, San Francisco, California, U.S.A. is pleased to announce the publication of this volume.

Heme Group as displayed on a Sigma terminal on a GEC4090 computer (Figure produced using programs from the molecular computer graphics system developed by Mr. D.Richardson in the laboratory of Dr.P.Pauling (University College London) modified by A.M.Lesk (while a visitor at the MRC Laboratory of Molecular Biology, Cambridge) [Max no of atoms 2400]

The International Union of Crystallography and the Cambridge Crystallographic Data Centre announce the publication of the latest volume in this series: Volume 13, entitled Bibliography 1980-81, Organic and Organometallic Crystal Structures. This volume contains references to 3610 structure determinations published during this period.

Volume 13 sees the introduction of the new Chemical Diagram Index. Chemical diagrams for virtually all compounds referenced in the book are included in the new 218 page index.

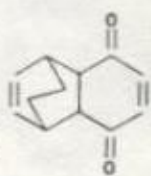
The price of the new volume is 135 Netherlands guilders. Copies are available from the publishers: D. Reidel Publishing Company, P.O. Box 17, 3300 AA Dordrecht, The Netherlands. Orders may also be placed with Polycrystal Book Service, P.O. Box 11567, Pittsburgh, Pennsylvania 15238, U.S.A. To ensure speedy receipt of new volumes readers are advised to make use of the standing order service. Information about personal purchase reductions and standing orders may be obtained from the publishers.

O. Kennard

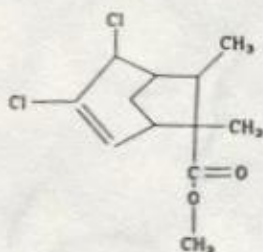
## BRIDGED RING HYDROCARBONS



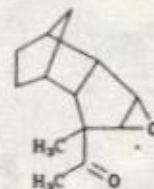
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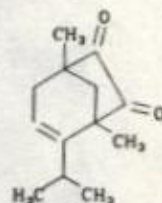
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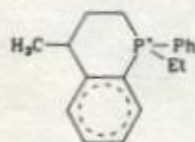
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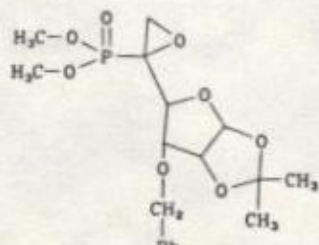
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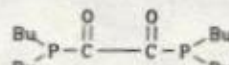
3116



64.89

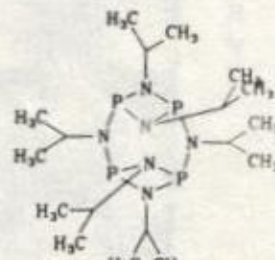


64.90

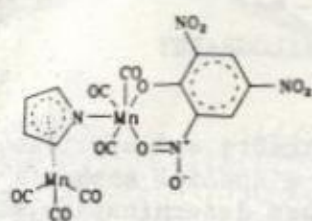


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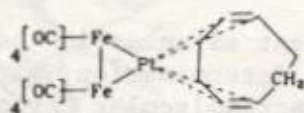
## PHOSPHORUS COMPOUNDS



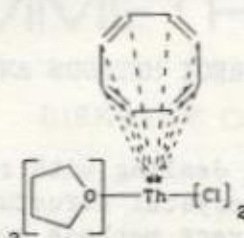
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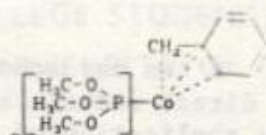
7513



7514



7515+



7517

12.

## INTERNATIONAL SCHOOL OF CRYSTALLOGRAPHY

The 9th Course, X-Ray Crystallography and Drug Action: Current Perspectives will be held at Erice-Trapani, Sicily from 21 March to 1 April, 1983.

The topics will be: introductory X-ray crystallography, crystal forces, host-guest complexes, drug-receptor binding forces, receptors, drugs and nucleic acids,  $\alpha$ -helix dipole and electrostatic interactions, dihydrofolate reductase inhibitors, haemoglobin, prealbumin hormone complexes, influenza virus haemagglutinin, rigid drug analogues, folic acid, polypeptide hormones steroids, benzomorphans, benzodiazepines, antibiotics, neuromuscular blockers, chemotherapeutic agents, drug conformation, drug development, molecular modeling, conformational analysis, and computers in drug design.

The lecturers are: F. Arcamone, Farmitalia, Milan, Italy; V. Austel, Thomae, Biberach, W. Germany, FRG; C. R. Beddell, Wellcome Laboratories, UK; J. Bernstein, Ben-Gurion University, Israel; C. Blake, University of Oxford, UK; T. L. Blundell, University of London, UK; M. Brufani, University of Rome, Italy; A. Camerman, University of Washington, USA; S. F. Campbell, Pfizer Research, Kent, UK; C. De Ranter, University of Leuven, Belgium; W. Duax, USA; P. Goodford, University of Oxford, UK; D. R. H. Gourley, E. Virginia Medical School, USA; P. Gund, Merck, Sharp and Dohme, USA; T. A. Hamor, University of Birmingham, UK; W. Hol, University of Groningen, The Netherlands; A. S. Horn, University of Groningen, The Netherlands; P. A. Kollman, University of California, USA; G. Marshall, Washington University, USA; H. Merz, Boehringer Ingelheim, FRG; S. Neidle, University of London, UK; G. Richards, University of Oxford, UK; D. Savage, Organon, UK; J. Tollenaere, Janssen, Belgium; K. N. Trueblood, University of California, USA; and I. A. Wilson, Harvard University, USA.

Contact: Professor Alan S. Horn  
Laboratorium voor Farmaceutische en Analytische Chemie  
A. Deusinglaan 2  
9713 AW Groningen, The Netherlands

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

The closing date for applications is November 20, 1982.

to Prof. D.N. Slay, FRU, who can provide further information.

13.

## SCHOOL ON DIRECT METHODS AND MACROMOLECULAR CRYSTALLOGRAPHY

A ten day school dealing with recent advances in the theory and application of direct methods of crystal structure determination, with a special emphasis on the application of direct methods to macromolecular structure determination will be held July 20-30, 1983, in Buffalo, New York. It is sponsored by the Medical Foundation of Buffalo, Inc., Research Laboratories.

The school will be devoted to theoretical advances and practical applications of direct methods of crystal structure determination, with a special emphasis on the integration of the direct methods philosophy with existing techniques of macromolecular crystallography. By bringing together students and lecturers interested or expert in one or both of these fields, we hope to inform the participants of the potential importance of recent developments and to stimulate interest and further work in this emerging field. The meeting will have the format of a workshop; there will be oral presentations as well as a heavy emphasis on tutorial sessions. Participants are encouraged to bring data sets with them, and time will be available for hands-on computing.

For further information contact: Dr. Jane F. Griffin  
Medical Foundation of Buffalo, Inc.  
73 High Street  
Buffalo, New York 14203

14.

## MOLECULAR STRUCTURE AND BIOLOGICAL ACTIVITY

Jane F. Griffin, Ph.D., and William L. Duax, Ph.D., Editors  
Medical Foundation of Buffalo, Inc., Buffalo, NY

This volume represents the proceedings of a meeting held in honor of David Harker, Buffalo, New York, August 26-28, 1981, as a satellite meeting of the IUCr Meeting in Ottawa, Canada.

This volume is now available. The authors are: David Harker; A. Camerman, et al.; D. Matthews and K. Volz; W. Saenger, et al.; J. J. Birktot, et al.; A. Arnone, et al.; T. L. Poulos; R. H. Ebright; F. H. Allen; P. Murray-Rust; G. A. Jeffrey; J. Kroon; H. J. Schneider, et al.; B. J. Oleksyn; M. N. Liebman; I. L. Karle; G. N. Tishchenko; J. J. Stezowski and E. Eckle; G. Gilli, et al.; W. B. T. Cruse and E. Egert; S. Neidle and H. M. Berman; O. Kennard; G. J. Quigley; R. M. Wing, et al.; R. Parthasarathy, et al.; A. Kalman, et al.; and J. P. Glusker.

1982 450 pages 0-444-00751 \$75.00

Dfl. 175.00/\$81.50 outside North America

# SYMMETRY SOCIETY

BIRKBECK COLLEGE STUDENTS' UNION  
UNIVERSITY OF LONDON



mike stanford (chairman)  
crystallography dept.  
birkbeck college  
malet street  
london wc1e 7hx  
tel. (01) 580 6622

15.

Anyone interested in the activities of the Symmetry Society should contact Mike Stanford at Birkbeck College. Besides the inherent beauty of symmetry, the Society is interested in the fun and fascination of the subject. Past speakers at meetings have been Dr David Singmaster on Rubik's Magic Cube and Professor Stewart Robertson on Symmetry Classification of Convex Polyhedra.

16a.

Biophysics Section - Department of Physics, Imperial College

## RESEARCH ASSISTANTSHIP IN MOLECULAR GRAPHICS

A one-year post-doctoral Research Assistantship (SERC-funded, Range IB) is available for an experienced computer programmer. The work includes development of displays of molecular structure and electron density for macromolecules using a PERQ computer and raster display, taking data from the SERC distributed computing network. A compatible pen-plotter system and colour display are also to be established.

Applicants should have appropriate background in computing, X-ray crystallography or molecular biology. An extension of the appointment will be possible if further Research Council support can be obtained.

Please apply as soon as possible

to Prof. D.M. Blow, FRS, who can provide further information.

166.

KING'S COLLEGE

(University of London)

Department of Physics

RESEARCH ASSISTANT

Applications are invited for an SERC supported Post Doctoral Research Assistantship to work on studies of phonon spectra using x-ray diffraction techniques. The project is funded for two years and involves working mainly at King's College but also at the Daresbury Laboratory of SERC using the UK Storage Ring Source of synchrotron radiation.

The post is available immediately. Salary on the standard 1A scale starting at £7925 including London Allowance.

Further particulars are available from :

Professor M Hart Department of Physics, King's College  
Strand London WC2R 2LS

17.

CRYSTALLOGRAPHY NEWS

Camera-ready copy for the December issue should reach the Editor by November 20 : Dr Moreton Moore, Department of Physics, Royal Holloway College, Egham, Surrey, TW20 OEX. Telephone: Egham 35351 extension 36. Telex: 935504.

FORTHCOMING MEETINGS (M) AND COURSES (C) Additional to  
those listed in the June issue

1982

- 20 October Tailoring of Crystal Growth (M)  
Grand Hotel, Manchester  
Dr M J Cliff, ICI Pharmaceuticals Division,  
Macclesfield Works, Cheshire, SK10 2NA
- 22-23 Oct. Crystal Related Arthropathies (M)  
Bristol Polytechnic  
Dr Paul Dieppe, Dept of Medicine  
Bristol Royal Infirmary, Bristol, BS2 8HW  
(see this issue)
- 10-12  
November 40th Annual Pittsburgh Diffraction Conference:  
(1) Liquid crystals, (2) phases in macromolecular  
structure analysis (M), Pittsburgh.  
Prof. C D Stout, Dept of Crystallography,  
Univ. of Pittsburgh PA 15260, USA
- 20-22  
December Solid State Physics Conference: Phase transitions;  
calculations of atomic arrangements, lattice  
vibrations & magnetism; quasi 2-D semiconductors;  
IR & Raman spectroscopy (M).  
Bedford College, London  
Dr M Lea, Physics Dept, Bedford College  
Regent's Park, London, NW1 4NS

1983

- 5-11 January Imaging and Microanalysis with High Spatial  
Resolution (C)  
Arizona State University.  
The Secretary, HREM Facility, Center for Solid State  
Science, Arizona State University, Tempe, AZ 85287, USA
- 18 March -  
1 April International School on Materials Science & Solar  
Energy (C) Cairo and Alexandria  
Prof. S Arafa, Science & Engineering Dept  
The American University in Cairo,  
113 Kasr El-Aini Street, Cairo, Egypt.
- 21-23 March Microscopy of Semiconducting Materials (M)  
St Catherine's College, Oxford  
Dr A G Cullis, RSRE, St Andrew's Road, Malvern,  
Worcs, WR14 3PS
- 21 March -  
1 April X-ray crystallography & drug action: current  
perspectives. (C)  
Erice, Sicily.  
L. Riva di Sanseverino, Piazza Porta San Donato 1  
40127 Bologna, Italy (see this issue)

1983

- 11-13 April Proterozoic 83 (M)  
Lusaka, Zambia  
The Organizing Secretary, Proterozoic 83  
Geological Society of Zambia, P O Box 50135  
Lusaka, Zambia.
- 13-15 April Molecular Graphics Society Annual Meeting (M)  
Dr Andy Morffew, IBM UK Scientific Centre,  
Athelstan House, St Clement Street, Winchester,  
Hants, SO23 9DR
- 17-22 April Scanning Electron Microscopy 1983 (C)  
Dearborn, Michigan, USA  
Dr. Om Johari, SEM, Inc., P O Box 66507,  
AMF O'Hare (Chicago), IL60666, USA
- 18-22 April InterMag (M)  
Philadelphia, Pennsylvania  
Dr W Doyle, Sperry Univac, P O Box 500,  
Blue Bell, Pennsylvania, 19424, USA
- 17-19 May 21st Meeting of the European High Pressure Research  
Group (M)  
Copenhagen, Denmark  
Dr B Andersen, Chemical Lab. IV,  
H.C. Ørsted Inst., Universitetsparken 5,  
DK-2100 Copenhagen, Denmark.
- 31 May -  
2 June 4th International Conf. on CVD  
Eindhoven, Netherlands  
G. Verspui, Philips Centre for Technology,  
Building SAQ,  
5600 MD Eindhoven, The Netherlands.
- 21-30 June 5th Summer School on Computing Techniques in  
Physics (C)  
Bechyně Castle, Czechoslovakia  
Dr J Badrchal, Institute of Physics, ČSAV,  
Na Slovance 2, 18040 Praha 8, Czechoslovakia.
- 20-30 July School on Direct Methods and Macromolecular  
Crystallography (C)  
Buffalo, New York  
Dr Jane F Griffin, Medical Foundation of Buffalo, Inc.  
73 High Street, Buffalo, New York 14203, USA
- 24-29 July 15th Meeting of the Federation of European Bio-  
chemical Societies (M), Brussels  
15th FEBS Meetings, Brussels International  
Conference Centre, Parc des Expositions, B-1020  
Brussels, Belgium.
- 7-10 August Applications of X-ray Topographic Methods to  
Materials Science (C), Snowmass, Colorado, USA  
Prof. S. Weissman, Dept of Mechanics & Materials  
Science, Rutgers Univ., Piscataway, New Jersey 08854,  
USA
- 
- 1984 29 July-  
4 August 8th International Biophysics Congress (M),  
Bristol, England. Dr H C Watson, Dept of Biochem.,  
Univ. of Bristol, Medical School, University Walk,  
Bristol BS8 1TD.



19.

SYMPOSIUM

CRYSTAL RELATED ARTHROPATHIES

Bristol Polytechnic, Coldharbour Lane, Frenchay, Bristol BS16 1QY  
22nd - 23rd October, 1982.

PROGRAMME

<u>Friday</u>	Introduction - "Crystals and Crystal Deposition Disease"	Dr. P. A. Dieppe (Bristol)
	Uric Acid Metabolism	Pr. G. Nuki (Edinburgh)
	Nucleation and Growth of Monosodium Urate Monohydrate Crystals	Dr. P. Calvert (Sussex)
	Gout - Recent Advances	Dr. J. Scott (London)
	GENERAL DISCUSSION	
	*****	
	LUNCH and POSTER VIEWING	
	The Pathology of Articular Deposition of Calcium Salts Their Relationship to Osteoarthritis	Pr. D. Mitrovic (Paris)
	Metabolism and Crystallisation of Calcium Pyrophosphate Dihydrate	Pr. G. Russell (Sheffield)
	Pyrophosphate Arthropathy - Recent Advances	Dr. M. Doherty (Bristol)
	*****	
	TEA	
	Growth of Calcium Phosphate Crystals in Normal and Osteoarthritic Cartilage	Dr. Y. Ali (London)
	Periarticular Hydroxyapatite Deposition and Calcific Periarthritis	Dr. G. Faure (Nancy)
	Intra-Articular Hydroxyapatite and Related Diseases	Pr. R. Schumacher (Philadelphia)
	GENERAL DISCUSSION	
	*****	
	COCKTAILS      POSTER VIEWING      DINNER	
	*****	
<u>Saturday</u>	Radiodiagnosis of Crystal Deposition Diseases	Dr. I. Watt (Bristol)
	Polarised Light Microscopy	Dr. J. Chayen (London)
	Physical Methods of Identifying Crystals	Dr. J. Shah (Bristol)
	Laboratory Handling of Crystals	Dr. P. Dieppe (Bristol)
	Crystal-Induced Inflammation	Dr. C. Dick (Newcastle)
	CASE PRESENTATIONS      Drs. Dieppe, Macfarlane and Doherty	
	LUNCH      POSTER VIEWING	

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\*

REPLY SLIP

CRYSTAL-RELATED ARTHROPATHIES

22nd and 23rd October, 1982

Bristol Polytechnic, Coldharbour Lane, Frenchay, Bristol BS16 1QY

I/We would like to reserve ..... places at the above Symposium at a cost of £35 per person. I enclose a cheque, made payable to "Crystal-Related Arthropathies" for.....

NAME(S) .....  
(Block capitals please)

POSITION.....

ADDRESS .....

.....

Please return form, with cheque, to:

Mrs. M. A. Clarke,  
Rheumatology Research Secretary,  
University Department of Medicine,  
Bristol Royal Infirmary,  
Marlborough Street,  
Bristol BS2 8HW

RETURN AS SOON AS POSSIBLE, PLEASE