Crystallography News

British Crystallographic Association

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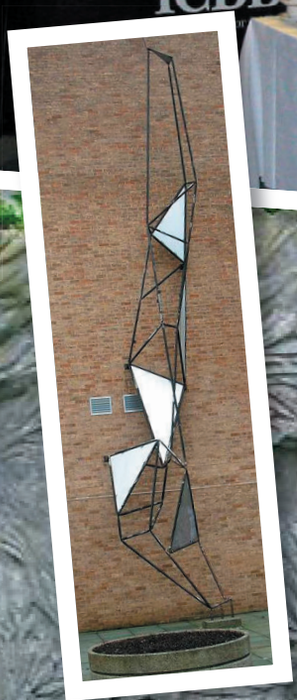

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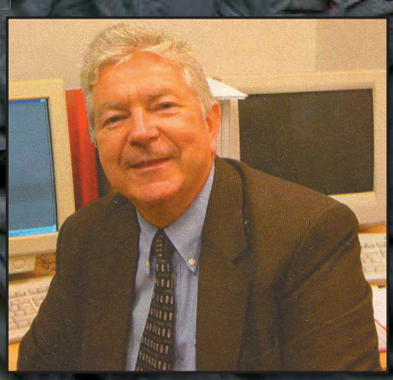

Crystallography News June 2006

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association.

Text should preferably be sent electronically as MSword documents (any version - .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files.

Items may include technical articles, news about people (e.g. awards, honours, retirements etc.), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.

Please ensure that items for inclusion in the **September 2006** issue are sent to the Editor to arrive before **25th July 2006.**

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From the President

WRITING this, my first column, shortly after the Spring Meeting at Lancaster, I would like to start by thanking all those people whose hard work and dedication contributed to making the Meeting such a success. It was very much a team effort, and thanks go to the BCA Officers, the programme committee, the group representatives and the session chairs for producing such a multifaceted and interesting programme. The contribution from the British Association of Crystal Growth is also very much appreciated, and we hope that the success of the synergy between the two groups will lead to further joint meetings. We are also most grateful to Northern Networking Events for the whole of the conference organisation, the staff of the Lancaster Conference Centre for providing able support, and all our sponsors without whose support the Meeting could not have taken place. My final thanks, specifically relating to the Meeting, go to the 360+ of you that attended and contributed through giving lectures, presenting a record number of posters, asking questions and interacting with the rest of the community.

You will be pleased to know that the planning for the Spring Meeting next year that will be held at the University of Kent at Canterbury between 17-19 April is already well under way. The Programme Committee, under the chairmanship of **Lindsay Sawyer**, is meeting in early May. The Programme Committee brings together representatives of the BCA subject groups and others, this year including colleagues from the XRF community and the British Association of Crystal Growth as well as from the Young Crystallographers who formed their own Special Interest Group during the Lancaster Meeting. The Meeting at Canterbury next year represents a milestone in the development of the BCA, as it will be our *25th Anniversary Meeting*, and I am particularly looking forward to a programme that celebrates our successes and reflects the "cutting edge" science that is being carried out by the community.

This year there have been quite a number of changes to the membership of Council. I would like to thank the retiring members **Sandy Blake**, **Peter Moody**, **Judith Shackleton**, **John Evans** and **John Helliwell** for all their contributions to the organisation over their terms of office. Particular thanks go to the outgoing president, **Chick Wilson**, whose contribution to the BCA has been enormous. The initiatives regarding the Young Crystallographers and the expansion of the meetings to involve other organisations have been largely at his instigation. His overwhelming enthusiasm and good humour will be missed, but I am very pleased to say that he will be remaining on Council for another year to show the "new boy" the ropes. I would also like to welcome onto Council **Bill Clegg**, **Richard Cooper**, **David Beveridge** and **Matt Tucker**, and congratulate **Elspeth Garman** on her re-election. It is also a great pleasure to welcome **Garry Taylor** onto Council as a co-opted member (when my enthusiastic co-opting has been ratified by Council). Finally, with Council permission, I welcome **Simon Coles**, who will represent the Young Crystallographers.

We also welcome two honorary members, who have made great contributions to Crystallography and to the BCA, **Chris Gilmore** and **Peter Main**. There will be more about them in the September Issue.

It is with great sadness that I have to report the recent passing of two distinguished members of the BCA, **Pat Tollin** and **Uli Arndt**. They will be greatly missed, and their contributions to crystallography will be recognized in full obituaries in a future edition of Crystallography News.

I have been giving some thought to my period as BCA President. I would certainly wish to strengthen the BCA by making it as inclusive an association as possible, and continue the work to form links with other associations and societies that have common interests with us, whilst not forgetting the strengths of our core membership. I would also like to further develop the theme of crystallographic education by promoting crystallography at the undergraduate and secondary school level now that the postgraduates are excellently catered for by the Young Crystallographers. I would certainly welcome thoughts and suggestions in these areas from the membership.

The summer will be busy crystallographically. We have the ECM23 in Leuven between 6-11 August as the focal point. The programme looks to be wide ranging and should have areas of interest for everyone. I look forward to attending the meeting and renewing contacts with colleagues from the UK and mainland Europe in our crystallographic community.

Paul Raithby

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2006-07

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www.crystallography.org.uk

Acknowledgements: The British Crystallographic Association is grateful to Birkbeck College, University of London, who host and manage the server for our website.

From the Editor

A warm welcome to these pages to our new President, Paul Raithby. It will be a little difficult getting used to the idea that the President is no longer in Glasgow after **Chris Gilmore** and **Chick Wilson**, but Scotland continues to be well represented with **Garry Taylor** on Council and **Lindsay Sawyer** chairing next spring's programme committee.

It was a great meeting at Lancaster, and I hope that some of the spirit sublimes over to recrystallise nicely in Crystallography News. As last year, most of the sessions have been written up by our bursars, and nearly all of them have been very good at sending in reports. I have had a good time sewing them together into what I hope look more or less like seamless accounts. Given the nature of our membership and the students who apply, there were many accounts of some sessions and few of others. I was glad to see, however, that most of the students made an attempt to go to something right outside their immediate interests, and were often pleasantly surprised by the results. Three students' reports, representing a range of age and interest, are also reproduced in full. And it wasn't just the important, scientific things that went well. The coffee service was excellent and readily available – no need to queue while someone insisted on pouring each cup. And the cookies! We've never had it so good, and I only hope that no one indulged to the extent of being affected afterwards by spyware!

One of the student reports on the Lancaster Meeting mentions "our learned Editor's constant presence with his digital camera". I cannot, sadly, be everywhere at once, and would again like to thank **Douglas Moore** for his help in shepherding speakers together!

Many thanks to all who wrote in with identifications of the 1938 photograph from Cambridge, the most complete of which came from **Andrew Lang**. Several correctly identified **Robert Evans**, but the best known was definitely **W.A. Wooster**, who looked much like that when I met him in the 1970s. Others spotted by at least one person included **F.C. Phillips**, **A. Harker** and **N.F.M. Henry**. It was good to hear from **Sidney Abrahams** in Oregon, who wrote: "the US crystallographer in the rear row, second from the right …. looks very much like a rather younger **I. Fankuchen** of Brooklyn Polytech than the one I initially met at the first IUCr Congress." And indeed he is, albeit in disguise. Even in those days, American ties sloped from upper right to lower left (as seen by the wearer), so Fankuchen was trying to go native! The photograph is reproduced with the obituary notice for Robert Evans, along with the actual identities.

In order to even out the size of individual issues, group material has been kept back for the September issue, when it will be a major component.

David Watkin's article on "Judging a Poster Prize" is something that should be compulsory reading for all future poster composers! I too have suffered from the stress of trying to make something of posters that seemed to contain as much information as the Handbook of Chemistry and Physics. Back when we used to bring the poster on bits of card and assemble it on the spot, it was possible to make a correction. Not so with beautifully unreadable hunks of A0!

The fact that next year will be the 25th Anniversary meeting means, by a simple calculation, that next March will see the 100th issue of Crystallography News. More about that later, but ideas are always warmly welcomed!

Finally, most of you will have received a message about "Chemistry in Great Britain and Ireland" – our latest name for our submission to the IUCr Newsletter. For more information, or to make a contribution, please contact the appropriate committee member:

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Bob Gould

Puzzle Corner

AFTER a bumper set of entries last month, this month's competition again salutes International Tables, on the appearance of Volume G. This is to a large extent concerned with that rapidly developing language CIFspeak. Please compose a job application in CIF. Credit will mainly be given for the adventurous use of as many statement types as possible – in particular, things other than special details. Have a go!

Last month's puzzle had a good number of entries, most of them from abroad, where International Tables clearly form a larger part of bedtime reading than they do in Great Britain and Ireland! Honourable mentions in particular to **Ulli Englert** (Aachen) and **Klaus Bartels** of Marresearch. The winner, though, by a good margin was **Howard Flack** (Geneva) (Yes, the Flack of the parameter!). I'll reproduce his answer more or less unchanged, complete with warnings about careless usage, engaged in sometimes even by your editor…..

2
- 1D space group types
- 3D triclinic geometric crystal classes / 3D triclinic point groups
- 3D triclinic space group types

4
- 3D point groups isomorphous to 622
- 2D crystal families

5
- 3D trigonal geometric crystal classes / 3D trigonal point groups
- 3D cubic geometric crystal classes / 3D cubic point groups
- 2D hexagonal point groups

7
- 3D lattice systems
- 3D crystal systems
- 3D tetragonal point groups
- 3D hexagonal point groups

14
3D Bravais flocks

17
Plane group types i.e. 2D space group types

32
3D geometric crystal classes sometimes called 3D point groups.

65
3D Sohncke space group types i.e. the number of 3D space group types containing only symmetry operations of the first kind (translations, pure rotations and screw rotations). Of these 65 space group types, 22 (i.e. 2 x 11) are chiral and 43 are achiral. Anyone who says that there are 65 chiral space groups should not be given the prize.

73
3D arithmetic crystal classes

230
3D space group types (not space groups as given in example to the question. There are an infinite number of space groups)

Letters to Ed.

From Professor Pam Thomas

Dear Bob,

I was both interested and concerned to read the entry for the ECM24 in 2007 at the bottom of page 32 of the March issue. It seems that George Bush has secretly annexed Morocco and incorporated it as the latest state of the USA.

I was really looking forward to my first visit to North Africa next year. Am I to be disappointed ?

Yours,
Pam Thomas

Ed. Dear Pam,

"From the halls of Montezuma to the shores of Tripoli,
We fight our country's battles in the air, on land and sea!"

So goes the US Marines' "Hymn", (sung, bizarrely, to the tune of Offenbach's "Les deux Gendarmes"!) so the takeover has long been planned.

Seriously, though, I'm at a loss to know what gremlin took over here. I did put MA for "Maroc" (I think it's the standard symbol but should have known better than to use it) and somehow, something thought it was Massachusetts.

Well, at least we can correct that in the next issue before anyone buys tickets to Boston...

Bob

From Professor Lindsay Sawyer

Bob

I've enjoyed the cosy between you and Tony and wonder if he has bowfed at you for misquoting his oft quoted North, Phillips and Mathews (Scott from WashU, St Louis, so spelled, not Brian from Oregon)?

North ACT, Phillips DC, Mathews FS, A Semi-Empirical Method Of Absorption Correction,*Acta Crystallographica Section A* **24**, 351(1968)

So where/who 'Williams'?! Seems to have been a good quarter, though without anything from Bill Duax. Yet.

Lindsay

Ed. Lindsay

My apologies all round – another senior moment, I'm afraid, and I'm glad to give the full reference here!

Bob

From Nicola Ashcroft and Louise Jones

Dear Bob,

Although we should probably not be allowed to send in a entry for March's Puzzle Corner, because we work as Technical Editors for the IUCr and could in theory have obtained the answers by searching the typesetting files for International Tables Volume A (we promise we didn't!!), we'd like to submit the following answers just out of curiosity, to see if we know our own publications as well as we'd like to think we do.

2 = number of one-dimensional space groups (line groups)
4 = number of crystal families in the plane groups
5 = number of Bravais types of lattices in two dimensions
7 = number of lattice systems (or crystal systems)
14 = number of Bravais types of lattices in three dimensions
17 = number of two-dimensional space groups (plane groups)
32 = number of geometric crystal classes
65 = number of Sohnke space-group types
73 = number of arithmetic crystal classes
230 = number of crystallographic space-group types ('space groups')

By the way, International Tables will be available online soon (see http://it.iucr.org), at which point any puzzles for which the answers could be found by searching the full text online might have to be avoided!

Please make sure we don't win (this might be embarrassing for the IUCr!) - we'd just like to know how we did.

Best wishes,
Nicola Ashcroft and Louise Jones IUCr

BCA Corporate Membership

The BCA values its close ties with commercial companies involved with crystallography. To enhance these contacts, the BCA offers Corporate Membership. Corporate Membership is available on an annual basis running from 1 January to 31 December and includes the following benefits:

- Up to 10 free BCA memberships for your employees.
- A 10% discount on exhibition stands on the annual BCA Spring Meeting, OR - A promotional poster at the annual BCA Spring Meeting.
- Free insert in the annual Spring Meeting delegate bag.
- Two free full registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly BCA Newsletter.
- Corporate Members will be listed in every BCA Newsletter and on the BCA Web Site with links to your corporate site.

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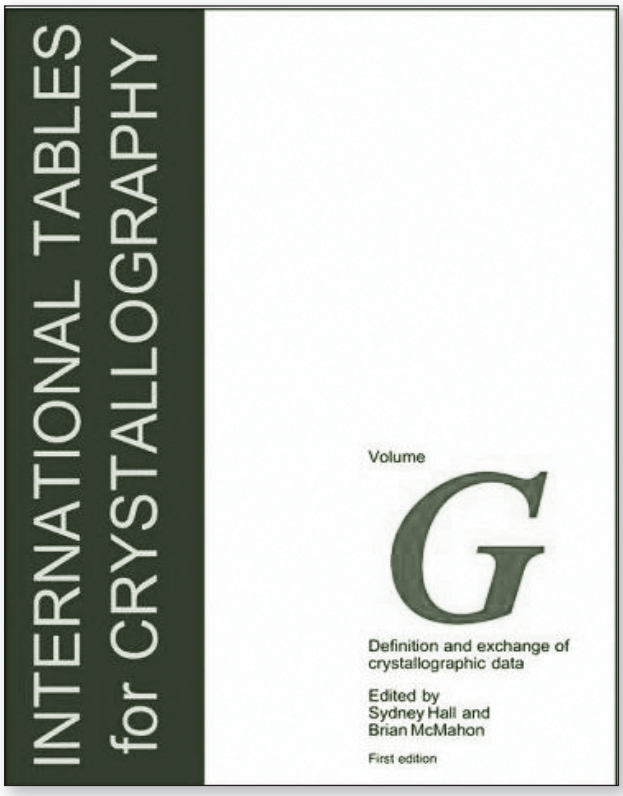
Books

International Tables for Crystallography

Volume G:

Sydney Hall, University of Western Australia and **Brian McMahon**, IUCr, Editors
Published for the International Union of Crystallography by **Springer Verlag**, 2005
Price £135, Euro205, $220 (institutions/libraries) – half-price for personal use.

ISBN 1-4020-3138-6, 594+xii pp.



THIS latest Volume of International Tables for Crystallography deals with the definition and exchange of crystallographic data. The intended audience comprises working crystallographers, programmers who write crystallographic software and data managers. The volume describes the standard CIF format for exchanging and archiving crystal data. It is divided into five Parts covering the historical context; concepts and specifications; the definition and classification of CIF data; the core and supplementary CIF dictionary and finally CIF applications.

The first Part details how electronic handling of crystallographic data has undergone just as much change over the past 15 years as have X-ray sources, detectors or software. In 1990 there were only limited facilities for electronic data exchange, and a lack of standardisation seriously limited the ability of one application to read and understand the output from another. However, the impact of the introduction of the CIF format was such that by 1996 Section C of Acta Crystallographica was able to require that all standard material for a paper except Figures and Schemes be submitted in that format. The widespread acceptance of CIF has also transformed the deposition of supplementary data: to those who can remember them, the days of having to submit multiple hard copies of structure factor tables now seem to belong to prehistory.

The second Part describes the challenge of developing a language which can convey precisely and reliably the complexity and variety of scientific results. This language also has to be flexible and capable of being extended to cope with new developments. The CIF is therefore a subset of the Self-defining Text Archive and Retrieval (STAR) format. Standardisation of data items is clearly of vital importance to the successful application of the CIF format, and this is the responsibility of an IUCr committee. The STAR format has been extended to cover related areas, including molecular information, macromolecular crystallography, powder diffraction and modulated structures. CIF fits well into the broader area of scientific data and is easily transferred to and from XML (extensible markup language). However these links develop, CIF is already firmly established in its central role within crystallography. The specification of a STAR syntax lies at the heart of the CIF format: it must be free-format and contain sequential lines of ASCII characters comprising text strings. Paired data names and data values comprise data items which convey the information, with a loop facility to allow the specification of multiple data values for a single data name.

The third Part deals with the definition and classification of CIF data. After a general overview, it describes the core CIF dictionary containing the data items common to most CIFs, for example those relevant to a standard laboratory X-ray structure determination of a small molecule. Subsequent sections cover powder diffraction, modulated and composite structures, image data and symmetry information.

Part 4 defines all the data names for the core and other dictionaries. These names include not only experimental information but also other data such as the author details for a paper. The data items are arranged alphabetically by category (such as atom_site) within which data items are also listed alphabetically (e.g., from _atom_site_adp_type to _atom_site_Wyckoff_symbol).

Part 5 deals with the creation of new "CIF-aware" applications, as well as the adaptation of existing applications to render them capable of dealing with CIFs. A program which has to be able to read CIFs, perhaps from a variety of sources, is much more of a challenge to write than one which has simply to output data in CIF format. A number of types of application are then outlined, including STAR file utilities which are capable of handling any data in the format: such programs might include ones which extract selected data from the CIF; allow editing of the contents of the CIF; transform the STAR format to HTML, etc. Syntactic utilities for CIF include syntax checkers, interactive editors, visualisers and validators. For programmers, a Fortran function library (CIFtbx) covers the common operations likely to be needed in order to deal with a CIF. A separate section of Part 5 deals with the application of the macromolecular CIF architectures to the management of Protein Data Bank information, while another describes an ANSI C library allowing the manipulation of binary files and image CIF files. Finally, there is a case study of the publication of small molecule crystal structures using CIF, as practised by Section C of Acta Crystallographica since 1991 and by Section E since its inception. This study outlines the advantages to authors, editors, referees and the journals of the highly automated procedures for submission, validation and publication which are possible because of the adoption of the CIF standard.

The accompanying CD is a important resource which contains machine-readable versions of STAR and CIF specifications, the various CIF dictionaries, along with a collection of software libraries and applications. It also provides extensive supplementary information for each Part.

Although this is primarily a work of reference, with Part 4 requiring over 260 pages to describe the data dictionaries, it also contains substantial narrative and explanatory sections which are very effective, for example in describing the evolution of the handling of crystallographic data and the concepts which underpin the operation of the STAR and CIF formats. The volume will clearly be indispensable for any programmers writing applications which need to read or write information in CIF format, but the pervasive nature of CIF in everyday crystallographic work means Volume G will be a useful addition to any crystallographic laboratory.

Sandy Blake

Michael Polanyi - Scientist and Philosopher

William Taussig Scott and **Martin X. Moleski, S.J.**
Oxford University Press, 2005
Price: £26.99 (hardback)
ISBN-13 978-0-19-517433-5, xvi+364 pages

THE first full biography of Polanyi describes well the early life and subsequent career of one of the pioneers in Berlin of metal structure and deformation and of X-ray fibre analysis. It relates how Polanyi, moving as a refugee to a chair in Manchester, enhanced his scientific reputation developing the transition-state theory of reaction kinetics but later gained even wider celebrity as a social scientist and philosopher of science.

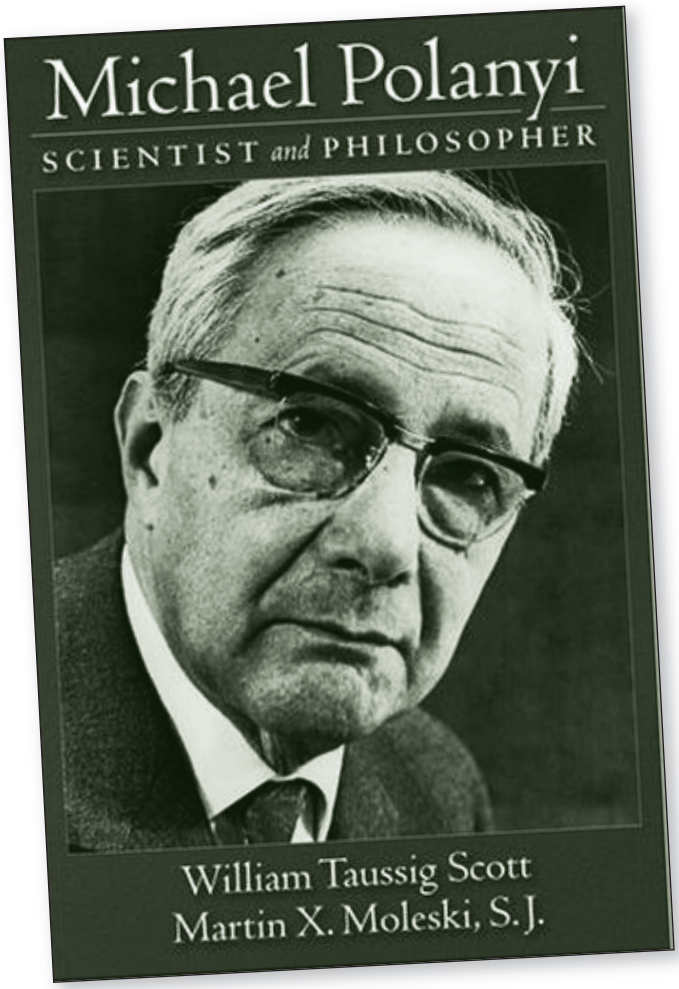
Michael Polanyi (1891-1976) qualified first in medicine in Budapest (although publishing in thermodynamics on the way). He then spent nearly thirty years in Berlin and Manchester in front-rank research in physics and physical chemistry (but concurrently wrote, lectured and campaigned on social sciences), and in his later years became an international figure in philosophy and the humanities. During World War I, Polanyi was a medical officer in the Austro-Hungarian army and in the latter part of World War II he was able in Manchester to investigate catalytic polymerization to form synthetic rubber, while his son George served in the British forces. Following consecutive full-time chairs at Manchester in Physical Chemistry (1933-1948) and in Social Studies (1948-1959), one of Polanyi's later Professorships was in the Department of Religion at Duke University! By then, in what he regarded as his chief contribution to intellectual life, Polanyi had become a philosopher of science, writing and lecturing across the world and embracing economics, aesthetics, political theory and theology. His close friends included Arthur Koestler and the economist John Jewkes.

It has taken an American physicist and philosopher, W.T. Scott, and a Professor of Religion, M.X. Moleski, many years and the resource of 150 interviews across several disciplines, but including some distinguished British chemists, to compose a fine comprehensive biography of this remarkable man. Scott, the senior author, knew Polanyi for the last seventeen years of Polanyi's life. The chronological list of books and papers (with titles translated into English where necessary), compiled by Polanyi's son John, a Nobel prize winner in Chemistry in 1986, in itself provides a measure of the contributions to diverse fields. Eleven chapters cover phases of family, scientific and philosophical life successively in Hungary, Germany, Manchester and, though based mainly in Oxford, effectively in the world at large. Polanyi' s scientific period, which, with his education, takes up two-thirds of the book, is covered well (thanks partly to detailed advice from an eminent physical chemist) and at a level that should be intelligible to the non-specialist. Strictly chronological biographers have their opponents but, for a life that was influenced by political attitudes and always carried parallel intellectual threads, I felt that it was appropriate to interleave the account with family events, generally happy, but occasionally tragic.

For crystallographers and solid-state scientists, the crucial period of Polanyi' s scientific creativity began in 1920 when he moved from the Karlsruhe Technische Hochschule (where he had gone to escape persecution in Hungary) to Berlin. Despite having experience of neither X-rays nor fibre chemistry, Polanyi was assigned the problem of interpreting the X-ray pattern of cellulose fibres at the new

Institute of Fibre Chemistry. Thus he became the first to suggest that the unit cell of cellulose could be interpreted in terms of a long-chain molecule. With this success, he was able to engage Brill, von Gomperz, Mark, Schmid and Weissenberg as assistants, and the rotating-crystal method was established. Polanyi commended Mark, who was to devote his career to high polymers, for manipulative skill and Weissenberg, whose name is linked with X-ray and rheological instruments, for mathematical ability.

Scott and Moleski describe how the emphasis of Polanyi's group then shifted from fibre structures to the strength and plastic flow of solids through stretching of zinc and then crystals and microcrystalline wires. Experiments with Ewald on cold working of a rock-salt prism led to notions of dislocation or "Versetzung". Among several references to Polanyi in The Crystalline State, WL Bragg credits him as the pioneer in single-crystal deformation and the theory of metal crystals. Although he transferred in 1923 to the Institute of Physical Chemistry and Electrochemistry in Berlin to concentrate on reaction kinetics, Polanyi continued to publish on the solid state, especially with Bogdandy, Sachs and Schmid on plasticity and annealing of metal crystals and the deformation of ductile materials through the 1920s.



Publications on rates of chain reactions and sodium-flame reactions steadily increased as the concepts of activation energy and transition state emerged and were developed at Manchester after 1933. However, many of the papers from groups that he had set up and directed, such as those led by Bawn and Fairbrother did not carry Polanyi's name. His FRS came in 1944 for a broad catalogue of achievement that specifically included rotating-crystal analysis and the strength of metal crystals.

Students in the 1940s attending Polanyi's first-year lectures on X-ray diffraction and the equipartition of energy were barely aware of his early contribution to both topics, still less that much of his thinking time was now spent on social sciences rather than physical chemistry. On economics, his views on Employment and Money, on which he produced two films as well as books and many papers, were close to these of Keynes. In social science, Polanyi made one of the most spirited responses, opposing central planning of science, to the influential 1939 book *The Social Function of Science* by the crystallographer J.D.Bemal (who, in the 1920s, had been one of the first to take up Polanyi's rotating-crystal X-ray method).

From 1948, having transferred to a chair of social studies at Manchester, Polanyi was able to devote all his attention to economics, social studies and philosophy. In science he raised doubts about absolute objectivity and recognized the importance of "tacit knowledge" in interpretation. After formal retirement in 1958, Polanyi became a celebrated world scholar with many visits to the USA. Emphasising freedom and responsibility in science, Polanyi's published lectures revealed a mind groping towards a relation between scientific knowledge and religious knowledge and faith.

We also learn from the biography that in the 1930s and 1940s, professors at Manchester, such as Polanyi and his contemporary WL Bragg, enjoyed large houses staffed by several servants, were enveloped in a vigorous social-cum-intellectual life, and had considerable freedom for leave. In his new chair, Polanyi "gave over 1949 to writing" (for prestigious lectures at another University), spending lengthy periods at a country inn in Wales!

The reproduction of old photographs is mediocre and the captions are inadequate, while the absence of a brief date-summary of Polanyi's career is regrettable. However, the book is well annotated and indexed and has a clear biography of Polanyi's scientific and other publications. Overall, this bibliography gives a fascinating account of a polymath who established his scientific credentials in X-ray analysis, went on to be a major contributor to the transition-state theory of reaction rates and then emerged as an acclaimed philosopher of science.

Derry W. Jones

Obituary

Robert Crispin Evans
(1909-2005)

ROBERT CRISPIN EVANS died peacefully on 18th December 2005 at the age of 96. As well as being the oldest of our Honorary Members, he was senior Emeritus Fellow of St. Catharine's College, Cambridge, and was also the last surviving founder of the IUCr.

Robert Evans was born in November 1909 in Wallington, Surrey, to a business family. He was educated at Repton School, Derbyshire, and Clare College, Cambridge, which he entered in 1928. He also had a B.Sc in physics from London University, which he apparently took as an external student while he was an undergraduate at Cambridge! He was a research student in physics at the Cavendish Laboratory and gained his Ph.D. in 1934 for a thesis was entitled 'The evaporation of ions and atoms of the alkali metals from hot surfaces'. Two of the papers from this work were communicated to the Royal Society by his official supervisor **Lord Rutherford**.

Evans became a member of the staff in the Department of Mineralogy and Petrology at Cambridge in 1933, serving as Demonstrator 1933-1945 and as Lecturer 1945-1977. During World War II, from 1940 to 1945, Evans was with the Ministry of Supply where he worked on shell ballistics and experimental firings. He returned to Clare College in 1945 and was elected a Fellow of St Catharine's College in 1947.

He gave extremely well received lectures that he illustrated with models mainly conceived and constructed himself. His lecture demonstrations of crystal optics and microscopy were notable. He built an electromagnetic mineral separator that was a great improvement on previous instruments and was much used by research students. Among other devices that he worked on with colleagues were a mechanical machine for the computation of two-dimensional structure factors and a concentrating X-ray monochromator. In essence, he was a tutorial don, who was not driven, as university staff are today, by the need to research and publish. Rather, he was a teacher and mentor to generations of students. His major academic contribution was his comprehensive book on *Crystal Chemistry*, published in 1939. The idea for this book arose from his translation of the short book *Kristallchemie* (1934) written in German by O. Hassel of Oslo. The preface acknowledges that he had been actively aided and encouraged by **J.D. Bernal**, who in 1937 had left Cambridge for Birkbeck College, London. The chapter on molecular compounds had been discussed with **Dorothy Crowfoot** (Hodgkin).

Crystal Chemistry omits any discussion of X-ray methods. It opens with chapters on the crystal lattice, interatomic binding forces, and quantitative lattice theory (Born, London, Pauling, Bloch, Seitz et al.) One can see how his thesis work would have stimulated his interest in these topics. Much the larger part of the book is on systematic crystal chemistry. When his tasks with the IUCr had finished in 1960, he was able to complete a second edition of *Crystal Chemistry* in 1964.

Evans was a key figure in the first years of the International Union of Crystallography and carried undoubtedly the largest single work load. XRAG, the predecessor of the BCA and led by **Sir Lawrence Bragg**, arranged an international scientific conference 'X-ray Analysis during the War Years' in London in July 1946. Afterwards, the Provisional International Crystallographic Committee of 31 persons from 11 countries met on 12 and 13 July with **Lawrence Bragg** and **David Harker** as joint Chairmen, and Evans as Acting Secretary. This meeting, which decided to create a Union and develop a journal and other publications, was effectively the 'Zeroth General Assembly of the IUCr'. Evans and **Paul Ewald** were heavily involved in launching the new journal ***Acta Crystallographica***. Money had to be raised, including grants from UNESCO, and from industrial and other sources in the UK and USA. A publisher had to be chosen: Cambridge University Press was selected. Manuscripts had to be sought and printed. Remarkably, the first issue of *Acta Crystallographica* appeared in April 1948.

Robert Evans was Secretary of the Provisional International Committee (1946), then General Secretary of the interim Executive Committee (1947), and then General Secretary of the Union from its formal inauguration in 1948 for the first two triennia until 1954. In addition, he was a Co-editor of *Acta* from its launch in 1948 until 1960, and carried the very demanding load as Technical Editor until 1958 by which time *Acta* was three times its initial size.

Evans' responsibilities concerned the arrangement of the formal business of the Union to be transacted at the sessions of the General Assembly. Actually, this formal business was transacted without real difficulty, despite Ewald's initial attempt as Chairman to create the Union by the acclamation of the entire audience of Congress participants rather than by the votes of the official delegates. "Evans somehow rescued me" Ewald wrote later. In fact, at that time there were only four members – the Adhering Bodies of Canada, Norway, UK and USA – indeed when Evans was making preparations, the number of formal members, as he wrote later, "could be counted on the thumb of one hand". Ewald and Evans, with their different styles, formed a very effective duo for the accomplishment of the necessary business.

Evans was a careful scientific and technical editor. He had a genuine interest in all aspects of print production. I remember being invited to his office in Cambridge in 1949. In those days, the text of papers was typewritten, but equations and symbols were inserted by hand. He pointed out kindly the ambiguities in my handwriting and showed me something of the way a paper should be marked up for the printer. In 1954 he gave a talk at an XRAG meeting in Cambridge about the work of an editor. He illustrated his talk by mentioning some of the problems in submitted papers. As each infelicity was mentioned, he raised his head a little and nodded gently to the relevant culprit in the audience.

In 1955 he married **Betty Bond**, whom he had met when she was a librarian in the Scientific Periodicals Library. She survives him; they had no children. Their home in Elsworth, a village outside Cambridge, was an important focus for hospitality of all kinds, and not least, hospitality to students.

After retirement in 1977 he had two hobbies, one keeping bees and the other opening his small workshop to encourage the youths of the community to learn skills in wood work activities. He was a kindly person, generous with his wisdom, but somewhat reserved in manner. However, on a public platform there was a side of Robert that could perform to great effect. He was not a joke teller, but he could make a remarkably effective and witty speech, simply by his choice of words and timing.

For his 90th birthday celebrations at St Catharine's College, the anecdotes he related included the following. The Cavendish Laboratory, where he was a research student, was enjoying its most illustrious epoch "not only because I was there" but because no fewer than 8 Nobel Laureates were there too. On one occasion Einstein was visiting Cambridge and made a tour of the Laboratory accompanied by Lord Rutherford and J. J. Thomson, who was Rutherford's predecessor and discoverer of the electron. The party visited a practical class in which Robert was demonstrating and after their departure he was asked by one of the students "Who were those other gentlemen with Einstein?"

On Monday 7th April 1997, fifty years after its inception, the IUCr invited Evans to visit Chester to open the latest extension to its offices. He spoke of the creation and early days of the Union. One of the major reasons for inaugurating a new Union was the desire to launch a journal of the highest standards to serve the entire crystallographic community. Appropriately, the Union's first half-century was celebrated in the place where its family of six journals was being produced with the most modern of computer technology. Very fittingly, the celebrations were enhanced by the presence of the last surviving founder of the Union: Robert Evans.

Durward Cruickshank

Robert Evans on the occasion of his 90th birthday in 1999.

Department of Mineralogy and Petrology, University of Cambridge, May 1938

Back row:
T. Deans, F. Walker, A.J. Hall, I. Fankuchen, R.T. Prider

Middle Row:
A.T.J. Dollar, S.O. Agrell, R.C. Evans, N.F.M. Henry, R.S. Nockolds, C.O. Hutton

Front Row:
F.C. Phillips, A. Harker, C.E. Tilley, R.H. Rastall, W.A. Wooster.

BCA Spring Meeting 2006

Lancaster Reports

Alan Cheung

IT is 6.30am in Sheffield on the first day of the main meeting and the Sheffield contingent of groggy protein crystallography students hop into the car for the two hour drive to Lancaster, hopefully arriving for the first lecture of the biological structures group. Unfortunately, one wrong turn by the hapless driver (which was me, but I blame my navigator) and three hours later, we check in, hunt for the strongest coffee available and wait patiently for the first keynote talk on novel protein crystallisation technologies by Larry de Lucas.

He showed us there is much more to crystallisation than a lab bench with pipettes, plates and solutions, incorporating both computational and biophysical techniques into improving your chances. This was a thoroughly interesting and entertaining lecture, especially on zero-gravity crystallisation and related toilet anecdotes and better yet, gave us hope for our future successes as budding crystallographers, although perhaps not as astronauts! This optimism repeated itself throughout the meeting, with excellent talks spanning useful techniques we could try at home, new technologies to look forward to and impressive biological stories.

Terese Bergfors' and Allan D'Arcy's lectures on crystallisation strategies, nucleation and seeding were especially informative and encouraging for despondent students and gave us new tricks we could try immediately on returning home. Terese's comparison of getting and optimising crystals to getting and optimising boyfriends brought hearty chuckles from the female audience, and shifty looks from the males. Elspeth Garman also gave a very practical and enlightening talk about cryo-cooling and I had to admit to making some of the mistakes she warned about! Jonathon Grimes' talk on Virus Crystallisation and his awesome viral structures showed us the extremes of what was achievable with protein crystallography, albeit with some serious determination and work – requiring thousands of crystals for heaven's sake! But it was breath-taking stuff. The structural genomics talks by So Iwata, Frank Von Delft and Tassos Perrakis were highly impressive and were even useful for students like myself, as their methods of expediting crystallisation and structure solution on a large scale seemed equally applicable to single-protein work.

Technology also played a big part, with both exhibitors and academics showing off their latest toys, stuff I really hope I'll get to try one day, like the free-mounting system from Proteros and the free-interface diffusion chips from Fluidigm. And I got my free mug from Rigaku, although the stand was unattended at the time – sorry guys!
Moving away from biology, we did make the odd foray into non-protein talks, the most notable (and comprehensible) one for me was the crystallisation of polymorphic drugs. Admittedly, we didn't move too far from biology! I have no experience of small molecule crystallography, and Ulrich Griesser gave an excellent introductory talk to the trials and tribulations of drug crystallographers and the effect polymorphism can make to the efficacy of medicines, an issue I was unaware of and that further highlighted the complexity of making new drugs.

So was the meeting a success? I have to admit, prior to the meeting I thought this BCA meeting would be one of the more dowdy academic conferences I would go to, but was completely surprised by how entertaining the speakers were – especially during the conference dinner! More importantly, it's given me new ideas for my own project and inspiration for the future and that is the most important thing from a student's perspective. Whilst I have a few new items I'd like to beg my supervisor for, there's plenty of new ideas to keep me going in the meantime!

Alan Cheung, University of Sheffield

Gary S Nichol

THERE are many factors which seem to be integral parts of all BCA meetings. One is our learned Editor's constant presence with his digital camera, and requests for non-embedded photographs. Another is the petulant refusal of laptops to talk to projectors until it's almost time for coffee. A third is the casual and informal atmosphere of the meeting, exemplified by much clapping and cheering when the outgoing president makes a mild Freudian slip during the AGM, and by the ability of the BCA membership to empty a bar of all draught beer within two days. I doubt whether other meetings of other scientific associations are quite so relaxed; as was noted at the AGM, membership of the BCA really is value for money.

This was my fourth and longest BCA to date, incorporating the main meeting, the Young Crystallographers meeting and the Hursthouse Event. For those hardy folk who stuck it out until the end, this meant five days of science which, thanks to a good balanced programme, never seemed to drag.

The week started with the second Young Crystallographers meeting, designed to run on alternate years to the CCG Durham School and to provide a forum for Ph.D. and post-doctoral crystallographers to give presentations on their research to their peers, along with a few longer seminars

by some of the so-called Old Gits of crystallography. This also included the two-minute Oral Poster session under the enthusiastic chairmanship of Andy Parkin, who had done much to make the meeting a success. There was a good spread of topics in a meeting dominated by high-pressure research, with presentations by Alex Griffin on crystal synthesis, and Anna Collins on analysis of structures with Z' = 2 being particular highlights for me. For future meetings I would recommend that the seminars given by the more senior crystallographers focus more on teaching, rather than merely being a pure research seminar. For example, a talk on the basics and practicalities of high-pressure crystallography by an acknowledged expert would be useful to those who do not work in this area (particularly biologists) and would be good preparation for the research-focussed seminars given by the students showing how high-pressure crystallography is used in research.

Arising the next morning to the gentle hum of traffic hurtling down the adjacent M6 and stumbling through the building site to the breakfast room, I decided to attend the full-day workshop on phase identification from powder diffraction. As a complete novice to powder diffraction, and keen to learn more, I found the workshop very useful and informative. Attended by a mixture of experts and first-timers, the day started with an introduction to the powder diffraction file (given the unfortunate abbreviation PDF which can be confused with a popular document format, although the powder file is far older) and the different methods of searching the vast database either by computer or by hand (for the time-rich!). The workshop also included a discussion of some practical matters regarding sample preparation, data collection and machine calibration and ended with a hands-on computer session with practical examples and exercises in searching powder diffraction databases.

The next day started with a keynote talk by Mark Spackman on the program Crystal Explorer. This uses the Hirschfeld surface of a molecule to analyse how the molecules pack in a crystal by means of differing shapes and colours of the surface. This would be a particularly useful tool for anyone with a keen interest in packing of organic molecules and about the only thing we weren't told was where to get the program from! http://www.theochem.uwa.edu.au/CrystalExplorer/ is the answer. Other highlights of the day came from Sally Price with a talk on progress in crystal structure prediction in her research group, and a particularly engaging talk by Terry Threlfall on crystal growth, polymorphism and growing polymorphs. The concept of disappearing polymorphs is quite well documented, but when one considers the unlikely idea of a single crystal travelling 3000 miles across the Atlantic and then penetrating a steel vessel containing crystals of a less-stable polymorph, and that the dissolution of this single crystal is enough to seed all the others to change to a different form, then perhaps we don't quite understand disappearing polymorphs after all! The last lecture of the day was another illuminating talk by Mike Glazer on the optical properties of crystals. New stuff to some of us, but for the old gits is was a stroll down memory lane.

The final day of the meeting started off with an introductory keynote talk on protein crystallography, complete with temperamental laptop. Following this was a useful session on charge density analysis, with good presentations by Louis Farrugia and Piero Macchi. As with high-pressure crystallography, charge density analysis is an area where some know much more than others and this would perhaps also be a candidate topic for a teaching-based Young Crystallographers session. The final afternoon was spent in the Crystal Engineering session, which with six speakers was quite long without a short break. Highlights from this afternoon session were presentations by Christer Aakeröy, Dario Braga and Joshua McKinnon.

For those for whom four days are not enough, a symposium organised in honour of Mike Hursthouse took place after the main meeting. Featuring a mixture of science, memories and holiday photographs this symposium was to mark the 65th birthday and retirement of Mike. However, as was noted by several speakers, retirement for Mike is a mere formality since he intends to continue on with research and the National Crystallography Service for a few more years to come.

I thank the CCDC, the BCA and Bill Clegg for funding to enable my attendance at all three meetings.

Gary S Nichol, University of Newcastle

Duncan Sneddon

THIS was my first real conference; I had previously attended one day symposia, but this was the first time I was destined to spend days listening to people talk science. There was a degree of trepidation during the build up towards Lancaster; as my background is not in Chemistry let alone Crystallography I was worried that I was facing four days of unrefined boredom. How wrong I was.

The young crystallographers satellite meeting was good for a number of reasons. Firstly, it offered a stage for the less senior (in most cases!) crystallographers to give a nice overview of the scope and depth of research being carried out by Ph.D. students and post-docs around the country. The meeting also gave an opportunity for all the people presenting posters to put a plug in for them, finally the poster session was a great opportunity to meet my fellow Ph.D. students and of course drink wine.

I attended the crystal stories session, which as I am a theoretical crystallographer is about as far from my field of study as you can get. Having friends who have attempted to crystallise proteins in the past, it was nice to see some applications of the techniques that caused them to lose so much sleep. The vapour batch technique was an interesting solution to problems in protein crystallography,

but it was especially refreshing to hear of international collaboration between groups to overcome similar problems. The lecture 'Protein crystallisation – an anecdotal approach' gave an interesting view that the early (19th and early 20th century) crystallographers had, in some cases, the right end of the stick. It was an interesting example highlighting what the early literature can tell you about your subject. The other talks I enjoyed were the groups that automated the process of crystallisation; my background is in genetics and bioinformatics where one of the largest undertakings in molecular biology was the human genome project and the automation of DNA sequencing. Getting an overview of the current status of the large-scale proteomics projects, while not being really relevant to my work, was interesting from the perspective of how far the field has advanced in a short period of time.

One of the highlights of the conference for me was the keynote lecture from Larry De Lucas. Apart from the obvious highlights such as being fired into space to make crystals, and creating plans to send the current President of the United States to Mars, his group's use of neural networks to simulate crystallisation conditions in order to ensure that all possible conditions under which crystals could form were covered. This was a fascinating use of a computational method married to high throughput crystallisation using novel techniques in order to maximise the chances of producing good quality crystals.

Overall, I thoroughly enjoyed myself in Lancaster. The conference served to disprove many of my assumptions – such as, posters are there solely to irritate the people that have to make them! I really liked being around so many enthusiastic scientists and feel fortunate that I have joined a community of dynamic and outgoing scientists. I can only hope that future BCA meetings will measure up to Lancaster 2006.

Duncan Sneddon, University of Glasgow

Judging a Poster Prize

CHARLIE BRODER and I were given the task of awarding the Chemical Crystallography Group Poster Prize at the Spring Meeting in Lancaster. Seemed quite an honour until we discovered that there were 75 posters to read!

We started by going round the displays during the buffet and wine evening, each of us independently rating the posters on science and presentation. Bad move! There were so many to read that I only found time to snatch one glass of wine and a bit of cheese, and that still worked out at just over two minutes per poster. At the end of the evening, we compared our shortlists, and found only one poster in common. We then combined the shortlists, and re-visited and independently re-ranked those posters. There was still only one poster in common in our top fives.

We quickly realised that it was quite impossible to compare the *quality of the science* - it would have been like trying to compare cabbage and apples. Equally, judging ***artistic merit*** was like trying to compare Rembrandt and Picasso. Since we were awarding a poster prize, we decided to choose the poster that conveyed its message most quickly and effectively.

Being forced to read 75 posters gave me some insight into how to prepare one to appeal to a judge:

1. Remember that you are preparing a poster, and not a 'learned paper'. Don't try to get everything you know into the space allocated.
2. It is probably best to avoid a cluttered background image, but if you must use one, be sure that the text is easily readable, that is, in a strongly contrasting colour. Black on dark blue or dark green were poor combinations.
3. Present both the aims and the conclusions in the top 1/4 of the poster. It's not a natural thing to do, but it enables the judge to see what you have done before delving into the detail.
4. Divide the body of the poster into two or three columns. One column means long lines of text which are uncomfortable to read, more columns makes the document look fragmented.
5. Put pictures in a frame with their explanatory text so that they can be understood without having to locate details in the main text.
6. Put really important text in a frame, possibly with a different background colour to the rest of the poster.
7. Keep tables simple - no judge will have time to assess shed loads of numbers.
8. Avoid novelty fonts and choose ones that are easy on the eye.

Finally, when you have drafted your poster, give a colleague three minutes to study it, and then ask them what it was about.

David Watkin

Exhibitors BCA 2006 Sprin

Alpha Helix UK

Beevers Miniature Models

Bruker AXS

Crystal Engineering Communications

Crystal Maker Software

Fluidigm

Genomic Solutions

Hecus X-Ray Systems

Hiltonbrooks

ICDD

INEL UK

IUCr

Marresearch

Molecular Dimensions

Oxford Cryosystems

g Meeting, Lancaster

Oxford Diffraction

Oxford University Press

PANalytical

Photonic Science

ReactArray

Rigaku

Taylor & Francis

Thermo Electron

Wyatt Technology

Xenocs

Certificates of appreciation for donors of Bursaries

ICDD

Oxford Diffraction

Rigaku

Lancaster Sessions

Charge Density

IT was the final day of the meeting, and everything was running perfectly on time, until the technical problems occurred in the plenary lecture, consequently delaying the starting time of the parallel-session. **Dr. Mary Mahon** (chair) introduced the first speaker, **Louis Farrugia**, whose talk was entitled *Experimental aspects of charge density studies.* Louis talked about the importance of collecting good data: at ultra-high resolution, with cryo-temperature, and using a synchrotron radiation source. He talked up the advantage of picking a short wavelength such as 0.5Å or shorter (i.e. much shorter than Mo Kα at 0.71Å). Thus, absorption and extinction errors in the diffraction data are even smaller, and both of these can badly affect valence density studies. Louis then demonstrated the benefits of having high quality data with examples of transition metal complexes and the direct experimental measurement of the electron distribution in molecules (charge density), providing detailed information about the chemical bonding between atoms. Louis continued his talk with the display of topological images of charge densities in Mn-Mn and carbonyl bonds.

The next speaker was **Piero Macchi**, who focused his talk on The *XD software package for charge density analysis*. Piero presented the main features of the XD program package, which is capable of multipole refinement and topological analysis of charge densities from both X-ray and neutron diffraction data. He showed various topological images (after carrying out multipole refinement) of deformation density on a theoretical model of benzene, and explained why out of the six different types of refinements the quadrupole refinement was the best. Piero also explained the anharmonic motion in a cobalt metal complex, and the difficulty of defining anharmonicity as temperature increases. He concluded his talk with the evaluation of electrostatic (e.g. multipole-multipole) properties and interaction energies (e.g. lattice energies) between molecules in crystals.

Sebastien Pillet presented a talk on *Electron density distribution of metastable states.* Sebastien emphasised the equipment details, measurement conditions and sample characteristics that are required in order to obtain accurate electron density maps. He talked about laser light perturbation and the importance of choosing a wavelength that will cause excitation (of the molecule) and in turn initiate a light induced transformation mechanism. This was followed with examples of Fe(II) complexes and their electron density distribution going from a high spin to a low spin state. Sebastien described how one can trap the metastable state of a complex by quenching the temperature, and how it is possible to measure the photomagnetic properties at temperatures as low as 30K. Discussion after the talk included whether standard uncertainties on the population percentages might be viable and how they might vary as a function of the experimental challenges such as sample mosaicity arising from the laser beam interaction (as well as the X-ray beam).

The session ended with the final speaker **Paul Popelier**, addressing *Quantum Chemical Topology (QCT)*. Paul revealed how the novel theory QCT can rigorously define atoms in molecules and how that information can be transferred from small molecules to proteins, carbohydrates, lipids and DNA. He then went on to show relief maps of electron density in methanol, water and ethene. Using the examples of ethene and glycine, Paul identified the critical bond points, and the 1,3-1,4 interactions that are involved in glycine. At the end of his talk he summarized how "Atoms in Molecules (AIM)" can be seen in a wider context and why Quantum Chemical Topology is an appropriate name for this approach. Discussion after the talk included whether atomic displacement parameters could be included in QCT in the future.

Ahmed Helal, Manchester

Louise Male, Piero Macchi, Louis Farrugia, Mary Mahon and Paul Popelier

Crystal Stories

FOLLOWING Lunch on Tuesday, **Lesley Haire** (NIMR) kicked off 'Crystal Stories – Session 1' with a talk in which the vapour batch method was discussed for use in crystallization using volatile organics. It was the story of her successes with vapour-batch on amino terminal domain (NTD) capsid protein, which came about after many other trials failed, trials with vapour-diffusion the crystals dissolved when the coverslip was lifted and micro batch also gave

no results. Using a mixture called Al's oil (a 50:50 mixture of silicone and paraffin oil to the uninitiated) she designed a vapour batch experimental set up that had given crystals within a couple of days, avoiding exposure to the air. This interesting solution to a difficult crystallization problem could be adapted to other crystals that are sensitive to air exposure.

Lindsay Sawyer of the University of Edinburgh gave a great chronological story of protein crystallization, which brought a few smiles to people's faces. He offered a nice break from all the techniques with a historical overview of crystallization, starting with the crystallization of Earth-worm haemoglobin and looking at several other landmarks in crystallization and the resulting structures. It was an insightful history of protein crystallization, with lots of interesting references.

The session ended with **Frank von Delft** (Structural Genomics Consortium) who was a little terrifying with his high throughput screening, allowing the solution of around 180 structures in 19 months! He gave an account of the SGC's collaborative attempt to solve as many structures as possible whilst limiting costs where possible, by working from family groups and using core screens and designed follow ups in a three stage work flow. Firstly they do an initial coarse screen. Then, for any hit, they vary its dilution and its pH. Finally, they design a custom screen, using initial screen results and family knowledge using their Beehive table based knowledge data base. They solve most of their proteins within two stages and to the same standard as the PDB and PSI averages.

A quick cup of coffee later, we were sitting in on 'Crystal Stories – Session 2' to which was all on the shoulders of **William Hunter** of the University of Dundee, as **James Murray** (Vernalis) was unable to attend. Bill gave an impressive talk entitled 'Accidental Discoveries in Crystal Complexes' with some nice videos of his accidental discoveries in crystals of complexes. He described his work on the epoxidase catalayse, FOM4, that catalyses the fourth step in fostomycin biosynthesis, using disk studies to find a cofactor that gave an improved crystal form. There was then plenty of time at the end of the day to look though the large array of posters on display during dinner.

Amy Shaw, Keele University
Mathew Martin, Exeter University
Chris Sayer, Exeter University

Frank von Delft, Lindsay Sawyer, Lesley Haire and Neera Borkakoti

William Hunter and Anrea Hadfield

Crystal Structure and Growth at the Nano Scale

THE conference dinner made for a very enjoyable evening, but despite the rather too much wine, the Crystal Structure and Growth at the Nanoscale session the next morning was well-attended!

To open the session, **Peter Laggner** presented his talk on *How crystals are born: Novel insights from SWAXS*, in which he described combining the use of wide and small angle X-ray scattering (WAXS and SAXS) to probe the processes involved in crystallisation, without the need for a synchrotron source.

The second speaker was **Kevin Roberts** whose lecture on *Solution phase nucleation: Cluster size and shape and its correlation with crystallisation kinetics and polymorph selection* discussed the importance of surface and interface factors when predicting polymorphs. The POLYPACK software has been developed for molecular modelling of size, shape and anisotropy dependency characterisation for particles, which may be of use when considering the stability of particles during crystallisation.

Moti Lal's lecture on *Metal nanocrystallites in supercritical fluids – the solvation process and its impact on the nanostructure* described how supercritical fluids can act as tunable solvents for nanoparticles by making the propensity of particles to remain dissolved size dependent by changing solving density through varying pressure. His work involves the simulation, using a molecular dynamics approach, of the nanostructure of particles from supercritical fluids, and the factors affecting their self-organisation.

The final speaker in this session was **Klimentina Pencheva** whose talk *Quantifying solubility enhancement due to particle size reduction and crystal habit modification: Case study of acetyl salicylic acid* described the need to obtain reliable interfacial tension data in order to determine how particle size affects the solubility of potential drug molecules. Calculations are usually based on classical nucleation theory, involving isotropic particles, however, in reality they are more likely to be anisotropic. Using an

approach involving *POLYPACK*, it is possible to calculate a more realistic surface area and volume to determine a more reliable vacuum interfacial tension. By then docking a solvent molecule on each face of the crystallite, an interfacial tension in the solvent can be calculated using the resultant binding energies. This allows a more quantitative picture of the enhancement of the solubility of acetyl salicylic acid as the particle size is reduced.

Sam Chong, University of Birmingham

Moti Lal, Richard Murray, Kevin Roberts, Klementina Pencheva and Peter Laggner

Crystallisation and Polymorphism of Pharmaceuticals

IT is good to report that there were a large number of high quality presentations on the timetable on the subject of polymorphism, including two keynote lectures.

Mark Spackman introduced the potential applications of his program Crystal Explorer, which while not exclusively targetted at polymorphism can be a powerful tool for the qualitative evaluation of the different intermolecular interactions present in polymorphs.

Ulrich Griesser gave an enlightening keynote lecture *Relevance and analysis of polymorphism in drug development*, showing exactly why pharmaceutical companies are so interested in the full characterisation of all solid forms of active pharmaceutical ingredients, to mitigate against unfavourable phase transformations having undesirable medical effects. Included in this lecture was some quantification of the prevalence of polymorphism (36%), hydrates (28%) and solvates (10%) in organic molecules. A reliable quantification of these phenomena is usually fraught with difficulty due to lack of thorough investigation of a large enough set of molecules and Prof. Griesser is possibly one of few people who could attempt to provide numbers based on the large body of work performed at the Innsbruck school, using hot stage microscopy as the primary analysis tool. This talk led seamlessly into the first Crystallisation and Polymorphism of Pharmaceuticals session.

Prof. Griesser's lecture was reinforced by a session devoted to Crystallisation and Polymorphism, which included lectures by several noted figures in the field of polymorphism research. **Roger Davey** presented research that focussed on the self-assembly of molecules in solution and the relationship of the self-assemble units to the supramolecular synthons present in the crystalline form grown from the solution. It was found that the initial particles appear to be amorphous and became more crystalline as nucleation progressed. This discovery opened up the possibility of selectively inhibiting particular polymorphs by judicious choice of solvent, or enantiomeric enrichment by inhibiting the formation of initial racemic clusters. Using a method developed by consideration of the phase diagram, enantiomeric enrichment was possible by making an initial solution at high temperature with an enantiomeric excess of either R or S, and then cooling. The talk by **Sally Price**, *Progress and problems in computational prediction of crystallisation and polymorphism*, gave an impressive overview of work in the rapidly developing area of crystal structure prediction. There were examples of successful cases such as 3-oxauracil, where the energy landscape was close to ideal and there was a large energy gap between the best predicted structure and the rest. There were also examples of more challenging cases, such as 5-fluorocytosine where particular aspects of the crystal structure, such as a preferred hydrogen bonding motif were correctly predicted, but not the complete crystal structure. She was followed by **Terry Threlfall** bursting some myths about the critical factors that can affect the outcome of a crystallisation experiment. Prof. Threlfall gave useful advice about understanding the thermodynamic processes occurring in crystallisation, how to optimise crystal size using heat-cycling and how to cross-seed solutions. He ended his though-provoking talk with a quote that was perhaps uncomfortable for crystallographers: "in isolation, the least useful piece of information you can have about a polymorph is its crystal structure"! The last lecture in the session was from **Caroline Day** from GlaxoSmithKline, who exemplified the lengths to which the pharmaceutical industry are prepared to go to fully characterise the solid state forms of drug molecules. She gave an overview of the use of a diverse range of crystallisation conditions in an automated crystallisation set-up to produce as many forms as possible within the time constraints imposed by the pharmaceutical development schedule and also how their set up allows a high through-put of molecules to compensate for the high attrition rate of candidate drug molecules during development.

Two talks from researchers at the Centre for Science at Extreme Conditions at Edinburgh University, **Colin Pulham** - *Exploring Crystallisation Processes at High Pressures*, and **Simon Parsons** - *The Effect of High Pressure on the Topologies of Molecular Crystals* showed that high pressure techniques are an untapped resource for the generation of new polymorphs. Simon Parsons' lecture gave some very interesting examples of the rearrangements of known crystalline forms of glycine

at higher pressure to give new crystal modifications which avoided the generation of short hydrogen bonds, producing different hydrogen bonded topologies instead.

In summary this BCA conference gave plenty of "food for thought" about polymorphism and judging by the posters there are plenty of other young researchers who are equally interested in this growing and industrially important field.

Ashley T Hulme, University College, London
Sam Chong, Birmingham University

Caroline Day, Anne Kavanagh, Terry Thelwell, Sally Price, Roy Copley, Roger Davey and Ulrich Griesser

Customised Crystallisations

Allan D'Arcy (Novartis) got the ball rolling; he gave an excellent talk and insight into techniques involved in nucleation and seeding in protein crystallisation. He began with nucleation and what variables we can alter to try and control it. The rest of his talk focussed on seeding, describing standard techniques but then moving on to discuss how materials such as horse hair can be ground up and added to the crystallisation drop to act as a seed and induce nucleation. I believe he sent people home with a few new approaches to mull over whilst staring down the microscope.

The next speaker was **Jonathan Grimes** from the University of Oxford, who gave a very interesting account the long and hard road to the crystallisation of whole viruses. He showed us how he and his colleagues achieved a 1998 *Nature* publication, through thousands of careful crystallisations in quartz capillaries, and many trips to the ESRF. This work on PRDI bacteriophage, was continued with lipid bilayer published 2000 and equine rhinitis virus in 2005. The amount of work put in by the group to obtain these structures, was for want of a better word(s) 'very impressive'!

The final talk of the session was that of **Terese Bergfors** of RAPID Centre, Uppsala University. Terese seemed to put everyone at ease giving us the low-down on her centre and relating how her group have optimised screening to give the most results from only the minimal conditions. She also gave us a brilliant metaphor 'Screening for crystals is like finding a boyfriend, you look everywhere. Once you found a boyfriend, you optimise and optimise, and if he's still no good, you then dump him'. Brilliant.

After lunch we continued with Session 2. **So Iwata** of the University of London gave us a compelling talk on a range of challenges faced in membrane protein crystallization, overcoming problems by the use of an antibody or artificial binding to introduce crystal contacts.

The next talk was by **Monika Spano** (Grenoble), which was based around crystallisation for neutron diffraction, namely the improvement of quality of crystals for neutron diffraction, by the use of temperature and seeding to improve size and mosacity of crystals, understanding and controlling chemical properties of solution to do this.

The final talk of the session was given by **Anne Cleasby** (Astex), who described an industrial approach to crystallography for drug design, by subjecting biologically active fragments to high-throughput screening, giving us an insight into the 'cocktail' approach search for compounds.

Mathew Martin, Exeter University
Amy Shaw, Keele University
Simon Willies, Exeter University

Allan D'Arcy, Terese Bergfors, Jon Cooper and Jonathan Grimes

Katy Brown, Anne Cleasby, Monika Spano and So Iwata

High Pressures, Liquids and Surfaces

After the presentation of the PANalytical thesis prize to **Dominic Fortes** (University College London), he gave the first talk of the High Pressures, Liquids and Surfaces session entitled '*Crystallisation of ammonia hydrates under high pressure*'. Titan is an example of an icy moon with a thick atmosphere of nitrogen and methane, and the research presented involved looking into the volcanic activity on moons like Titan, by studying aqueous solutions of ammonia at high pressure. Dominic also provided a detailed description of the problems that occurred during the research, in particular the tendency for samples to vitrify instead of crystallise. He also presented powder results obtained from the Paris-Edinburgh cell.

Back down to earth, **Colin Pulham** from the University of Edinburgh gave a detailed talk on the exploration of crystallisation processes at high pressures. The research is fundamental as it provides not only an insight into intermolecular interactions, but a view into life at the bottom of the earth's deepest oceans or energetic materials under extreme conditions. Crystallisation at high pressure can also be a way of forming new polymorphs and solvates, which has important industrial implications. The research involved the use of the diamond-anvil cell to not only monitor single crystal - single crystal phase transitions but also to monitor crystallisation from solution under pressure, hopefully producing new high pressure phases directly. Case studies involving acetamide, maleic acid and paracetamol were used to illustrate the formation of new polymorphs previously undetected using these techniques.

Daniel Bowron (ISIS Facility, CCLRC) had the third talk of the session. The subject was: "*Changing the structure of water using pressure*". He showed how the four-fold "tetrahedral" hydrogen bonding in liquid or glassy water is highly resilient to perturbation by either pressure or chemical solutes. Although moderate pressure induces changes in the local structure of water through non-bonded interactions between the donor hydrogen bond sites, it is the "chemical pressure" induced by the solvation of acceptor rich / donor poor solute species that makes possible the change of the water structure around its hydrogen bond acceptor sites. Daniel showed his results effectively with the help of simulations, fits and interesting graphic representation of the spatial density function of the water.

Roy Wogelius (University of Manchester) finished the session by discussing "*Crystallographic controls on biofilm formation*". He reported that some observations have been made about how adsorption of "conditioning film" ligands is a necessary precursor to the attachment of microbes onto inorganic substrates and that some medical research has shown that crystalline silica and titania tend to act as better substrates for microbial growth than amorphous substrates of these oxides. He also made the hypothesis that long-range order of the crystalline substrates registers with the adsorbate to enhance adsorption and promote microbial colonization. Using techniques like EBSD, ESEM MIR-FTIR and, of course, X-rays, he pointed out that the mineralogical controls on conditioning film formation place clear controls on subsequent microbial biofilm development.

Alessandro Prescimone, Edinburgh University
Teresa Savarese, Bath University

Roy Wogelius, Colin Pulham, Daniel Bowron and Dave Allan

The Hursthouse Event

THE Hursthouse Event took place on the Thursday afternoon and Friday morning of the BCA Spring Meeting, and was organised to give recognition to the outstanding contribution that Professor Mike Hursthouse (University of Southampton) has made to advances in small molecule crystallography over the last four decades. The speakers at the symposium were former students and colleagues of Mike's who had collaborated with him during the last 30 years.

The first speaker was **Professor Alan Welch** (Heriot-Watt) who reminisced about his time as a Ph. D. student with Mike, at Queen Mary College, in the 1970s, and then went on to describe the structural and synthetic chemistry of heteroboranes which has culminated recently in the development of supraicosahedral heteroboranes. The second speaker was **Professor Martin Schröder** (Nottingham) who has been one of the main users of the EPSRC National Crystallography Service that Mike has founded. Martin described the chemistry of a range of inorganic and metal-organic porous frameworks, emphasising the structural types, and showing the importance of this class of material in catalysis and gas storage applications. The next lecture was given as a "double bill" by **Professors Maria Carrondo** and **Teresa Duarte**, both from ITQB, Lisbon, Portugal. They traced their collaboration with Mike since the late 1970s, indicated Mike's contribution to the development of crystallography in Portugal and, most of all, showed the great friendship that had been built up between Mike's family and their families over the years. The afternoon was rounded off with a splendid lecture by **Professor Robert Shaw** (Birkbeck) that traced the development of the chemistry of phosphorus-nitrogen heterocyclic ring systems from

the beginning of his collaboration with Mike, in the 1970s, to the present day, and judging by the rate of results and publications that are being generated at the present time the collaboration will continue long into the future.

The first session was followed by a gala dinner at which **Professor Donald Bradley** (QMC) presented Mike with a leather bound copy of an issue of Polyhedron that had been dedicated to Mike, and contained contributions from many of Mike's colleagues and collaborators. After dinner speeches were also given by **Terry Threlfall** (Southampton) and **Robert Shaw** (Birkbeck) and Mike replied on behalf of himself and his wife, Hanna.

On the Friday morning the proceedings started off with a lecture from **Dr Simon Coles** (Southampton), the manager of the EPSRC National Service and co-organiser of the symposium, who traced the development of chemical crystallography from the 1960s and showed how the National Service had grown over the past 25 years to become a key research facility. This was followed by **Professor Bill Clegg** (Newcastle upon Tyne) who pioneered the development of small molecule single-crystal crystallography using synchrotron radiation within the UK and now runs the synchrotron-based part of the National Service. Bill described the synthetic and structural chemistry of Group 1 and 2 elements with a variety of oxygen and nitrogen donor ligands and illustrated the importance of both X-ray and neutron diffraction in determining the nature of the packing and intermolecular interactions within the crystals. Then **Dr Philip Gale** (Southampton), a current colleague of Mike's, presented a very elegant lecture on a variety of anion receptor complexes, and showed the importance of crystallography in determining the nature of the intermolecular interactions within the materials, and how they related to the sensor properties of the systems. **Professor Paul Raithby** (Bath) completed the lecture programme with a lecture that traced the development of crystallography from data collections on the earliest diffractometers to modern synchrotron-based techniques, and showed that crystallography was no longer restricted to a static, ground state technique. **Alan Welch**, one of the co-organisers of the Event, then summed up Mike's contribution to chemical crystallography and reiterated the high esteem in which the community held Mike. Mike then closed the meeting with a few words of thanks.

Paul Raithby

Topology

TOPOLOGY is essentially a qualitative method to describe shape through the presence and geometric arrangement of nodes within a network, but as the program demonstrated it can be approached in a variety of ways.

Mark Spackman had the second main lecture on "*Visualising and exploring intermolecular interactions in molecular crystals: a new toolkit for crystal engineering.*" He described some useful tools that can be used to understand how molecules have to organise themselves into their crystalline structures: one of the most interesting tools he presented was the use of the "Hirschfeld surfaces". They are a graphical tool which uses different colours to give an idea about the way the molecules occupy space, highlighting the different kinds of interactions that some molecular areas can have, such as H-bonding or π-stacking. In particular, these surfaces are useful since they allow easy recognition of the different phases of the same compound, as different phases have different intermolecular interactions which Hirschfeld surfaces show clearly in various colours.

Simon Parsons talked about the effect of high pressure on the crystal packing of organic molecular materials specifically the amino acids, glycine, and serine. He discussed the way that the application of pressure causes anisotropic compression of the unit cell. Super-short contacts are however not formed up to 10GPa, instead a phase transition is often observed to relieve any short contacts. The use of topology techniques can provide some information on why some compounds exhibit phase transitions and others do not. This involves taking a central molecule and looking at where the other centroids associated with the nearest neighbours are located. This contracts the system into something simpler. The program TOPOS (Blatov et al) which looks at molecular coordination numbers has been used to investigate this. Hirshfeld surface analysis has also been used to visualise the molecular packing and identify the most significant interactions and their variation with pressure.

Subsequently, **Elna Pidcock** presented a method to obtain a broad view of crystal packing which ignores intra- and inter-molecular forces along with the exact atomic or molecular content of the unit cell, and instead describes the asymmetric

unit as a box with qualitative short, medium and long side lengths. The orientation of these boxes with respect to each other was studied and appears to show several interesting features, for example, the units tend to arrange themselves in manner to minimise the surface area of the unit cell.

The morning session was concluded by **Thomas Gelbrich**, who provided an illuminating insight into the similarities between the crystal structures of different polymorphic forms. Within the presentation he demonstrated the existence of comparable 1D and 2D packing motifs in the alternate forms of several structures, and showed that the variations in the 3D lattices could be accounted for by differing relationships (e.g. translation or rotation) between these motifs. The program XPac has been written to identify the supramolecular constructs and has been used to explore the structures of sulfathiazole, carbamazepine, olanzapine, and aspirin.

German Sastre began the afternoon talks with an examination of the different sizes of silicon-oxygen rings that have been found within the reported structures of zeolites. The study focused on the energetics of the systems and raised some interesting questions about the relative stabilities and strain within the zeolite frameworks. Several questions can then be raised. Are rings of different sizes equally stable? Are all rings of the same size equally stable? Are large SiOSi angles more frequent in rings of larger size? Force field atomistic simulations have been used to explore the energy of the ring and the energy of the Si state. It was observed that the energies do not depend on the ring size but on the conformation. The strain in rings comes from the deformation of SiO_4 tetrahedra.

The session was rounded off by **Carroll Johnson** who provided the audience with a challenging but fascinating examination of topology from a mathematical perspective. He stressed the idea that crystallography is progressing past the harmonic approximation. This leads to the need to work with higher order thermal motion, moving away from the Gaussian style thermal ellipsoids. The close relationship between the critical nets of graphite and hexagonal diamond was highlighted prior to an explanation of orbifolds and their construction. It also became apparent that the simple triclinic space group $P\bar{1}$ is topologically highly complex forming an eight fold suspension due to the presence of the eight inversion centres.

Lynne Thomas, Cambridge
Hazel Sparkes, Durham

Simon Parsons, Jacqui Cole, Elna Pidcock and Thomas Gelbrich

Jacqui Cole, Caroll Johnson and German Sastre

Powder diffraction in industry

THIS session was on Thursday afternoon. **Judith Shackleton** (chair) introduced **Jeremy Cockroft** who gave a brief introduction and awarded the Industrial Group prize to **Professor Paul Fewster**, in recognition for his sustained contribution to industrial crystallography including crystallographic and diffraction work in industry of all kinds. The award lecture was titled *It's all in the detail*. Paul initially talked about his previous jobs and the instruments they had to use thirty years ago, and how the technology has moved on since. A critical step had been interfacing of various pieces of apparatus to cheap PCs, "running in the face of management policy who preferred 'more standard' computer suppliers of the time". His work involved looking at superlattice structures, and the interfacial chemistry of Ga complexes. The accuracies of the structures were then analysed using the dynamical theory and reciprocal space mapping to see whether the materials would be suitable to make superconductor devices. These devices could be used as quantum dots (semiconductor nanocrystals) and then made into fibre optics for faster internet connections. Paul also included some work with a laboratory X-ray source on protein crystal perfection. He finished his talk with the analysis of polycrystalline thin film materials.

The second speaker of the session was **Dr David Beveridge**, and his talk was on *The precipitation of pigment red 57:1 from homogenous solution for X-ray powder diffraction.* David described the synthesis that was involved in producing the pillar box red pigment. The morphological properties of the pigment looked more crystalline than expected. So, with the help of powder diffraction, it was confirmed that the pigment was indeed crystalline. The red pigment is mainly used for colouring oil-soluble products such as make-up, powders, lipsticks and foundation creams. A question from the audience was asked regarding the numbering 57:1; David replied that it was chosen because it wasn't currently in use!

Before the session break, **Dr Mary Vickers** gave a lecture on *X-ray diffraction at Materials Science, Cambridge.* Mary talked about the typical samples that are analysed using

powder diffraction such as metals, ceramics, and carbon nanotubes. She mentioned the Rietvield refinement and the quantitative phase analyses and cell parameters in steel. Mary has also carried out experiments using Small Angle X-ray Scattering (SAXS) on thin film materials like polyurethane, which is medically important in replacing discs in the human spinal cord. Staying on the topic, Mary highlighted the weakness of SAXS when it comes to identifying water molecules in cellulose fibres. The talk ended with a nice discussion on how students can be encouraged to learn more about X-ray diffraction.

Helal Ahmed, University of Manchester

Martin Gill, David Beveridge, Judith Shackleton, Chris Staddon, Mary Vickers, Andrew Hodge and Paul Fewster

XRPD Workshop

ON the Tuesday I spent the day in the XRPD workshop on phase identification, which was run by John Faber from ICDD. I decided to attend this workshop because I had recently started to use XRPD and wanted to learn as much as possible about the subject. The first session was a lecture by David Rendle on the "History & Structure of the Powder Diffraction File". This lecture covered the history of powder diffraction; starting with its discovery by Bragg in 1913 and moving on to the first powder database of 1000 patterns, which was established by Hanawalt, Rinn and Ludo K. Frevel in 1938. The talk then moved on further to the creation of the PDF and its subsequent growth through the 20th century from 35,000 patterns to nearly 500,000 patterns. I found this section of the workshop to be very interesting because I was new to the field of XRPD; but for someone experienced in the field, it may have proved to be slightly less interesting.

The next section of the workshop was on Phase identification and was run by **Dave Taylo**r, another consultant at ICDD. This section gave practical tips regarding the correct use of the PDF for powder pattern identification. At the end of this section there was a question and answers session, to allow the audience to ask the three organizers any questions about XRPD or the PDF. This was a lively debate and proved to be very informative for me.

The final section of the workshop was Advanced Phase Identification and Quantitative analysis and was run by **John Faber** from ICDD. This section dealt with the best ways to collect your data for the purposes of phase identification and more importantly quantitative analysis. This was a much more technical session than the two previous ones and by far the most enjoyable and useful of the day. This was followed by computer workshop where we were able to use the PDF under the watchful eye of the event organizers.

Stephen Cairns, University of Glasgow

Dave Taylor, John Faber and David Rendle

Young Crystallographers

THIS years BCA spring meeting was preceded by the young crystallographers' satellite meeting. The meeting was opened by Andy Parkin (University of Glasgow) who was the head of the organisation committee. The meeting was so popular as to have attracted over 90 delegates. The satellite was made possible because of the support from the BCA, Bruker AXS, CCDC, Oxford Cryosystems, Oxford Diffraction and Rigaku.

Andy opened the meeting with a brief introduction in which he managed to call the more senior speakers "old gits" then straight in to the talks. First "old git" to talk was **Maryjane Tremayne** who used an interesting theme of mullets to show her group's work on using evolution processes to predict structures from powder patterns. She was followed by five students giving 20min talks which covered a suitably wide range of research interests to provide both a treat for the audience and to represent the varied nature of crystallographic research: **Chris Spanswick** on a high pressure study of urea-phosphoric acid, **Alex Griffin** on crystal engineering where she was trying with moderate success to form straight hydrogen bonded chain of molecules depending on their size, **Alistair Davidson** talking about more high pressure work, but this time involving polymorphism of thiourea dioxide, **Guillermo Minguez** on molecular ionic networks, and then the last in the session **Lynne Thomas** telling us about the disorder in pentachloronitrobenzene where she is using a computational study to try and match the different features of diffuse scattering observed in the diffraction images. Lynne managed to convey the science in an interesting and easy to understand way, including Mickey Mouse and kangaroos to keep even us entertained.

The second session was also opened by an invited speaker, **Bill Hunter** (Dundee). He is currently based in the division of Biological Chemistry and Molecular Microbiology where he is interested in the crystallization of biological complexes. A particular class of enzyme which participates in the biosynthesis of sugars and isoprenoid precursors was shown to form crystals with specific metals.

John Warren's (CCLRC Daresbury) talk entitled '*Nasty things happen to nice crystals*' showed us how he tortured a poor crystal with an imaginative set up on Station 9.8 at the Daresbury synchrotron, that is when it is not being flooded with water! He described some results of SO_2 uptake on single crystals of 'Chinese lantern' type molecules

An interesting study of the hydrogen bonding patterns in base pair systems was discussed by **Susie Harte** (Glasgow). The information was gathered by the use of diffraction and computational studies and allowed identification of anomalous hydrogen behaviour.

The interesting effect of high pressure on crystals of nitric acid and its hydrates was **Martin Walker**'s (Edinburgh) topic of discussion. The structure was predicted first using computational techniques; neutron diffraction data were then collected with the two results used in comparison.

Anna Collins (Oxford) discussed the occurrence of Z' = 2 structures, which account for 10% of organic structures in the CSD. Some are thought to be pseudosymmetric, but the problem lies when identifying the extent of divergence from the true symmetry. Using computational techniques such as RMS deviation and a MATCH routine in CRYSTALS, the extent of pseudosymmetry could be assessed.

After a short break, it was time to formally inaugurate the young crystallographers special interest group, short and sweet, everyone just mumbled in agreement and it was done. Andy Parkin had also found (or bullied) people to be the organizing committee so that future events could be run as smoothly as this one. These are as follows: **Lee Brooks, Simon Coles, Alex Griffin** and **Mike Probert**. A tradition from last time involved everyone presenting a poster (excluding those who had given a talk) to give a two-minute oral presentation. They ranged from the professional pitch trying to gain the audience's interest through intellectual conversation to the funny and amusing, with moles, smurfs, stickmen and cow noises all making their own distinct point! The most amazing thing was that no one ran over the allotted time, so we got to go for the wine and buffet early and to see who had actually fallen for our two minute poster spiel and visited us in the poster session.

In the morning after the night before, **Simon Coles** (Southampton) gave an overview of the EPSRC National Crystallography Service and how it can help groups with difficult samples which require specialist equipment and knowledge. **Victoria Money** (York) showed us crystal structures of *Clostridium thermocellum lichenase*, an enzyme which hydrolyses the glycosidic bond, with different inhibitors complexed within its structure. **Lee Brooks** (ESRF & Keele) discussed the relevance of insect recognition pheremones and how they are made up from a mixture of unbranched monoalkenes and methane-branched alkanes. Last but by no means least, **Francesca Fabbiani** (Edinburgh) rounded off the meeting with another high pressure study. A polycyclic aromatic compound pyrene was shown to exhibit polymorphic behaviour at pressures of 0.5GPa.

On behalf of the organising committee, we were overwhelmed with the number of people wanting to attend this event, and even more amazed at just how well prepared and knowledgeable the crystallographers of the future are. It is our aim that this will become a yearly event and that we will see even more 'youngsters' in Kent, 2007.

Chris Spanswick, Edinburgh
Martin Adam, Glasgow
Alexandra Griffin, Bristol

A group of young crystallographers

Definitely the youngest crystallographer at the meeting!

Prize winners

Richard Pauptit presenting the famous bluejohn BSG Poster Prize to S. J. Ahmed

Paolo Radaelli and Simon Parsons presenting the PCG and CCDC/CCG Prizes to Matt Tucker and Graeme Day

Richard Cooper presenting the CCG poster prize to Peter Wood

Dario Braga presenting the new Crystal Structure Engineering Poster Prize to Guillermo Garcia Minguez

Andy Parkin and Jeremy Cockcroft presenting the IG poster prize to Gordon Barr

Jeremy Cockcroft presenting the IG Prize to Paul Fewster

Chick Wilson presenting the Lonsdale Lecture Award to Mike Glazer

Reg Nicholl of PANalytical presenting the prize ipod to Mairi Haddow

Reg Nicholl of PANalytical presenting the PANalytical Poster Prize to Andrew Goodwin

BCA Accounts 2006

The British Crystallographic Association

Summary Financial Statements for year ended 31 December 2005

Examining Accountant: R A Young, BSc. FCA
The Young Company, Lakeview Court, Ermine Business Park, Huntingdon PE29 6XR
These are consolidated accounts and include the BCA, BSG, IG, CCG and CCG School funds, expressed in pounds sterling (£)

INCOMING RESOURCES:	2005	2004
Grants and sponsorship	7,548	2,300
Donations	1,986	1,633
Annual Conference(5)	74,977	58,945
Meetings of groups	2,287	6,144
Crystallography News	24,802	23,706
Membership Subscriptions	12,636	17,322
Course fees	10,261	(600)
Net Income from trading	115	(235)
Investment income	6,180	4,047
Interest received	2,877	2,746
IUCr Bursary	-	-
Sundry Income	71	-
Total Income	**143,740**	**116,008**

EXPENSES:	2005	2004
Direct Charitable expenditure(2)	129,460	116,125
Management & administration(3)	24,321	21,292
Total Expenditure	**153,781**	**137,417**

	2005	2004
Net Income:	(10,041)	(21,409)
Unrealised gains (losses) of investment assets	6,869	3,305
Net Movement In Funds	(3,172)	(18,104)
Balances brought forward at 1 January	197,126	215,230
Balances carried forward at 31 December	193,954	197,126

ASSETS

Fixed assets	2005	2004
Tangible assets	32	367
Investments	99,109	97,048
Total	99,141	97,415
Current assets		
Stocks	520	425
Debtors	375	732
Cash at Bank	99,355	113,280
Total	100,250	114,437
Liabilities: amounts falling due within one year	(3,764)	(12,818)
Liabilities: amounts falling due after more than one year	(1,673)	(1,908)
Net Assets	**193,954**	**197,126**

INCOME FUNDS:	2005	2004
Restricted funds (4)	64,393	71,158
Unrestricted funds (4)	129,561	125,968
Total	**193,954**	**197,126**

Notes To The Summary Financial Statements

1. Accounting Policies.
These summary statements are based on financial statements which have been prepared under the historical cost convention, with the exception of investments which are included at market value. The financial statements have been prepared in accordance with the Statement of Recommended Practice, "Accounting and Reporting by Charities" published in October 2000 and applicable accounting standards.

All incoming resources are included in the Statement of Financial Activities when the charity is legally entitled to the income and the amount can be quantified with reasonable accuracy. All expenditure is accounted for on an accruals basis and has been included under expense categories that aggregate all costs for allocation to activities. Investments are stated at market value at the balance sheet date.

Tangible fixed assets are stated at cost less depreciation. Depreciation is provided at rates calculated to write off the cost of fixed assets, less their estimated residual value, over their expected useful lives. Stocks are valued at the lower of cost and net realisable value after making due allowance for obsolete and slow-moving stocks.

2. Direct Charitable Expenditure

	2005	2004
Previous year conferences	-	45
Subscription to International bodies	3,363	3,701
Annual conference (5)	71,493	54,972
Meetings of groups	1,503	3,004
Crystallography News	24,491	24,912
Course fees and accommodation	20,000	-
Grants and sponsorship	1,000	1,000
Prizes	50	1,050
Crystallography Reviews	4,000	4,000
Arnold Beevers Bursary Fund	3,560	1,200
Bursaries from restricted funds	-	22,241
Total	**129,460**	**116,125**

3. Management And Administration

General expenses		
Depreciation	335	335
Administration fee	16,420	14,950
Accounting fee	3,316	3,143
Insurance	378	378
Bank and security charges	298	240
Special Interest Group administration	2,684	553
Council Members' expenses	504	612
Officers	324	759
Other Council expenditure	62	322
Total	**24,321**	**21,292**

4. Statement Of Funds

	Brought Forward	Incoming Resources	Resources Expended	Transfers In/(Out)	Gains (Losses)	Carried Forward
UNRESTRICTED FUNDS						
General Fund	125,968	121,223	124,499	-	6,869	129,561
RESTRICTED FUNDS						
IUCr bursary fund	1	-	-	-	-	1
Arnold Beevers bursary fund	18,033	842	3,560	768	-	16,083
Dorothy Hodgkin prize fund	7,308	502	-	-	-	7,810
Chemical group teaching school	11,902	17,249	21,606	-	-	7,545
Chemical group fund	5,682	1,588	779	-	-	6,491
Industrial group fund	7,015	1,525	1,586	-	-	6,954
Biological Structures group fund	21,217	811	1,751	(768)	-	19,509
Subtotal	**71,158**	**22,517**	**29,282**	**-**	**-**	**64,393**
Total of Funds	**197,126**	**143,740**	**153,781**	**0**	**6,869**	**193,954**

5. Spring Meeting 2005 Loughborough

INCOME	
Sponsorship	3,400
Registration	50,442
Exhibition	20,050
Bursaries	1,085
Total	**74,977**
EXPENDITURE	
Accommodation & Meals	16,446
Facilities	10,287
Catering	10,953
Social Event	2,955
BCA Speakers Expenses	5,292
Refunds	1,106
Abstract Book	4,181
NNE Fee	11,464
Administration	3,718
Printing &Stationery	1,800
Bursaries	3,291
Total	**71,493**
TOTAL INCOME	74,977
TOTAL EXPENDITURE	71,493
MEETING SURPLUS	**3,484**

Treasurer's Report 2005

THE Association had an overall deficit of £3,172 during the year ended 31 December 2005 but it has no material commitments or guarantees which could affect its future solvency. Our investments are continuing to perform well, and brought in an income of £9,057 this year. We also were grateful to receive a legacy of £1,000 from the estate of Professor Mary Truter, and this was donated to this year's Young Crystallographers symposium.

The unrestricted funds show a deficit of £3,276 over the year before revaluations. A revaluation of investment assets of £6,869 gives the unrestricted funds an overall surplus of £3,593. The Spring Meeting surplus and the good investment performance were very welcome.

Council members have conducted a review of the major risks to which the Association is exposed. The only consideration is with regard to its major reserves, namely its investments, and to mitigate those risks the Association has all its investments placed with an independent professional management company.

These investments, valued at £99,109, also provide useful but fluctuating income for sustaining the Association's objectives, which are to advance the education of the public in the sciences of crystallography, and to promote its teaching and applications in academia and industry. The Council's review of the reserves indicates that we need to generate more income to maintain our present level of educational and scientific activity.

Our agreement with Taylor & Francis to publish highlights of the Spring Meeting proceedings in "Crystallography Reviews" resulted in all members receiving a copy in June 2005 at a cost of £4000.

2005 was the year of the XX triennial International Union of Crystallography Congress, held this time in Florence, Italy. This was a big occasion for the crystallographic community, and we were very pleased to be able to award 11 bursaries from the Arnold Beevers Bursary Fund to help our young crystallographers to be there and to sample the fun and challenges of our scientific community. There were plenty of other conferences happening in 2005 and we awarded bursaries to 8 people attending meetings on a wide variety of crystallographic topics. The total amount awarded from the Arnold Beevers Bursary Fund was £3,560. The Spring Meeting at Loughborough had fewer applicants for bursaries this year as it was the year of the Congress. We awarded bursary funding of £3,291 to benefit 21 students with 7 being commercially sponsored. The IUCr Bursary given to help the Congress in Florence was also much appreciated, and its repayment will appear in the 2006 accounts.

Crystallography News has broken even this year on a turnover of £24,802, very much the same as last year. The BCA owes a debt of gratitude to its advertisers and sponsors who generously support our activities.

Subscriptions to International bodies were £3,363, a little lower than last year due to currency variations. Administration costs are a little higher this year at £16,420, up by £1,470.

Membership income is down by £4,686, with thirteen organisations paying Corporate Membership dues in 2005 (up from 11). The total membership numbers are down, and this is also reflected in the drop in Gift Aid that we were able to claim from the Inland Revenue. This sum of £842 was again allocated to the Arnold Beevers Bursary Fund. The Fund was also boosted by a transfer of £768 investment income from the BSG.

In my first report as Treasurer, I would like to thank many people for their goodwill and understanding – members of Council, **Gill** and **Elaine** at Northern Networking Events, our accountant **Bob Young**, but particularly I would like to pay tribute to **Dave Taylor**, who handed over a system up and running beautifully, and who has patiently dealt with all my questions at all times.

Sheila Gould

The full BCA accounts for 2005 are available as an e-mail attached file from the BCA administrative office.

Secretary's Annual Report to the AGM 2006

COUNCIL has had another busy year, culminating in this highly successful Spring meeting which has over 350 registered participants. We would like to thank **Professor Paul Raithby** for agreeing to take on the role of Programme Chair and for arranging such an excellent and wide-ranging programme. We are fortunate to have been able to welcome a new Treasurer, the wise and experienced **Dr Sheila Gould**, whose first frustration was attempting to transfer the bank accounts, but who has now settled into her demanding role. At the present AGM we have elections for a new President and for three Ordinary Members of Council.

Just after the last Spring Meeting, **Elaine Fulton** joined Northern Networking Events Ltd. as our main contact person, and you will have all had a chance to meet her during this meeting. She and the Treasurer plan to undertake a review of the membership database in the near future, which should help to improve our membership statistics. This is an important task : we have 704 paid–up members as of yesterday, compared with 705 in November 2005, whereas we have been talking about a target of 1000 members for the last few years. This number breaks down as follows (November 2005 figures in brackets) : Corporate 98 (37), Ordinary 413 (558), Retired 39 (36), Student 140 (111), Unemployed 5 (3), Honorary 13 (15), Life 30 (33). Membership by groups is as follows (last year's figures in brackets): the Biological Structures Group have 178 (216) members, the Chemical Crystallography Group 190 (241) members, the Industrial Group 126 (97) members , and the Physical Crystallography Group 114 (89) members, with 81 (66) members having no stated group affiliation.

It may well be that your records are out of date as regards your group affiliations in the membership database. You can check your entry with Elaine Fulton, and you are encouraged to do so.

We have two new Honorary Life Members, **Professor Chris Gilmore** and **Professor Peter Main**. We welcome nominations for more. Constitutionally, we are allowed to have 20 such members.

Council met twice, before this meeting and in Birkbeck (London) in November 2005. On both occasions there was a long agenda, and there is never enough time for detailed debate. Issues which continue to concern Council include the long-term financial viability, the level of membership subscription and the membership numbers. These issues are obviously related.

All the groups have organised meetings during the year. The Biological Structures Group organised a successful Winter Meeting in Bristol on 'Structural Enzymology', which attracted 109 participants. It will host a Summer School in Oxford, and a Winter Meeting in Birmingham. The Chemical Crystallography Group held their Autumn Meeting in Daresbury on 'Applications of Computational Chemistry related to Crystallography' which attracted over 80 attendees. Their next Autumn Meeting will be in Glasgow, on Crystal Engineering. They will host the Chemical Crystallography School again in 2007. The Industrial Group held a two-day meeting for 34 delegates on industrial pharmaceuticals. The Physical Crystallography Group did not hold a meeting, but plan to do so on 26th October 2006, with the title 'A Snapshot of Physical Crystallography in the UK'.

Our Crystallography News editor, the immensely capable **Bob Gould**, has just completed work on his 17th issue of this extremely professional publication, whose length averages at 32 pages. Council has previously been concerned that this publication was a drain on funds, but this year it has even resulted in a financial surplus of £796. We are all very appreciative of the work involved. Bob always welcomes contributions, especially those with high-quality pictures attached (and not embedded the document).

Since the last AGM we have sadly lost four members by death, **Robin Shirley**, **Robert Evans**, **Patrick Tollin** and **Uli Arndt**. Appropriate tributes to all these will appear in Crystallography News.

Finally, as always, we are a voluntary organisation and could not exist without our hardworking unpaid volunteer workers. This year we have to thank our dynamic but modest and approachable President for his three years' service. Chick is a Glaswegian to the core, and has actively nurtured the young crystallographers. This has been a very healthy emphasis on the role created for us by our founders, that of an educational charity. The formal creation this week of the Young Crystallographers SIG is just one outcome of his many efforts on behalf of our UK community. Thank you, Chick!

Christine Cardin, Secretary to Council

Membership Subscriptions

THE AGM of the BCA passed a motion to raise the membership subscription rate w.e.f. 1st January 2007 by £5.00 per annum, from £15.00 to £20.00, with the other rates increasing proportionately. Thus, from 1st January 2007 the membership subscription rates for the BCA are

£20.00 per annum Full membership
£10.00 per annum Student, retired and unemployed
£7.00 per annum IOP CMMP members
£27.50 3 yr term Students only
£100.00 5 yr term Overseas members only

We will be getting in touch with everyone on our membership database to let them know of these changes, and to ask for new standing order mandates etc., but in the meantime you can sit back and enjoy all the exciting programmes and informative issues of Crystallography News coming your way!

Sheila Gould, Treasurer, BCA

Meetings of interest

Further information may be obtained from the website given. If you have news of any meetings to add to list please send them to the BCA Web Master **cockcroft@img.cryst.bbk.ac.uk** or to the Editor, **gould@ed.ac.uk**. The help of **Dr Simon Parsons** and the IUCr listing is gratefully acknowledged.

1-3 June 2006
XIII Annual Conference of the Serbian Crystallographic Society, Novi Sad Serbia. **http://www.iucr.org/cww-top/mtg.anc3.doc**

1-3 June 2006
36th Mid-Atlantic Macromolecular Crystallography Meeting, Winston-Salem NC USA
http://csb.wfu.edu/midatlantic06/

5-9 June 2006
Fundamentals of X-Ray Powder Diffraction: ICDD, Pennsylvania, USA.
http://www.icdd.com/education

9-18 June 2006
The Structure Biology of Large Molecular Assemblies: the 38th crystallographic course at the Ettore Majorana Centre, Erice, Italy, **crystalerice.org/futuremeet.htm**

12-16 June 2006
Advanced Methods in X-Ray Powder Diffraction: ICDD, Pennsylvania, USA.
http://www.icdd.com/education

14-17June 2006
Eighth International Quasi-Elastic Neutron Scattering Conference(QENS2006), Bloomington, IN, USA **http://www.iucf.indiana.edu/events/qens2006**

14-18 June 2006
The Fifteenth Slovenian-Croatian Crystallographic Meeting. Jezersko, near Ljubljana Slovenia. **http://abra.fkkt.uni-lj.si/fn01leban/slkr15/**

18-22 June 2006
2006 American Conference on Neutron Scattering, St. Charles, IL USA **http://www.acns2006.anl.gov/**

18-24 June 2006
Eighth International Workshop on the Physical Characterization of Pharmaceutical Solids, Rhodes, Greece
http://www.assainternational.com

26-30 June 2006
NCNR/NSF Summer School on Small Angle Neutron Scattering (SANS) and Neutron Reflectometry (NR). Center for Neutron Research, Gaithersburg MD USA
http://www.ncnr.nist.gov/summerschool/ss06/

9-13 July 2006
The XIII-th International Conference on Small-Angle Scattering. Kyoto, Japan.
http://www2.scphys.kyoto-u.ac.jp/sas2006/index.html

10-13 juillet 2006
Colloque de l'Association Française de Cristallographie, Toulouse, France
http://www.afc2006-toulouse.org

10-19 July 2006
2006 ACA Summer Course in Small Molecule Crystallography, Indiana, PA, USA.
http://www.hwi.buffalo.edu/ACA/ACA2006SummerCourse.html

10-22 July 2006
ACA Summer School in Macromolecular Crystallography, Chicago, IL, USA
http://acaschool.iit.edu/

16-21July 2006
2006 Gordon Research Conference on Diffraction Methods in Structural Biology, Bates College, Lewiston ME, USA., **http:// www.grc.uri.edu/06sched.htm**

22-27 July 2006
ACA 2006 - The American Crystallographic Association Annual Meeting (2006). Honolulu, HI, USA, **http://www.hwi.buffalo.edu/aca/**

23-28 July 2006
IMA 2006 - 19th General Meeting of the International Mineralogical Association. Kobe, Japan. **http://www.congre.co.jp/ima2006/index_e.html**

24-28 July 2006
8th International Conference on ancient DNA and Associated Biomolecules, Lodz, Poland. **http://csk.umed.lodz.pl/~dmb/DNA8/doc/?plik=3Dinv**

30 July - 2 Aug 2006
ZMPC 2006 - International Symposium on Zeolites and Microporous Crystals. Yonago, Japan
http://www.chem.tottori-u.ac.jp/~zmpc2006/main.html

30 July - 2 August 2006
SRMS5 - Fifth International Conference on Synchrotron Radiation in Materials Science. The Drake Hotel, Chicago IL USA
http://www.aps.anl.gov/News/Conferences/2006/SRMS/index.html

1-4 August, 2006
X-EI 2006 - School on structure determination by the combination of X-ray powder diffraction and Electron Crystallography: Antwerp, Belgium.
http://www.emat.ua.ac.be/**XEI2006/XEIhome.htm**

4-5 August 2006
Structural Bioinformatics & Computational Biophysics. Fortaleza Brazil
http://3dsig.weizmann.ac.il/

4-6 August 2006
ECM-23 Satellite Meeting on Mathematical and Theoretical Crystallography, Leuven Belgium
http://www.lcm3b.uhp-nancy.fr/mathcryst/leuven2006.htm

5-6 August 2006
The 1st TOPAS User's Meeting. Denver Marriott Tech Center Hotel, Denver, CO USA
http://www.bruker-axs.de

6-11 August 2006
ECM-23, European Crystallographic Meeting, Leuven, Belgium.
http://www.ecm23.be

13-18 August 2006
Sagamore XV: The fifteenth international conference on Electron Charge Spin and Momentum Densities, Bosworth Hall Hotel, Warwickshire
http://www.sagamore2006.com

15-21 August 2006
11th International Conference on the Crystallization of Biological Macromolecules. Laval University, Quebec QC Canada
http://www.iccbm11.com/

19-26 August 2006
5th PSI Summer School on Condensed Matter Research: Neutron, X-ray and Muon Studies of Nano Scale Structures Zuoz, Engadin Valley Switzerland
http://num.web.psi.ch/zuoz2006/

20-25 August 2006
Indaba 5: Models, Mysteries and Magic of Molecules. Kruger National Park South Africa.
http://www.sacrs.org.za/indaba5/

27-31 August 2006
1st European Chemistry Congress. Budapest, Hungary.
http://www.euchems-budapest2006.hu

27 August - 2 September 2006
Siena 2006 : IUCr School on Basic Crystallography, Certosa di Pontignano, Siena,Italy
http://www.iucr.org/iucr-top/comm/cteach/siena2006/

31 August – 9 September
Neutron Techniques In Molecular Magnetism, Jaca, Spain
http://magmanet.unizar.es/

1 September 2006
EPDIC 'Under the Bonnet' Powder diffraction Workshop: University of Geneva, Geneva, Switzerland.
http://www.pa.msu.edu/cmp/billinge-group/Geneva2006Software

1-4 September 2006
EPDIC 10, European Powder Diffraction Conference, Geneva
http://www.sgk-sscr.ch/EPDIC10/EPDIC10.html

3-8 September 2006
13th BCA Summer School in Protein Crystallography, Biochemstry Department, Oxford University
http://www.crystallography.org.uk/bsg

4-8 September 2006
44th European High Pressure Research Group meeting, Prague, Czech Republic. **http://kfes-80.karlov.mff.cuni.cz/EHPRG/**

7-14 September 2006
SHELX/MAXINF Workshop - Workshop on Experimental Phasing of Macromolecules. Göttingen Germany
http://shelx.uni-ac.gwdg.de/workshop2006/

10-12 September 2006
BACG Annual Meeting, Heriot Watt University, Edinburgh
http://www.bacg.org.uk

10-13 September 2006
5th European Conference on Computational Biology - ECCB '06, Eilat, Israel
http://www.eccb06.org

10-15 Septembre 2006
Summer School - Ecole thematique: Analyse structurale par diffraction des rayons X, cristallographie sous perturbation. Nancy, France.
http://www.lcm3b.uhp-nancy.fr/nancy2006/

11-16 September, 2006
XX Conference on Applied Crystallography and Summer School on Polycrystalline Structure Determination, Wisla, Poland.
http://crystallography.us.edu.pl/satel.php

13-15 September 2006
ECRS 7 - The 7th European Conference on Residual Stresses. Berlin, Germany.
http://www.ECRS7.de/

13-15 September 2006
13th CCP4 Protein Structure Workshop, Galashiels
http://www.ccp4.ac.uk/

15-16 September 2006
5th International NCCR Symposium on New Trends in Structural Biology, Zürich Switzerland
http://www.structuralbiology.unizh.ch/symposium06.asp

17-22 September 2006
ISRP-10 - 10th International Symposium on Radiation Physics. University of Coimbra, Portugal.
http://pollux.fis.uc.pt/isrp10/

19-22 September 2006
XTOP 2006 8th Biennial Conference on High Resolution X-Ray Diffraction and Imaging, Baden-Baden, Germany,
http://xtop2006.fzk.de

25-28 September 2006
PNCMI 2006 - The sixth International Workshop on Polarised Neutrons in Condensed Matter Investigations, Berlin, Germany.
http://www.hmi.de/bensc/pncmi2006/

29-30 September 2006
WINS2006 - 3rd Workshop on Inelastic Neutron Spectrometers. Hahn-Meitner Institute, Berlin Germany
http://www.hmi.de/bensc/wins2006/

2-5 October 2006
Polymorph Screening: Techniques and Applications. Stamford, CT, US.
http://www.assainternational.com

4-6 October 2006
German Conference for Research with Synchrotron Radiation, Neutrons and Ion Beams 2006, Hamburg, Germany.
http://www.sni2006.de/

16-19 October 2006
Polymorph Screening: Techniques and Applications. Ettlingen, Germany,
http://www.assainternational.com

22-26 October 2006
4th International Conference on Structural Genomics, Beijing, China
http://www.sino-meetings.com/icsg2006/

23-25 October 2006
Basic and Advanced X-Ray Powder Diffraction: Pharmaceutical Applications,Part I: Basic crystallography. Stamford, CT, USA
http://www.assainternational.com
23-26 October 2006.
Polymorph Screening: Techniques and Applications Mallorca, Spain
http://www.assainternational.com

23-30 October 2006
EMBO Practical course - Solution Scattering from Biological Macromolecules. EMBL, Hamburg Germany
http://www.embl-hamburg.de/workshops/2006/embo/

24-27 October 2006
First African Structural Biology (FASB) conference, The Wilderness, South Africa.
http://sbio.uct.ac.za/conference

25-27 October 2006
Argentine Crystallographic Association - The second gathering of the Argentine Crystallographic Association (Asociacion Argentina de Cristalografia, AACr). Puerto Madryn, Chubut Argentina
http://www.tandar.cnea.gov.ar/~vega

26-27 October 2006
Basic and Advanced X-Ray Powder Diffraction: Pharmaceutical Applications, Part II: Basic and advanced structure-solving solutions from X-ray powder patterns. Stamford, CT, US
http://www.assainternational.com

18-19 November 2006
Theoretical Crystallography and Materials Science - Satellite Conference of the AsCA'06 / CrSJ meeting. Tsukuba, Japan.
http://www.lcm3b.uhp-nancy.fr/mathcryst/asca2006.htm

14-19 January 2007
International School on Mathematical and Theoretical Crystallography. The University of Havana, Cuba.
http://www.lcm3b.uhp-nancy.fr/mathcryst/havana2007.htm

17-19 April 2007
BCA Annual Meeting, University of Kent, Canterbury
http://crystallography.org.uk

7-17 June 2007
Engineering of Crystalline Materials Properties: the 39th crystallographic course at the Ettore Majorana Centre, Erice, Italy **http://www.crystalerice.org/futuremeet.htm**

21-26 July 2007
ACA Annual Meeting - Salt Lake City, UT, USA.
http://www.hwi.buffalo.edu/ACA/

13-17 August 2007
BSR2007 - Ninth International Conference on Biology and Synchrotron Radiation. Manchester, UK
http://www.srs.ac.uk/bsr2007/

22-27 August 2007
ECM-24, European Crystallographic Meeting, Marrakech, Morocco
www.ucam.ac.ma/fssm/ecm24

31 May – 5 June 2008
ACA Annual Meeting - Knoxville, TN, USA
http://www.hwi.buffalo.edu/ACA/