CRYSTALLOGRAPHY NEWS

BRITISH CRYSTALLOGRAPHIC ASSOCIATION

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Contents

B.C.A. SPRING MEETING

The venue for the second Spring Meeting, held 2-5 April 1984, was the Department of Chemistry at the University of Nottingham. The scientific programme followed the general pattern of the 1983 meeting, aside from some re-ordering of the main topics, but for the first time individual sessions were all arranged by the Association's specialist groups.

The meeting opened with a symposium on physical crystallography, chaired by Dr Paul Fewster. This was in two sections. The first, on instrumentation, covered two important developments at the SRS, Daresbury, for the study of powder samples and protein structures. The second was devoted to the theory and various applications of EXAFS.

On Tuesday it was the turn of the Industrial Group. The first session, chaired by Mr Glen Smith, included papers on applications of powder diffraction which were of interest to geologists and mineralogists. Dr Brian Isherwood presided over the second session on the use of topography in quantifying the degree of perfection in electronic crystals.

The Chemical Crystallography Group arranged a general symposium on structure refinement. This session, led by Dr M. B. Hursthouse, included a review of current practice which was particularly useful for non-specialists in this field.

The symposium on biological molecules, held on Thursday morning, again contained two sessions. The first was concerned with the principles and application of maximum entropy to phase determination and this was followed by a session devoted to recent structural research.

Posters on a variety of topics complemented the oral sessions. On Tuesday afternoon the theme was physical and industrial crystallography, with posters on chemical and biological subjects on Wednesday. These were displayed in the same room as a commercial exhibition and it is gratifying to note that this valuable and important aspect of the meeting attracted sixteen exhibitors.

The plenary lecture was given on Wednesday evening by Dr D. Sayre, President of the ACA, who surveyed the development of crystallography since 1900 and included several personal reminiscences, with a few thoughts for the future. This was followed by the excellent conference dinner in Lenton Hall. A highlight of the meeting was the entertainment provided during Thursday evening by the talented and versatile Emanon Singers.

The fact that a fair proportion of the 170 or so participants attended most sessions is indicative of the success of the 2nd Spring Meeting. Those who had a hand in arranging it, particularly Drs Michael Begley and Stephen Wallwork, are to be complimented on providing the Association with another memorable event; the high standard set at the 1983 meeting was equalled in every respect.

J. Ian Langford.

REPORT ON THE BIOLOGICAL MOLECULES SYMPOSIUM

Nottingham - April 5, 1984

The symposium on biological molecules was held on Thursday morning. It contained two sessions. The first was concerned with the principles and application of maximum entropy to phase determination; this was followed by a session devoted to recent structural research.

The opening lecture "Maximum Entropy and the Foundation of Direct Methods" was given by Gerard Bricogne (LURE, Paris). In this the established principles of direct methods were first reviewed. Their limitations were identified as essentially failure to cope with the "branching problem" in phase determination. Maximum entropy was shown to be a technique applicable to the phase problems for exploiting prior knowledge of some structure factors in the construction of the joint distributions of other structure factors. The branching property of the system is clearly identified and described through this formalism which also leads to an equivalent and optimal formulation for the basis of direct methods.

The crucial advance in the use of maximum entropy ideas, which challenges the pessimism that established methods are weaker for large structures, is the handling of joint probability distributions. Bricogne developed the notion that a joint probability distribution for a structure factor set must be handled as a collection of conditional probability distributions, local

in character and each derived from one member of a large set of incompatible prior assumptions. In contrast conventional direct methods do not construct a joint probability distribution for any large set of structure factors; they are limited to low order formulae which describe individual phase invariants. Thus the great success of direct methods has rested on an incomplete basis; its success may well be greater in the future when prior information can be applied along every branch of the generated phase sets.

An example of the application of maximum entropy to a filamentous virus of MW 29000 was described by Don Marvin (Biochemistry Department, Cambridge University). The procedures followed in determining the structure of the virus in its fibre organisation and the calculation of the electron density were gone through in detail. Thus the practical working of the algorithm written by Bryan from Cambridge could be followed and its very great promise appreciated. The helical structure of the molecule was nicely represented in its electron density in a series of coloured slides.

There were some interesting experimental aspects to this study; the most intriguing one was the use of an intense magnetic field to orient the fibres. Presumably the intrinsic dipoles in the helix responded to the field in this very special case of axially oriented helices.

The discussion that followed on the maximum entropy method was led by David Sayre (IBM, New York) who also threw further light on how Bricognes approach to the phase problem differed from earlier treatments. Gerard Bricogne illustrated a trial application of the maximum entropy method to a calculated error free crambin structure. The improvement in effective resolution was clear and the method's potential for extracting full information from the structure factors was underlined. There was obviously great interest in this discussion and there is no doubt that an important development in crystallographic theory and practice has taken place.

The second session opened with Tim Richmond's description of the nucleosome structure at 7A spacing. This structure is made up of about 146 base pairs of DNA double helix, twisted into two turns of super helix. Packed into the DNA are eight histone molecules. With 7A spacing data the electron density revealed the chracteristic "propellor wake" structure of the DNA double helix. The histone proteins interactions with the DNA could often be followed, they were seen to fit nicely into the double helical groves. There were several rods of density in the histone structures that indicated their helical folding. The details of the complex are still being analysed but it is clear that important insight into DNA structure and how it is affected by protein interaction will emerge.

The experimental problems in preparing and growing nucleosome crystals are formidable and the size of the molecules in the crystal presented more than the usual problems in phase determination. The conventional procedures of heavy atom derivatives again proved sufficient, though metal clusters were introduced to increase their scattering power. Thus protein crystallographic methods continue to have the capacity to cope with these larger and increasingly complex structures.

The other end of the protein crystallographic spectrum was covered by Dr. Herman Watson of Bristol University who reviewed his work on phosphoryl transferase mechanisms in the phosphoglycerate kinase and mutase enzymes which are adjacent in the glycolytic pathway. These studies were based on analysis of various substrate analogues and cofactors residing in the parent enzymes. The analysis concentrated on the structure and contacts of the small molecule substrates within the framework of the enzymes. Careful crystallographic refinements and inspection of the electron density led to a model for the structural pathway for the phosphate groups and substrates. The "in line" mechanism fitted the crystal structures nicely and made excellent chemical sense. In the case of phosphoglycerate kinase catalysis is associated with the opening and then shutting of the two domains in the enzyme onto the substrates. In the closed environment the phosphoryl transfer from the diphosphoglycerate to adenine diphosphate takes place in a water free environment. The products are then released on the opening up of the enzyme.

The phosphotransfer mechanism in the mutase enzyme is also assisted by structural change. In this tetrameric molecule an N terminal segment is found to be free and flexible in the absence of substrate. On the binding of substrate the N terminal residues twist into a helix and close off the active site from the surrounding solvent. Thus water is excluded permitting the transfer of the phosphate group via a diphospho intermediate from the 3 to the 2 position of the glycerate. Steric and chemical arguments implicate two histidines in the catalytic mechanism, they lie parallel and adjacent in the active site.

It was very satisfying but not surprising to see how effective the structural arguments can be when based on the electron density of large complexes like the nucleosome. Just as pleasing however was the chemical and structural insight derived from study of the small molecule substrates in an enzyme system. This provided a nice illustration of the power of crystallographic analysis to further our understanding of enzymatic processes. Thus the biological molecule symposium closed with a clear picture of why we need to know the crystal structure of proteins and why therefore phase determining methods both traditional and newly developing are at the centre of the subject.

ggd/dl

Dr W H TAYLOR

Dr William Hodge Taylor, who died on May 14 aged 79 was Reader in Crystallography in the University of Cambridge, and an outstanding member of the school of British structural crystallographers who developed many aspects of this approach to the understanding of the atomic architecture of matter.

He was the leader of a numerous and international school of young crystallographers whose influence on the science was second only to the school of W. L. Bragg which preceded it.

Born on September 25, 1904 Taylor was educated at Chorley Grammar School in Lancashire and appeared destined for further study in the classics. But university scholarships in classics were not numerous at that time and in his final year he switched to science and mathematics, entering the University of Manchester as a science scholar in 1923 to read Physics under Bragg. He graduated in 1926 in the process setting his examiners the problem of finding reasons why he should not be declared to be perfect in all his papers.

Bragg's influence was immediate and Taylor began to make his own mark, publishing his first paper on the structure of caesium and ammonium sulphates in 1928.

His perfection in detail, coupled with a deep instinct for logic and insight, were allied to an accurate experimental technique and made him one of the most active members of the Bragg team which was extending X-ray analysis to compounds of an increasingly complex character. He made contributions to the study of the aluminium silicates, but the paper on the "Structure of Sanidine and other Felspars" in 1933 was the crowning achievement of the investigations at Manchester on silicate structure. Taylor returned later in life to investigations of the felspars and was regarded as the leading expert on their complex and interesting varieties.

In Manchester, where Taylor was head of the physics department in the College of Technology for ten years, his influence on the running of the college was direct. When at the end of the war Bragg wanted someone to take charge of the Crystallographic Laboratory in the Cavendish he was the obvious choice.

The appointment preceded an exceptional influx of young scientists from the Commonwealth and the United States, and Taylor set about the task of laying down the foundations of a centre in his subject which influenced the teaching of physics, chemistry and the earth sciences in universities throughout the world.

In the 1950s he was chairman of the X-ray Analysis Group of the Institute of Physics and vice-president of the Institute and the Physical Society for seven years. He also served on a number of government scientific committees. During this period it became commonplace advice to anyone in the profession with a problem, "to have a word with Taylor".

He was an inexhaustible participant in the International Union of Crystallography over a number of years and at the end of this time his own university found further need of his leadership appointing him chairman of the Faculty Board of Physics and Chemistry until his resignation in 1970. In 1956 he had been elected Senior Fellow of Clare Hall.

In addition to his teaching, Taylor contributed much to the progress of his subject through his many papers and as editor of the *Philosophical Magazine* for many years.

His wife Annie was his companion from his undergraduate days and their home in Cambridge was a centre of international hospitality. They both relished in return the ability to travel the world refreshing friendships forged there. Both were exceptionally well cultured in music and her death in 1977 left him a very lonely man.

FELLOWS OF THE ROYAL SOCIETY

It is a pleasure to record the election of
Professor T. L. Blundell, Professor of Crystallography at Birkbeck College, London,
Professor J. B Pendry, Professor of Theoretical Solid State Physics at Imperial College, London and
Professor M. M. Woolfson, Professor of Physics in the University of York to the Fellowship of the Royal Society.

ILLUSTRATIONS AT NOTTINGHAM

David Watkin would like to acknowledge the following for illustrations to his talk at the BCA Meeting: Genius by John Glasham, Now We Are Six by Ernest Shepard, Bravo Ernest by Gabriel Vincent, and Where the Wild Things Are by Sendak.

CRUICKSHANK SYMPOSIUM

UMIST, 11-13 SEPTEMBER 1984

A programme and application form for the Symposium is enclosed with this issue of *Crystallography News*. The Symposium not only provides an opportunity to honour Professor Cruickshank, but will also provide state-of-the-art reviews of many important areas of structural chemistry. We hope, therefore, that the Symposium will be attended by both experts and students of the areas concerned.

Special arrangements for non-resident participants and students are described below.

Non-resident participants. For non-resident participants a symposium fee of £55 including lunches on 12 and 13 September will be charged; dinner on 11 September (£7) and the special Conference Dinner (£12) on 12 September are optional extras. Please state all requirements clearly on the application form and enclose appropriate remittance.

Students. The British Crystallographic Association has arranged for a number of places to be available for bona fide students at a reduced cost of £70 resident (or £30 non-resident, but includes lunches). Students wishing to apply for one of these places should write to the organisers, enclosing with their application form and remittance a letter of support from their Head of Department or research supervisor confirming their status.

BCA Council Members. It is anticipated that a Council meeting will be held on the afternoon of Thursday 13 September in the Chemistry Department at UMIST.

PHYSICAL CRYSTALLOGRAPHY GROUP

and THIN FILMS AND SURFACES GROUP

INSTITUTE OF PHYSICS

Surface Crystallography

ONE DAY Meeting - WEDNESDAY, 28th November 1984.

IMPERIAL COLLEGE

The last twenty years has seen a great increase in activity in structure determination at the surface of solids. The plenary talks in this one-day meeting will be highly tutorial in spirit, and will attempt to give a balanced view of the present state of the art in terms understandable both to bulk crystallographers and surface scientists:

Probes of Atomic Structure at Surfaces	J.Pendry (Imperial College)
X-Ray Diffraction from Physisorbed Layers	R.K.Thomas (Oxford)
Surface Crystallography with Incident Electrons	M.Prutton (York)
Non-Diffractive Approaches to Surface Structure	R.F.Willis (Cambridge)

Contributed papers are requested on any aspect of surface structure: low energy electron diffraction, reflection high energy electron diffraction, 2D X-Ray diffraction, surface extended X-ray absorption fine structure, neutron scattering, scanning tunnelling microscopy, theoretical prediction, etc. We are aware of a number of groups contemplating various kinds of highly surface sensitive X-ray diffraction experiments, and would welcome short papers even if things are still in the design or development stage. We plan to provide participants with a guide to the acronyms of surface structure determination (e.g. RHEED, NANES, SEXAFS) to keep confusion to a minimum!

NOTE AMENDED DATE

Jim Matthew

Mary Halliwell

International School of Crystallography
11th Course: STATIC AND DYNAMIC IMPLICATIONS OF PRECISE STRUCTURAL INFORMATION. Erice-Trapani- SICILY: 24 May - 6 June, 1985

TOPICS

An Interdisciplinary Approach to Molecular Structure. The Potential Energy Surface. Minimisation, Refinement and Constraints. Neutron Diffraction. X-ray Data Collection and Treatment. The Rôle of Electron Density in X-Ray Analysis. Thermal Motion in Crystals. Microwave Spectroscopy. Gas-Phase Electron Diffraction. N.M.R. and Precise Molecular Geometries. Quantum Mechanical Predictions of Geometry. Empirical Force-Fields. Retrieval and Analysis of Precise Structural Information from Data Files. The Role of Precise Structural Information in (i) Organic Chemistry, (ii) Inorganic Chemistry. Structural Correlation and Reaction Pathways. The effect of Crystal Environments on Molecular Structure. The Effects of Substituents on Molecular Structure. Statistical Techniques for the Analysis of Molecular Geometry.

Persons wishing to attend the Course should write to:

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

They should specify: (i) full name(s), address, age, nationality; (ii) present academic position and other qualifications; (iii) languages spoken; (iv) reference of up to five published papers (do not include papers!) and enclose four (possibly self-adhesive) labels with full address for further correspondence. Young persons with only a few years experience should enclose a letter of recommendation from the head of their research group or from a senior person active in the field.

CLOSING DATE FOR APPLICATION: 31 OCTOBER, 1984. No special form is required.

The total fee including board and lodging (arranged by the School) is 1,350 Swiss Francs.

Thanks to the generosity of the sponsoring Institutions, partial support can be given to those students who need financial help, but the amount required must be specified and justified in the application letter.

Imperial College of Science and Technology
Biophysics Section, Department of Physics.

RESEARCH ASSISTANTSHIPS IN PROTEIN CRYSTALLOGRAPHY.

Post-doctoral Research Assistantships are available on a programme of research into protein structure by X-ray crystallography. An initial appointment can be made for up to three years, but further extension is likely. Two posts are available. One requires an experienced protein crystallographer; the other would suit a young Ph.D. with a knowledge of crystallography.

Apply as soon as possible to Prof. D.M. Blow, FRS, Blackett Laboratory, Imperial College, London SW7 2BZ, including a brief c.v. and the names of two referees.

5.5.1984.

SILICATES IN SOLUTION

A short (about 15 minutes) introduction to the solution chemistry of silicates is available as a colour video-tape. It describes hydrolysis, polymerisation, and structure, and is suitable for undergraduate teaching, or as an elementary introduction to the subject generally. It is based on a computer generated film* made on the FR 80 at the SERC Rutherford Appleton Laboratories Atlas Centre, shown at the recent Nottingham meeting, but incorporates additional background material and a spoken commentary.

Copies are available from:

Aberdeen University Television Service,
Regent Walk
Old Aberdeen, AB9 1FX, Scotland.
[Telephone No. 0224-40241]

They may be rented (£25 p.w. for educational institutions/£32 p.w. elsewhere) or purchased (£60/£120). Hirers who decide to purchase within one month may deduct the hire fee from the purchase price; all prices are plus VAT. Please remember to state which system is needed (UMATIC or VHS).

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*Copies of the original film (silent with subtitles) may also be purchased, price £125 approx. Contact Mrs. K.M. Crennell at the Atlas Centre, Chilton, Didcot, OX11 0QX [Tel. 0235-446397].

FORTHCOMING MEETINGS AND COURSES

additional to those listed in the March issue (No.8)

13-14 Sept. 1984 : The Kinetics and Mass Transport Behaviour in Silicate and Oxide Systems : Geological Society, London : P F Dennis, Dept. of Geology, Imperial College, Prince Consort Road, London SW7 2BP.

14-15 Nov. 1984 : Fifty Years of the Patterson Function : Institute for Cancer Research, Philadelphia : Kathryn Gennett, Office of Public Affairs, The Institute for Cancer Research, The Fox Chase Cancer Center, Philadelphia, PA 19111, U S A.

28 Nov. 1984 : IoP Physical Cryst. Group + Thin Films & Surface Group : Imperial College, London : Dr Mary Halliwell, British Telecom Research Labs, Martlesham Heath, Ipswich IP5 7RE : SEE THIS ISSUE.

17-22 Dec. 1984 : International Symposium on Biomolecular Structure & Interactions : Bangalore, India : Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560 012, India.

9-13 April 1985 : VIII Internat. Conference on Solid Compounds of Transition Elements : Vienna, Austria : Gesellschaft Österreichischer Chemiker VIII S.C.T.E., Eschenbachgasse 9, 1010 Vienna, Austria.

8-11 Sept. 1986 : 16th European Solid State Device Research Conference (ESSDERC 86) : Cambridge : The Meetings Officer, The Institute of Physics, 47 Belgrave Square, London SW1X 8QX.

27 August - 6 Sept. 1987 : Crystal Growth in Science & Technology : Erice, Trapani, Sicily : Dr Lodovico Riva di Sanseverino, International School of Crystallography, Piazza Porta San Donato 1, 40127 Bologna, Italy.

CRYSTALLOGRAPHY NEWS

Camera-ready copy on A4 paper is welcome at any time. For inclusion in the September issue please send items by 15 August to the Editor (or hand them to him at Hamburg!) : Dr Moreton Moore, Department of Physics, Royal Holloway College, Egham, Surrey, TW20 0EX :(Telephone 0784-35351 extn 36 : Telex 935504).

SURFACE CRYSTALLOGRAPHY

IMPERIAL COLLEGE - WEDNESDAY, 28th November 1984

Please send a registration form when available

I would like to present a contributed paper entitled:

Signed:.....

NAME:.....

ADDRESS:.....

.....

TELEPHONE No.....

PLEASE RETURN TO:

Dr. Mary Halliwell
British Telecommunications Research Laboratory
Martlesham Heath
IPSWICH
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Telephone: 0473 643640