Crystallography News

British Crystallographic Association

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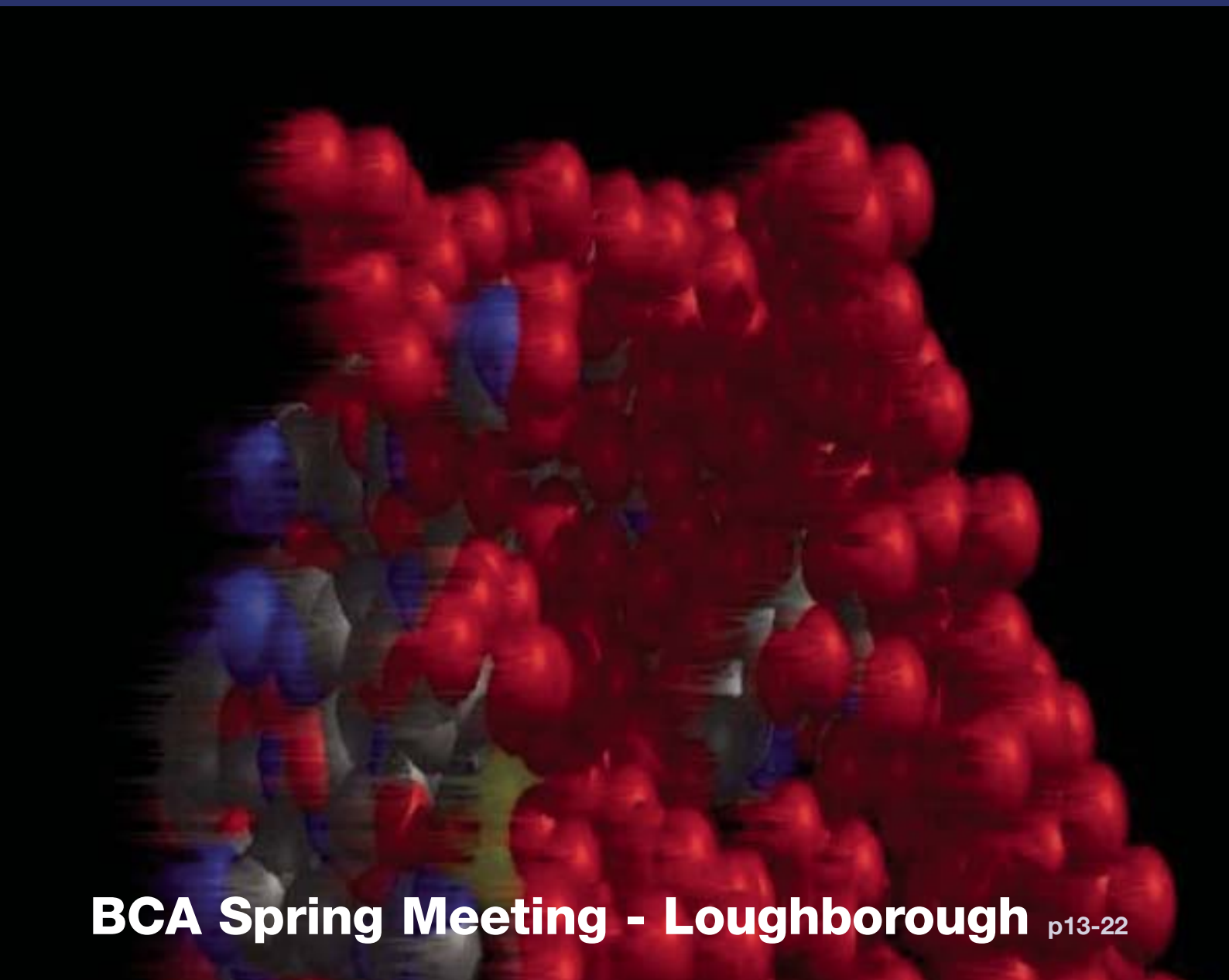
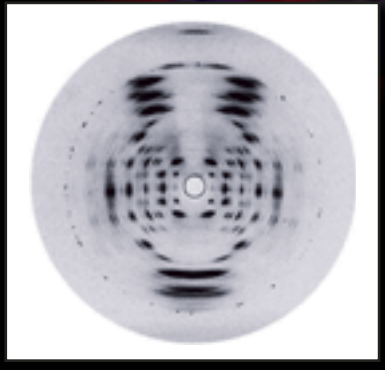


BCA Spring Meeting - Loughborough p13-22



CCDC at 40 p6-8

CCP4 at Reading p10-12

Francis Crick and Maurice Wilkins 1916-2004 p23-26

Book Reviews p27-29

Meetings of interest p40

Crystallography News March 2005

Contents

From the President 2

Council Members 3

From and To the Editor 4

Puzzle Corner/Corporate Members 5

Cambridge Cyrstallographic Data Centre at 40 6-8

IUCr Computing Commission / Global Watch 9

CCP4 at Reading 10-12

BCA 2005 Spring Meeting 13-22

Francis Compton Crick 1916-2004 23

Maurice Hugh Frederick Wilkins 1916-2004 24-26

Books 27-29

News from the Groups 30-38

New Honorary Members 39

Meetings of Interest 40

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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 **June 2005** issue are sent to the Editor to arrive before **25th April 2005.**

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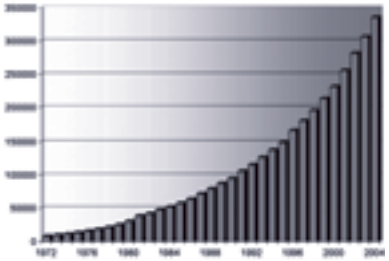
Hasn't it grown?



CCDC at 40 ***p6***

This month's cover:

Our cover features the poster for the BCA Spring Meeting in Loughborough.

The inset is an early DNA fibre photograph supplied by Struther Arnott for his appreciation of Maurice Wilkins.

From the President

THE 2005 Annual BCA Spring Meeting, the 23rd of the series, rapidly approaches, and you will find many details of the programme in this issue of Crystallography News. The Programme Committee under its chair John Finney has put together a full and diverse programme. I would encourage you and your colleagues to come along to what promises to be an excellent meeting - we look forward to seeing you in Loughborough.

One slight disappointment we have had assembling the programme has been the low response to our call for contributed talks. With a deadline set earlier than the normal abstract deadline, we aimed to allow colleagues to put their work forward and bid for spare slots which the programme organisers had kept free. We had identified this initiative as one way of continuing involvement from our younger colleagues in this "mid"-year when there is no Young Crystallographers' Satellite session. The reasons for the low response are not clear. A new initiative is always difficult, perhaps people were less well aware of this possibility since we have not traditionally called for contributed papers, but nonetheless we had a rather low response to this call. I have no doubt the poster sessions in Loughborough will still be full and exciting – it is just unfortunate that more people were not anxious to secure a possible speaking slot. That notwithstanding, the oral sessions are of uniformly high quality, with a range of high profile speakers attracted.

This year we have participation from the XRF and solid-state chemistry communities, and from the Facility user groups, helping to broaden our appeal and emphasising the central role of crystallographic techniques in structural science. In early planning for the 2006 Spring meeting, which will be held in Lancaster, I am pleased to say that we intend to link up once again with the British Association of Crystal Growth, following conversations with BACG Chair **Kevin Roberts.** The Programme Chair for Lancaster 2006 will be **Paul Raithby** (Bath).

With this issue of CN, we hope to include the latest BCA Review Symposium issue of the journal Crystallography Reviews, covering a selection pf papers presented at the last Spring Meeting (Manchester, 2004). The production and distribution of this issue has been part supported by page-sponsorship from CCDC, Bruker AXS and ICDD.

Towards the end of 2004, Council was pleased to invite three colleagues to become BCA Honorary Members, our highest membership accolade. I am delighted to say that **Professor Paul Barnes, Professor Mike Glazer** and **Professor George Sheldrick** have all accepted these invitations to honorary membership. Brief citations for these honorary members can be found elsewhere in this issue.

In closing, I would like to remind members that our treasurer of 5 years, **Dave Taylor,** is resigning from this post at the Loughborough Spring Meeting. More on Dave's massive contribution to the BCA and its operation will follow in a later issue; for now I would like to remind members that nominations for Treasurer are welcome. As of the time of writing, on a cold dark January morning, we have one nomination for this important post. As always in the BCA we encourage competitive election processes and invite further nominations.

Chick Wilson

Chick Wilson, Georgina Rosair, Jeremy Cockcroft, Judith Shackleton and Sandy Blake.

Bob Gould, John Finney, Elspeth Garman, Peter Moody, Andrea Hadfield, Christine Cardin and John Evans.

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www.crystallography.co.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

ISSUE 92 of Crystallography News looks toward our meeting in Loughborough in April, and you will find plenty about the programme in this issue, together with material for the A.G.M. of the Association and of the individual groups. Practical details appear in our December issue.

It is sad to have to record the deaths of two such eminent scientists as **Francis Crick** and **Maurice Wilkins** in this issue. We are very grateful to **Struther Arnott** for the appreciation he has given us of Maurice, and to **Connie Chidester,** editor of the ACA Newsletter for sharing her obituary of Francis with us.

We are very pleased to have **Frank Allen's** contribution on the 40 years of CCDC in this issue. The benefit this organization has been to crystallography in this country and throughout the world can hardly be overestimated. It is amusing to think back to one of the protests at the time it was started, "How can they want to spend so much money on librarians?" I suppose the reply could be, "Well, some library!"

There have been several excellent group meetings this autumn four of which are reviewed here. All of them attracted interest and attendance from outside the sponsoring group itself. I particularly enjoyed the Industrial Group's meeting on DIY crystallography, where "DIY" included not only excellent ideas to make do and mend in a small lab, but even the installation of the new diamond light source! The most memorable, though, was the very well-attended meeting in honour of one of our most missed former colleagues, **David Blow.**

We receive many E-mails about crystallographic developments. One which deserves wide publicity came to me from **Lachlan Cranswick:** The SCHAKAL structure plotting software (PC and UNIX) by **Egbert Keller** has been transferred into the public domain and is now freely available via the web: **www.krist.uni-freiburg.de/ki/Mitarbeiter/Keller/schakal.html.** This is the plotting program best known for the "frog-spawn" plots which neatly combine space-filling and ball-and-stick representations in the same figure. See the website for further information.

As I mentioned in the last issue, we have been asked to provide material for an IUCr issue on "Crystallography in Britain." Some excellent suggestions for this have been coming in, mainly from Chemical Crystallographers, but we could do with more! Please write to me or to one of the group representatives, **John Evans** (PCG), **Sheila Gover** (BSG), **Georgina Rosair** (CCG) and **Judith Shackleton** (IG).

Bob Gould

Letter to the Editor

Pointing things out in Powerpoint

From Professor Tony North

Dear Bob

As nobody has responded, I thought I had better do a bit more myself! Actually, I am a bit surprised that no-one has pointed out that there is something relevant in the official Powerpoint Manual (maybe, like me, people find the Microsoft Manuals indigestible to say the least). There are also some comments on the internet, which I found with a Google search. But it has also involved some personal experimentation. Here goes:

First, people need to know that Powerpoint 97 (which we have on Leeds University machines) and Powerpoint 2002 (which I have at home) differ. In the course of a 'slide show', with 97, the arrow cursor does not appear with each new slide until the mouse is moved ; it then stays on unless switched off - right-clicking produces a menu which allows the arrow to be hidden 'now' or 'always', i.e. for the rest of the slide show. With Powerpoint 2002, there is an additional option whereby the cursor can be switched permanently on for the whole slide show. As an alternative to right-clicking for the menu, ctrl+a will switch the arrow on, ctrl+h will hide it, in each case for the whole slide show.

The right-clicked menu allows a pen to be selected instead of the arrow. The point about this is that you can draw with the pen by moving the mouse with the left button pressed down. Resultant lines are usually a bit wobbly. but if you press 'shift' while moving the mouse, you can get nice straight horizontal or vertical lines. The colour of the lines can be changed via the 'pointer options' on the menu. With Powerpoint 97, the cursor reverts to the normal arrow when the next slide is shown; if the pen is again selected, it retains the colour that had previously been set. With Powerpoint 2002, the cursor remains set as 'pen' or 'arrow' for successive slides unless you deliberately change it (ctrl+p selects the pen).

I have not found a way to change the arrow pointer from within Powerpoint, but it can be done in Windows Xp>Control panel>Appearance and Themes>Mouse pointers>Pointers (there is an equivalent way with other versions of Windows). If you select 'browse', you will find a long list of alternative pointers stored in the folder C:/WINDOWS/Cursors. They mostly seem rather useless for our purpose; the most conspicuous is a spinning coin and this certainly is more obvious in a Powerpoint show than the usual little arrow. There are some rather charming galumphing dinosaurs, but it's rather difficult to see which part of their anatomies is the active pointer. The maximum size of a cursor is 32x32 pixels, so you cannot have a very big one. Using a program Imagedit (available free over the internet), I have generated 2 larger arrows (one white, one gold) and also one red one of the biggest size that will fit in. As a special treat for BCA members, I have also made a couple of versions of the BCA logo, the centre point of which is the active 'hot spot'.

I should be very happy for anybody to use my cursors if they wish to. I will be happy to send files of these 5 cursors to anyone who would like them - they just have to be put into the C:WINDOWS/Cursors folder.

The modified cursors appear in all relevant Windows programs, not just Powerpoint; it is easy to replace them with the normal default arrow via the Control Panel.

But just let me finish by saying that my objective is to encourage speakers to face the audience while they are using Powerpoint and not look at the screen while waving vaguely with a laser pointer. Additionally, I think that many people do not realise that you can turn the screen off by pressing 'b' or to a white screen by pressing 'w' - much better than sticking a piece of card in front of the projector!

Best wishes
Tony

[I loaded these pointers to Windows 2000 without any trouble. To me, the most effective is the gold arrow, which can be left on in normal computer use without problem. It does help emphasise Tony's main concern, that speakers keep audiences both in mind and in view! – Ed.]

Puzzle Corner

Congratulations to Tim Weakley, with the first correct solution to last month's puzzle:

a: Fluidigm
b: PANalytical
c: Astex Technology Ltd.
d: Bruker AXS
e: Chemical Computing Group
f: deCODE Genetics
g: Oxford Cryosystems
h: International Centre for Diffraction Data

He made me feel somewhat ashamed by asking, "Was there some subtle catch?" Well, sorry, there wasn't! Once again, my apologies to other corporate members whose logos are unfortunately impossible to dissociate from their names!

Now for this month – another of one of our more popular competition types. The following is a simple letter-substitution cryptogram. Each letter always represents the same letter throughout the text, and may represent itself. The source of the quotation should be given, and this month's issue contains a clue!

Qezzjose bah wjsryhrfroe bsj bzyan opj zyqo lbqfraboran bah fpbsbfojsrqorf wsywjsorjq yl fseqobxq de iprfp opje bsj hrqoranmrqpjh lsyz yopjs lyszq yl zboojs. Ya opj zbfsyqfywrf xjkjx, oprq qezzjose rq jgwsjqqjh de wyrao nsymwq, ipjsjbq opj wjsryhrfroe rq hjqfsrdjh de osbaqxborya nsymwq bah xboorfjq, bah opj lmxx qosmfomsbx qezzjose yl fseqobxq rq nykjsajh de qwbfjnsymwq.

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.
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The Cambridge Crystallographic Data Centre

40 years of database development, software and research

Beginnings

The CCDC was created to record crystal structures, and the Cambridge Structural Database was one of the first numerical databases created anywhere in the world. The CCDC originated from a small group set up in 1959 by **J D Bernal** and **Olga Kennard,** initially at Birkbeck College, London and from 1962 at the Chemistry Department in Cambridge, collecting data on organic and metal-organic crystal structures and using these to investigate intermolecular arrangements and forces. In January 1965 David Watson joined the group and later that year the CCDC was formally established with a grant from the Office for Scientific and Technical Information. The collection of data was greatly accelerated and both numeric and bibliographic data were transferred from edge punched cards to "machine readable" form. Subsequent CSD growth statistics suggest that, had this work started later, it is doubtful if it would have started at all. But it did, and 40 years later the CSD contains 335,276 structures.

The three directors of the CCDC:
David Hartley, Olga Kennard and Frank Allen

Development

By modern standards, early progress was horribly slow: computer technology was in its mainframe, card chewing, batch-processing era, and hardware was temperamental. On the human level, staff were needed to acquire, log and encode data, and crystallographer-programmers were needed to turn the vision into a reality. Scientific abstractors and data entry personnel, most of whom worked from home, were also vital early colleagues on the developing production line. The CCDC itself was partly a hub which managed a complex data preparation network, and partly a scientific analysis centre that processed the raw material into a growing database. Data acquisition itself has now completed its own transformation from the days when all coordinates were printed to the current nirvana of electronic deposition via the CIF. In between we had to cope with the myriad vagaries of hard-copy depositions, which even involved some in handwritten form!

An early need was for structure validation software, to guard against local data entry mistakes and to locate the errors that occurred in some 10% of typed or typeset tables. Many errors were trivial to correct, but in the pre-email era a significant number had to be referred back to authors by letter. Crystallographers took these 'CCDC letters' in good part, and this was the beginning of a special relationship with the community that has enhanced the development of the CSD throughout the past 40 years.

An electronic bibliographic file was being regularly updated by 1970, and was disseminated via the Molecular Structures and Dimensions book series – itself one of the earliest handbooks to be typeset directly by computer. Meanwhile, the first 5,000 crystal structures were being validated and entered into a CSD data file. Finally, it was realised that a system of chemical structure representation was needed and a third component, a file of chemical connection tables, was created. 2D and 3D substructure search capabilities were now possible, adding tremendous value to the underlying crystal structure information. These three separate files were eventually amalgamated into the CSD that we know today.

Millions of lines of code

Software development has always been at the heart of CCDC activities, and we have run the gamut from FORTRAN II to our current object-oriented C++ environment. FORTRAN, as its name implies, was never really created for text processing, and we pushed the available compilers to their limit and beyond in the early days.

The CCDC is responsible for three types of code: that which underpins CSD creation, that which forms part of the CSD System for search, analysis and structure visualisation, and applications software that uses crystal structure data to solve problems in structural chemistry and biology. CCDC software developers have blended the 3D representations of crystallography with the 2D representations of chemical

Views of the exterior and interior of the CCDC Building

informatics, and have been at the forefront in creating novel systems for 3D substructure searching, including searches for intermolecular interactions, and the statistical analysis and visualisation of parameter distributions retrieved from the CSD. More recently, we have generated knowledge-based libraries of structural information, and have diversified (often collaboratively) into software applications that use crystal structure information.

CSD System releases

By the mid-1970s, the first version of the CSD System had been released to academics in the UK, USA, Japan and Italy. Many other countries formed National Affiliated Centres and became subscribers to the service. The pharmaceutical and agrochemicals industries began to experiment with computational chemistry and modelling tools for rational molecular design, and the number of industrial subscribers began to rise during the 1980s. Early releases were on magnetic tape, and the number of 1600 foot tapes per release was certainly a challenge for the average postman, particularly the one who 'delivered' several CCDC parcels to a hedge 'somewhere in Europe'. Software was released as source code, to be compiled under the user's local operating system. Today all that has changed, with the universality of just a few operating systems, CDs and internet downloads, click-of-a-button installers, and e-mail support desks.

1,200 Applications Papers

The first papers that made use of the CSD for fundamental research began to appear in the late 1970s, inspired by the work of **Hans-Beat Buergi** and **Jack Dunitz** on structure correlation. Recognising the CSD as a growing library of geometric structures, there was a rapid acceleration in this type of research from about 1980. A key issue was to improve database searching and develop a proper statistical basis for data analysis, so that improvements in distributed software were often driven by current research needs.

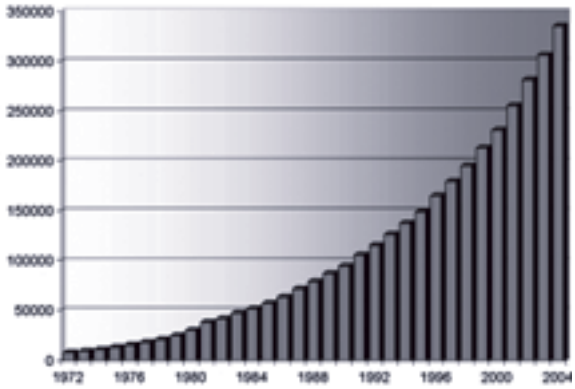
The CCDC itself has been heavily involved in this research effort, and has published applications papers covering both intramolecular and intermolecular topics. Tables of mean bond lengths published in J.Chem.Soc, Perkin Trans (1987, pp S1-S19) and J.Chem.Soc. Dalton Trans. (1989, ppS1-S83) have now jointly received more than 10,000 citations. In the study of intermolecular interactions, the CSD has underpinned many fundamental contributions. These have helped to provide tools for studying protein-ligand interactions, and played a part in the emergence of crystal engineering as a sub-discipline. The CCDC's most cited paper in this area – more than 1,000 citations and the 60th most cited paper ever in the first 125 years of JACS – is the categorisation of short C-H…O interactions as true H-bonds (Taylor & Kennard, J. Amer. Chem. Soc., 104, 5063-70, 1982), work that re-shaped the global view of weaker interactions.

The CCDC maintains a web-accessible database of published applications of its products, and the 1,200 current entries chart the many and varied uses of the CSD. The CCDC is well represented with over 150 papers, but more than 1,000 other references show the truly international impact of CSD-based research.

The CSD at 40

On 1 January 2005, the CSD contained 335,276 crystal structures and grew by nearly 29,000 structures in 2004. The size and complexity of structures has also increased steadily with time. The CCDC has excellent relationships with journals, and 84 titles now require electronic data deposition to the CCDC when a paper is submitted. These data enter the CSD when the paper is published, and the CCDC now maintains a growing parallel archive of more than 160,000 of the initial 'raw' CIFs.

Current CSD statistics are also available on the website, and although the CCDC encourages direct deposition of Private Communications, these statistics refer primarily to published data. The issue of the very large number of structures that languish unpublished in laboratory records is quite another matter, but one that must surely be addressed. Software for data processing and maintenance of both the CIF archive and the CSD are currently undergoing a major overhaul, and new software will incorporate much expert knowledge that has been gained over the past 40 years.



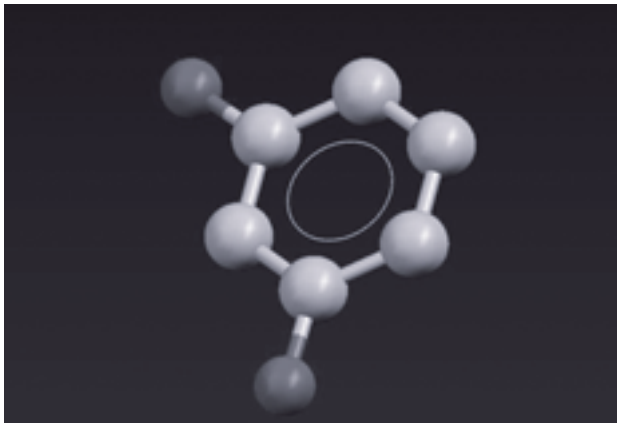
Growth of the CSD 1970-2004. *At this rate of growth, the CSD will record its 500,000th entry during 2009.*

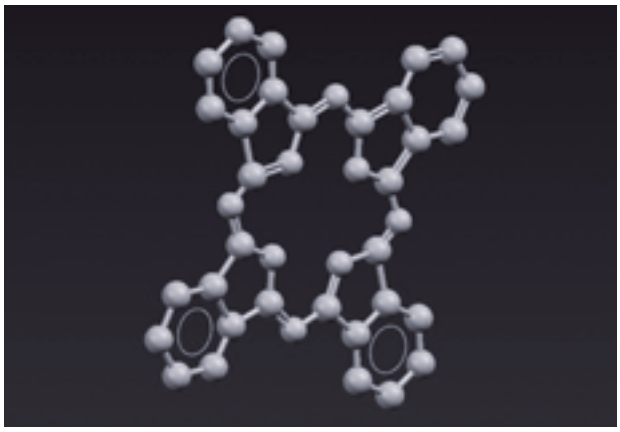
New Products

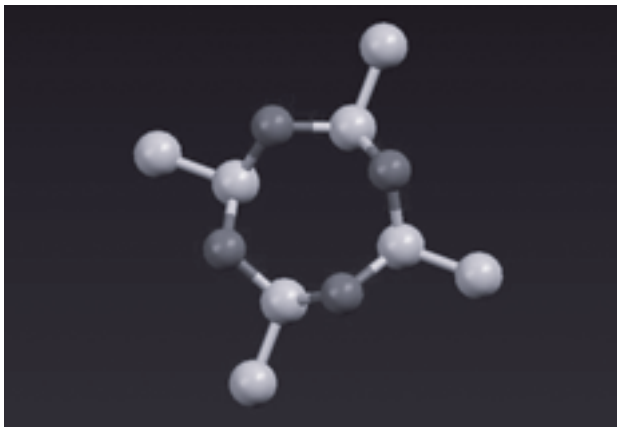
Two new components of the CSD System have been added since 1997. These are knowledge-based libraries of intramolecular geometry (Mogul) and intermolecular interactions (IsoStar). They provide click-of-a-button access to millions of individual pieces of geometrical and chemical information that can be derived from the CSD (and PDB protein-ligand complexes in the case of IsoStar). Further development, and integration of this structural knowledge with other software, is ongoing in both cases.

Recent years have also seen the CCDC diversify into developing and marketing specific software applications for rational drug design (GOLD, SuperStar, Relibase+) and for structure solution from powder diffraction data (DASH). All of these products make use of crystal structure data from

the CSD or PDB in some way, and all except SuperStar are being developed through collaborations with industry and academia. The life sciences products, concentrating essentially on protein-ligand interactions and protein-ligand docking, help to solve difficult problems, and promote the value of small-molecule crystal structure data in structural biology and in the pharmaceutical and agrochemicals industries. The CCDC continues to broaden its horizons, by seeking new areas of science in which crystal structure data adds value to research and development activities.







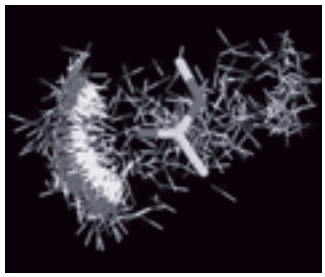
Published in 1936, these are the three earliest structures with full 3D coordinates stored in the CSD. Metaldehyde (L. Pauling & D.C. Carpenter, JACS, 58, 1274, 1936), Phthalocyanine (J.M. Robertson, J.Chem.Soc., p1195, 1936), and Resorcinol (J.M. Robertson, Proc.Roy. Soc.Lond., Ser.A, 157, 79, 1936). No R-factors are recorded for any of these structures! The earliest references, which do not report 3D coordinates, are from 1923: Beryllium oxypropionate (Bragg & Morgan, Proc.Roy.Soc.Lond., Ser. A, 104, 437,1923) and D-Mannitol (Backer & Rose, Z.Phys., 14, 369, 1923).

The CCDC as an Independent Institution

The CCDC was grant-funded from 1965 until 1989, when it became an independent institution: a non-profit Company Limited by Guarantee and with charitable status. This means that the CCDC must be financially self-sufficient, and that any surplus income must be ploughed back into the company (e.g. for new equipment) or into specific charitable activities. Thus, the CCDC provides grants-in-aid for access to the CSD System in developing countries, sponsorship to students who are working on projects allied to the CCDC's interests, and support for the activities of relevant professional organisations. The CCDC's affairs are overseen by an international Board of Governors, eight eminent scientists who, in their turn, are responsible to UK Companies House and to the Charity Commissioners for England and Wales.

Our most valuable assets: Staff, Customers and Collaborators

The CCDC has expanded steadily, and now has 50 employees divided between database creation, product development, research, scientific and technical support, and administration. The CCDC now has customers in academia and industry all over the world, and the nearly 2,000 CSD System licenses were distributed across 56 countries in 2004. The CCDC has a long history of scientific collaboration with academia and industry, and this work has fuelled our research output and fed into our product developments. Currently, the Pfizer Institute for Pharmaceuticals Materials Research, a major partnership involving the CCDC, Cambridge University and Pfizer Inc., is generating exciting results and further extending our areas of scientific interest.



IsoStar scatterplot of the distribution of O-H (donor) contact groups around ester central groups in the CSD.

We do not have a precise total of the number of staff and visitors who have worked at the CCDC over the past 40 years, but it must be 250 or more. What we do know is that they have left, or are leaving, their own mark on the organisation. It is the stronger for their contributions. Customers, scientific collaborators and data depositors also leave their mark, through their constructive input and feedback on our efforts. The CSD, our products, and ultimately all of our customers, have benefited enormously from these interactions, and we are grateful for their involvement.

We look forward to the next 40 years.

Frank Allen
www.ccdc.cam.ac.uk

IUCr Computing Commission – Aperiodic structures

The latest edition of the Computing Commission Newsletter is viewable via: http://www.iucr.org/iucr-top/comm/ccom/newsletters/2005jan/

Besides having articles of general interest, this edition has the theme: **"At Right Angles to Conventional Crystallographic reality: incommensurate structures, quasicrystals and pair distribution functions" - Editors: Simon Billinge, Gervais Chapuis, Lachlan Cranswick and Ron Lifshitz**

The Editors' Introduction and the list of articles in this edition are given below. For more than three decades, crystallographers have been faced with new, challenging crystalline materials with structures incompatible with the classical view of crystals with three dimensional periodicity. These new materials include incommensurately modulated and composite structures and quasicrystals with icosahedral or dodecagonal symmetry, to cite only the most representative examples of aperiodic structures as they are presently called. In most cases, these new structures are best described by embedding them in space of up to six dimensions. This approach is justified by the fact that periodicity can be recovered albeit in higher dimension.

The rapid evolution of this field is not only due to the innovative theoretical approach of the so-called superspace symmetry, but also to the enormous worldwide efforts on software development. This issue includes a range of articles on techniques that can explain diffraction data where the most appropriate model may not fit into an ordered, convenient, commensurate cell: Incommensurate Structures, Quasicrystals and Pair Distribution Functions. Besides encouraging exchange of ideas within different communities, we hope it might encourage crystallographers, who may prefer to deal only with ordered commensurate cells, to take these style of problems out of the "too unusual drawer" and onto their diffractometers and transmission electron microscopes.

At Right Angles to Conventional Crystallographic reality: incommensurate structures, quasicrystals and pair distribution functions (programming and general articles):

Procedures for the refinement of incommensurate structures using XND. Coding issues for the refinement of incommensurate structures - Jean-Francois Berar and Gianguido Baldinozzi

A Program Package for Aperiodic Tilings - Uwe Grimm

DIMS (Direct-methods program for solving Incommensurate Modulated Structures) on the VEC platform - Hai-fu Fan

DIMS (Direct-methods program for solving Incommensurate Modulated Structures) /VEC applications - Hai-fu Fan

Collection and visualization of single crystal data of incommensurate crystals - Rob Hooft

Visualization and Analysis of Single Crystal Time-of-Flight Neutron Scattering Data using ISAW - Dennis Mikkelson, Arthur J. Schultz, Ruth Mikkelson and Thomas Worlton

Graphical and interpretation tools for difficult incommensurate and composite structures in JANA2000 - Vaclav Petricek and Michal Dusek

Calculating the Pair Distribution Function from a Structural Model - Thomas Proffen

Other Articles:

Refinement in Crystals - Richard Cooper and David Watkin

Computing the Z-matrix for global-optimisation - Kenneth Shankland

cctbx news: Phil and friends - Ralf W. Grosse-Kunstleve, Pavel V. Afonine, Nicholas K. Sauter and Paul D. Adams

Lachlan Cranswick

Solving the Protein Puzzle in China and Japan

Global Watch is the monthly magazine of the DTI Global Watch Service, which helps UK businesses improve their competitiveness by identifying and accessing innovative technologies and practices from overseas. The following is, with permission, an extract from its December 2004 issue, where Dr Kimberley Watson of the University of Reading is talking about a recent Global Watch mission to rapidly emerging structural genomics centres in China and Japan.

What is structural genomics?

Structural genomics has evolved out of the human genome project, the idea being that if we can identify which genes are responsible for a particular outcome we can endeavour to modify and improve how the proteins produced by the genes work. It is proteins that actually perform the biological function. They are responsible, for example, for signalling events along a pathway of nerve stimulus, such as when the body perceives pain. Structural genomics aims to provide the ways and means for solving protein structures rapidly and thus the challenge is to do this in a very high throughput way - several hundreds of thousands of macromolecules are responsible for every biological process in the human body.

Why was the mission mounted?

It is known that structural biology has been a great UK strength since its inception and we have a really good, competitive industry, but we must continue to learn from others. This mission is the result of a bioinformatics mission to Japan which revealed that structural biology is an area of major interest and investment, and of awareness that China has also prioritised the field since 2001. The UK's Diamond Light Source - a state-of-the-art synchrotron radiation facility which can be used to study the structure of matter at the atomic level - comes on line in a couple of years and we should be seeing where there are opportunities for scientific collaboration and information exchange, particularly with Japan's synchrotron, SPring-So.

To discover information about the impressive technologies the mission witnessed, and to learn who will benefit from the mission's findings, please visit www.globalwatchonline.com/missions, and click on 'life sciences'. To obtain a copy of the mission report phone **Charlotte Leiper** on 01664 501 551 or email: **events@globalwatchonline.com**.

Ron Kirby
Global Watch Service

Meetings

CCP4 at Reading

AFTER many years in the North of England, the annual Collaborative Computational Project in Macromolecular Crystallography (CCP4) Study Weekend saw a move to the South where it was held at the University of Reading from January 7-8, 2005. This year's meeting focused on "Data Collection and Analysis" with a scientific programme organised by Gwyndaf Evans (Diamond Light Source) and Martin Walsh (European Synchrotron Radiation Facility, Grenoble, France). Approximately 450 delegates were registered including individuals from institutions based in Europe, the USA, Japan and China.

The meeting began with a few words from **Professor Eleanor Dodson** (University of York) remembering **Professor David Blow** who died last year and his contributions to the development and support of CCP4. **Zbigniew Dauter** (Brookhaven National Laboratory, Upton, NY, USA) then opened the scientific programme in his usual entertaining style and proceeded to overview the tremendous progress in macromolecular crystallography in the past few years and drew analogy with the developments in small molecular crystallography in the past few decades. Among the most notable current technological advances at synchrotron sites are microfocus beamlines and long-wavelength facilities for anomalous phasing on lighter atoms. With the help of this modern technology, it is often possible to obtain a complete structure of a novel protein within a day. Zbigniew, however, added that not all protein structures could be obtained using fully automated procedures and hence structural work on some of the 'high hanging fruits' will require more sophisticated and elaborate processes. **Andrew Thompson,** SOLEIL, France, gave a very precisely constructed and highly appreciated presentation about essential elements of protein crystallography beamlines. After a brief introduction, he overviewed the rapid evolution of the current beamlines where the appropriate hardware is tailored to provide fast and flexible data collection facilities without compromising the quality of the X-ray data.

Session 2, "Expression, Crystallization and Screening", opened with **Darren Hart** (European Molecular Biology Laboratory, Grenoble, Outstation, France). Darren posed the question "Is there a soluble form of my insoluble protein?" but his ultimate aim was to find crystallisable forms of uncrystallisable proteins. He then presented a method to achieve this aim a high throughput approach for expression construct screening called ESPRIT. This method is based upon the view that truncated forms of a protein, which may include individual domains, may be more soluble and hence more crystallisable than the complete protein. This method uses incremental truncation libraries sets of expression constructs which code for different parts of the protein under study. These constructs are used to produce multiple truncations of the protein, i.e. the protein truncated residue by residue from either the N or C- terminus. The expressed protein also contains a tag which enables rapid purification and a means of monitoring the yield of soluble protein. Screening is done using automated robotic methods which generate high density protein arrays that can be probed for identification of soluble variants. The timescale from expression construct generation to solubility screening is typically about three weeks. The current rate limiting step in ESPRIT is the sequencing of constructs. But the time invested is well worth it if one can achieve the production of soluble, crystallisable protein.

Janet Newman (an independent consultant based in Encintas, CA, USA) followed on with a lively presentation entitled "If you can't always get what you want, can you get what you need?" which covered a range of methods for enhancing production of "ideal" crystals. Points for discussion included whether the most efficient use of one's time was working with poor data versus re-screening for better crystals. Based upon industrial experience, Janet argued that getting better data was almost always more time efficient. It was also evident that persistence can "pay off" in terms of investing time in screening for crystals under different conditions and using different methods. However, another critical aspect for success she pointed out was the ability to know when to stop investigating a particular crystallization experiment. Indeed, this latter point reminds us of the empirical nature of protein crystallization, as Janet noted that "all crystallisation techniques are a series of published anecdotes".

This session was rounded out by a tour de force from **Elspeth Garman** (University of Oxford) who covered the development of cryo-cooling methods and issues surrounding radiation damage in protein crystals that occur during diffraction experiments. She pointed out that understanding why we cool and optimise cryo-methods was strongly driven by observations involving radiation damage in protein crystals irradiated using second generation "high flux" synchrotron radiation sources. Elspeth not only described HOW one experimentally carries out and optimises cryo-cooling of protein crystals, but gave clear explanations as to WHY these procedures are carried out in the first place (e.g., temperature of cryo-cooling, addition of cryo-protectants, storage and retrieval methods, etc). Based upon the work of her group and others, she also described how radiation damage can result in specific structural changes including decarboxylation of glutamate and aspartate residues, or destruction of methionine side

chains. She emphasised the importance of being aware of potential radiation-induced modifications, particularly in the context of interpreting biological function from structure where observed modifications of enzyme active sites, for example, may actually be an artefact arising from X-irradiation.

The final session of the first day focussed on "Data Collection and Integration." **Andrew Leslie** (MRC-LMB, Cambridge) showed us, almost from first principles, how diffraction images are converted to indexed intensities. He took the audience through indexing, parameter refinement, post refinement and integration in considerable detail and clarity. **Sasha Popov** (European Molecular Biology Laboratory, Hamburg, Germany) then described the program BEST, that uses limited (and quick) initial measurements to predict the optimum strategy for data collection, and how radiation damage could be compensated for. He stressed the importance of the ultimate use (MAD/SAD/MIR/MR/refinement) of the data in influencing the compromises of resolution, completeness and accuracy. **Michael Blum** (Mar USA Inc., Evanston, IL, USA) then reviewed both the history and current means of recording X-ray diffraction. He described how the various detectors work as well as the advantages and disadvantages of the each type. He showed how the sort of detector influences the way data is collected, and looked at future developments. He also considered how we compare different detectors and discussed the use of DQE for this purpose.

The following day opened with Session 4, "Data Collection in Practice" which contained two very interesting presentations. **Jim Pflugrath** (Rigaku/MSC, Inc., The Woodlands, TX, USA) began by comparing the time taken to determine structures in 1980 and the present day, and identified the main improvements in speed as occurring in the collection and subsequent "massaging" of data, which now takes hours rather than years. The improvements in data collection are due to more intense and sources which are also better focussed. Recent advances include microfocus rotating anode sources and multilayer mirrors, which both focus and monochromate, giving a very pure single line spectrum. Image plate detector technology has also improved, with more sensitive phosphors, improved scanning lasers and faster ADCs (which give rise to greater signal to noise); IP detectors can now be nearly 40 times faster than they were 15 years ago, and on a lab source easily compete in macromolecular crystallography with CCD detectors, though each technology has its own strengths. Automation in the lab relies on robotics and reliable crystal ranking. The MSC model applies a ranking based on a series of differently weighted criteria (in the same way as e-mail filters such as SPAM ASSASSIN work). Jim pointed out some of the potential pitfalls, e.g. errors in image headers (direct beam position, crystal to detector distance, etc). He followed this by discussing SAD phasing in the home lab, especially the use of longer wavelength radiation (e.g., Cr-Kalpha), which uses the significant anomalous signal from sulphur atoms in native proteins to be used. The take home message was that, while the current hardware is better than ever, problems in the home lab are still problems at the synchrotron. Intelligent design of the experiment and thoughtful implementation will allow even difficult problems to become tractable.

Sean McSweeney (European Synchrotron Radiation Facility, Grenoble, France) then discussed the particular characteristics of undulator radiation which are important for crystallography, and drew attention to the problems involved as well as the advantages. He pointed out that the spectrum is spiky, due to the radiation being produced via interference; this gives a central bright spot surrounded by interference rings. The beam has very low divergence - this means that, although the beam has quite low power, it is very concentrated in the central spot. He pointed out that if all the photons from a bending magnet source could be brought to focus at the sample, a bending magnet beamline could be competitive in terms of intensity with an undulator; in practice, both a wiggler and bending magnet source are much more divergent and it is this which explains the difference in large part. Because the radiation is produced through interference and the spikes in the spectrum are due to harmonics, it is possible (and also realised in practice) that some regions of the X-ray spectrum are unavailable. The high intensity means that sample lifetimes are relatively short (the Henderson limit is reached rapidly); it also means that data collection times can be (and in fact need to be) very short. Also, the low divergence and small focal spot mean that every flaw in the crystal will be revealed, where they might be hidden in experiments with X-ray beams with different characteristics. The short sample lifetimes give rise to another problem, which historically was important until the relatively recent advent of cryocooling, i.e. multiple crystals may be necessary for a single experiment. The advantages, though, are plain; data collection is possible from all sorts of samples which would previously have been unsuitable, such as crystals with large unit cells or those which are poorly diffracting. Also, screening and characterisation of multiple samples is now much more rapid.

Sean finished with some advice to users: do the simple things properly (crystal mounting etc); speed kills; everything dies; have a plan and don't trust to luck. He also suggested, regarding data collection: small but not tiny oscillations are better; fill the detector; process the data as you go; think about background scatter; and remember that mosaic crystals often give better data. He recommended that for each sample that one should have the basic crystal information; know what type of experiment you want to do; know the expected and desired diffraction limits. With regard to phasing one should be conservative (collect to lower resolution); collect a complete SAD data set (remote or peak) before changing wavelength; and aim for both multiplicity and completeness. Regarding molecular replacement, Sean recommended to collect the low resolution first (can be done with minimal dose); refine cell and mosaicity well to get a good strategy; data quality is not such an issue (some "bad" data are not useless).

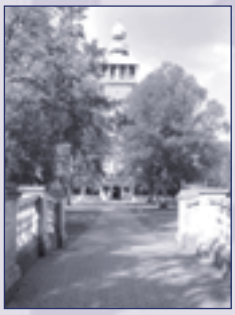
Session 5 on "Data Scaling and Quality Indicators" was held after coffee and started with a 'pointless' talk by **Phil Evans** (MRC-LMB, Cambridge). 'Pointless' is his program that scores possible point groups based on the symmetry observed in the reflections and the deviation from ideal lattice dimensions. This will be added into a new version of his scaling program 'scala' which is based on the philosophy that 'Scaling should reflect the design of the data collection experiment and vice-versa'. He outlined how scala does this. **Andrey Lebedev** (University of York) then discussed twinning of protein crystals and the various measures used to detect the presence in the data. They have been surveying twinning in those PDB depositions with proper structure factors deposited and showed that the files can be partitioned into clusters depending on whether there is twinning, pseudosymmetry or a combination of both. This work is leading towards implementing refinement against twinned data in 'Refmac'. **Kay Diederichs** (University of Konstanz, Germany) then rounded off the session by discussing the changes in individual structure factors with absorbed dose and his programs for calculating structure factors at different absorbed doses to allow extrapolation to the undamaged zero time structure and to look at structures on the decay trajectory.

In the final session entitled "Case Studies" opened with **Zygmunt Derewenda** (University of Virginia, Charlottesville, VA USA) describing his use of mutants, particularly of surface lysines to enhance the crystallisability of proteins. He reminded us that in general proteins have not evolved in order to crystallise. Proteins have an "entropic shield" of flexible side chains that prevent ordering of solvent. Many proteins appear recalcitrant to crystallisation, and increasing the size of the screen rarely improves the success rate. Taking proteins that express well but do not crystallise from structural genomics projects, a triage step of surface mutations has given a high rate of success in then getting crystals. In other cases mutations have improved resolution significantly by generating new crystal forms if poor crystals have been obtained.

Rob Esnouf (University of Oxford) then described the technical struggles involved in solving the biologically interesting semaphorin 4D structure. A soluble construct of around 650 residues was used, containing the 500-residue uncharacterised "sema" domain. Removal of a His-tag and deglycosylation proved counterproductive; crystals were only obtained leaving these modifications on! Only a 2648 image MAD experiment on BM14 that even the beamline scientist did not think would work, gave them the phases they needed. This was from the only crystal to show true C2 symmetry out of 150 which were P1 with pseudo C2. Robert was further blessed by incomplete selenomethionyl incorporation and non-isomorphism. No derivatives were found but some dehydration was seen to give better resolution. As in a number of other talks over the weekend, dehydration and screening a lot of crystals yielded the high resolution data needed for proper refinement resulting in structure determination revealing the predicted 7-bladed propeller dimer for the sema domain. Congratulations! Finally, **Tadeusz Skarzynski** (GlaxoSmithKline, Stevenage) gave an industrial perspective on data collection. GSK crystallographers at four international sites determine roughly 400 "successful" structures a year (many are solved with no ligand present), and there is considerable time pressure, such that automated structure solution pipelines become very attractive. It is necessary to develop a crystal system suitable for studying ligands – there is a strong focus on the ligand interaction; most of the underlying protein structure is of no consequence. It is hard to invest time perfecting crystals that are often severely compromised in quality when ligand is added, with a general philosophy of "structure today is better than better structure tomorrow". He sparked some controversy by suggesting some data processing packages could not deal with certain types of data sets in default mode, although the package concept was robustly defended by some of the audience. Most people are not used to dealing with bad data. Tadeusz openly challenged **Zbigniew Dauter** "You never collect bad data, do you?" (What could he answer?). Whereas most processing programs perform well with good data, Tadeusz showed some striking differences in interpretability of density for different software when data are marginal, possibly due to the different error models being used. In the high throughput situation in industry where many complexes of the same protein crystal are being solved, the choice of package used is guided by the problem and questions about why other packages do not work as well are not usually addressed. He then outlined the GSK system for linking together programs in an automated structure solution pipeline.

In keeping with tradition the meeting dinner was held at a racecourse – this time in Newbury with live music from a swing band which proved popular and drew many delegates onto the dance floor. As always, the smooth running of the meeting was guaranteed by the CCP4 organisation (Daresbury) which includes **Maeri Howard, Charles Ballard, Pat Broadhurst, Liz Kennedy** and **Sue Waller** with additional assistance from **Stuart Eyres** and **Laura Roe.**

Kate Brown
Imperial College, London



BCA 2005 Spring Meeting

Secretary's Annual Report to the AGM 2005

THIS year the report must start on a sombre note. The death of one of our founding fathers, Professor David Blow, who chaired the working group which led to the founding of the BCA, and then acted as President from 1984-1988, was a major sadness for the BCA, which we have already recognised with an obituary in the September 2004 issue of Crystallography News. The Biological Structures Group dedicated their Winter Meeting on 17 December to his memory. We also lost a previous Secretary, Dr Sam Small, who held this position from 1985-1987. We also, very suddenly, lost a much younger colleague, Sue Bayliss.

Next, the composition of Council: This year we welcomed a new Vice-President, **John Finney,** who has taken on the arduous task of organising Loughborough Spring Meeting, but who will not carry this responsibility for the whole of his three-year term. The Secretary's term of office also expired, but she was re-elected for a second term. The Ordinary Members of Council have remained the same, but **Chris Gilmore** is no longer a co-opted member of Council; instead we have co-opted **John Helliwell** following his candidature for Vice-President, and thank him for agreeing to co-option. We also owe a big debt of gratitude to **Kate Crennell,** for her many years of service as Education Officer, and before that, as the editor of Crystallography News.

Council met twice, in UMIST after the Spring Meeting and in Birkbeck (London) in September. On both occasions there was a long agenda, and there is never enough time for detailed debate. Issues which continue to concern Council, and which could be discussed at the AGM, include the future of the post of Education Officer, which was discussed by Council at its September meeting. One possible option is to move to an elected officer for this position. Other issues include membership fees and membership numbers.

Our current membership statistics are as follows: we have 867 paid–up members, but there a large number of former members not included in this figure who have not renewed

their subscriptions but who are kept on the database. This number breaks down as follows: Corporate 85, Ordinary 558, Retired 36, Student 140, Unemployed 5, Honorary 13, Life 30. Membership by groups is as follows: the Biological Structures Group have 297 members, the Chemical Crystallography Group 259 members, the Industrial Group 116 members, and the Physical Crystallography Group 118 members, with 77 members having no stated group affiliation. There has been at least one occasion during the year when a fully paid-up member was not receiving copies of Crystallography News: please make sure that the Administrative Office or I hear promptly about these hopefully rare glitches. We have previously recognised that there will always be student members who finish their courses and leave crystallography, but this means that every year we should be aiming to at least replace those we lose this way. Council has made a start in collecting names of people willing to act as local 'recruiting officers', we should be aiming to have a national network of enthusiasts. It is a particular concern that non-members do not receive Crystallography News and therefore miss the main publicity for the Spring Meeting. A suitable poster design would help here. September is the best time of year to add new memberships, at the start of the academic year. Membership remains a bargain, and cost cannot be a reason not to join.

We have three new Honorary Life Members, **Paul Barnes, Mike Glazer** and **George Sheldrick.** and we welcome nominations for more. Constitutionally, we are allowed to have 20 such members.

As already mentioned, the Biological Structures Group Winter Meeting was dedicated to **David Blow** and held in the Physics Department in Imperial College. The Physical Crystallography Group held a two-day meeting on 'Neutron Scattering from Biological Systems', on 13-14 December. The Industrial Group organised a Pharmaceutical SIG meeting on 5 October and a one-day Autumn meeting on 4 November entitled 'DIY Crystallography' in Birkbeck College, London. The Chemical Crystallography group held a one day Autumn meeting on In-situ Crystallography, Aston University, 17 November 2004. All these events are reported in Crystallography News.

Finally, as always, we are a voluntary organisation and could not exist without our hardworking unpaid volunteer workers. Nowhere is this perhaps more true than for the role of Treasurer. Dave, you are an angel, a wonder worker, and a tower of strength. As you come to the end of your term of office, THANK YOU.

Christine Cardin
Secretary to Council

2005 Annual General Meeting of the BCA

The Annual General Meeting of the British Crystallographic Association will be held on Wednesday 13th April 2003 at 4.35 p.m. in the University of Loughborough.

At this meeting we will elect a new Treasurer.

Draft Agenda

1. Approval of Agenda
2. Apologies for absence
3. Minutes of the last AGM (published in Crystallography News)
4. President's report
5. Secretary's Report to Council (published in Crystallography News).
6. Northern Networking's Report.
7. Report of the Treasurer to include Presentation of the Accounts for 2004 and the Examining Accountant's Report.
8. Acceptance of the Accounts
9. Elections to Council
10. Appointment of Examining Accountant for 2005.
11. Any other business.

Christine Cardin (Hon Secretary)

Central Facility User Meetings

Prior to the Spring Meeting itself, there will be a series of facilities User Meetings, including the SRS XRD and ISIS Crystallography User Groups. A Joint Facilities User Meeting is also planned, with involvement from ILL and ESRF as well as the UK-based Facilities.

SRS XRD User Meeting (11th April)
Organiser: **Mina Golshan,** Daresbury

This meeting will focus on discussion of issues of interest to SRS X-ray diffraction users.

ISIS Crystallography User Meeting (11th April)
Organiser: **Richard Ibberson,** ISIS

The programme will include reviews by **Steve Wakefield** on ISIS and the TS2 project and **Paolo Radaelli** on ISIS instruments. There will also be presentations on new instruments and instrument upgrades (WISH, HRPD, POLARIS, SXD optics and TS2 instruments), as well as a number of science presentations by users. The meeting will conclude with an open discussion, suggested topics being beamtime access modes, sample environment and software.

Bursary Report 2004 – From the Treasurer

GENEROUS membership donations have boosted the Arnold Beevers Bursary fund by over £200 this year. The BSG has transferred interest on its reserves of £608 to the fund and a GIFT AID refund of £998 has also been allocated to the fund. In October the Charity Commission agreed to a donation to the BCA of £1,451 following the wind up of the Reciprocal Space Venture Association and its associated trading company. Council has allocated £500 of this donation to the bursary fund.

In 2004 web based bursary applications were introduced. The system has worked well and is more efficient, with electronic transfer replacing the multiple paper copy distribution and associated postage costs.

The Manchester Spring Meeting saw the award of bursaries worth £5,250 to 35 students from 15 Universities. Eleven of these Bursaries were commercially sponsored.

The BCA is grateful to the following organisations for this valuable support: BrukerAXS (2), ICDD (1), PANalytical (3), Rigaku (3) and Syngenta (2). Each sponsor was presented with a certificate of appreciation.

Through the year there were 7 applications for Arnold Beevers Bursaries and all were accepted. However, one award, made subject to a shortfall in other sources of funding, was not required. So, in 2003 six bursaries totalling £1,200 were taken up.

In 2004 there were no applications to the BCA for "good works" funding.

IUCr Congress Bursary fund
In May 2004 the Euro equivalent of £22,241 was lent to the **2005 IUCr Congress in Florence** for congress bursaries with conditions set by BCA council and agreed by **Carlo Mealli** for the organisers.

Details of the Bursary scheme can be found under Membership at **www.crystallography.org.uk**

Name	University	Conference	Awarded
Miss Francesca Fabbiani	University of Edinburgh	35th Erice Crystallography Course - Diversity Amidst Similarity	£200
Mr Zhanhui Yuan	University of Newcastle	American Crystallographic Association (ACA) Annual Meeting	£200
Ms Luciana De Matos	Bradford University	Erice 34th International School of Crystallography on Polymorphism	£200
Miss Sophie Dale	Loughborough University	ECM-22 Budapest	£200
Dr Colin Seaton	University of Bradford	ACA annual meeting	£200
Mr Philippe Fernandes	University of Strathclyde	ECM-22 Budapest	£200

From the Secretary

Announcement of Election to Council - Treasurer

This year we have a vacancy on BCA Council for the Office of Treasurer. After 5 years of service, the current Treasurer, **Dave Taylor,** is standing down to assume another role outside the BCA. Please send your properly seconded nominations for this position to me as soon as possible. I will accept nominations until two weeks before the date of the AGM on 13th April 2005. If you nominate someone, it is your responsibility to make sure that the person you nominate is willing to stand for election.

Christine Cardin Secretary to Council

Minutes of Annual General Meeting

Held on Wednesday, 7th April 2004 at 5.00 p.m. in UMIST. The President (Chick Wilson) in the Chair.

112 voting members were present.

1. Approval of agenda. The agenda was approved

2. Apologies for absence. There were no apologies for absence.

3. Minutes of the previous AGM. These had been published in the March 2004 issue of Crystallography News. They were approved as a correct record of the meeting. Proposer: **Harry Powell.** Seconder: **Sheila Gould.**

4. Matters arising – the President asked the meeting for suggestions for increasing the membership, particularly among Ph.D. students. Suggestions included regional representatives to build a network, free memberships for students, 18 months for the price of 12 **(Sandy Blake),** flat fees for the whole of the Ph.D. course **(Tony Bell)**, and a flexible attitude to student bursaries for attending the Spring Meeting **(Richard Pauptit),** but not for general bursaries. Student members said what mattered to them most of all was the opportunity to attend a meeting
The meeting accepted the principle of a free student trial membership (proposed **Richard Pauptit,** seconded **Mike Glazer**) subject to a discussion in Council.

The President reported that our IUCr fund had been received back from the Geneva meeting and that its value would be maintained for the 2008 IUCr meeting in Osaka. He reported that **Christine Cardin** had agreed to be the BCA representative on the ECA, and that a bid to host the ECM in Edinburgh in 2009 had been prepared but not yet presented. The ECA have created a Max Perutz prize which will be presented in Budapest. He called for nominations for the BCA Prize lecture to be delivered at the Spring Meeting in 2005.

5. Secretary's Report. The secretary, **Christine Cardin,** presented her report, which had been published in the March 2004 issue of Crystallography News.

6. Northern Networking report. This report was presented orally. **Gill Houston** said that there were now only 771 members on the database. There are 11 companies as Corporate members (80 people). She reported that Crystallography News flourishes, and that the Spring Meeting had 270 registered participants. There were six new exhibitors. The Young Crystallographers sessions had been a great success with about 70 at the sessions. The 2005 meeting has been booked for Loughborough for the 12-14th April. Site visits will be arranged to select the venues for 2006.

7. Treasurer's report. The Treasurer, **David Taylor,** presented a detailed report, subsequently published in Crystallography News. He was asked why the accountants fee had risen by 50%, and said it was due to the extra work required by the Charities Commission. We should not expect the same increase next year. Gift Aid is a useful form of additional income, and so are legacies. Details of both of these are on the website.

Chick Wilson thanked David for his tireless work on behalf of members, and **Judith Howard** proposed that the accounts be accepted. This was seconded by **Chris Gilmore.** The reappointment of the accountant was also approved. David Taylor recommended that the Young Company be reappointed. **Graham Bushnell-Wye** proposed that the meeting accept this, seconded **Sheila Gould.** The discount given on membership subscriptions to IoP members was discussed, and it was noted that the PCG wish to maintain the present position.

The Treasurer finished by saying that he wished to stand down in 2005.

8. Elections to Council.
8.1 John Finney was elected unopposed as Vice-President, proposed **Paul Fewster** and seconded **Judith Howard.** Christine Cardin was re-elected as Secretary, proposed **Harry Powell** and seconded **Andrea Hadfield.**

.8.2. Presentation of prizes.
The Industrial Group poster prize was awarded to **Luciana De Matos,** presented by **Jeremy Cockcroft.**

The PCG poster prize was won by **X.B. Zeng,** (who was not present) presented by **Pam Thomas.**

The CCG poster prize, very generously donated by Oxford Diffraction, was awarded to **Stephen Crawford,** presented by **Simon Parsons.**

The David Blow BSG poster prize was awarded to **A.I. Margiolaki,** with second place going to **Constanze Breitfeld,** presented by **Phil Evans.**

There being no further business the meeting closed at 1745.

Christine Cardin
Secretary to Council

BCA 2005 Spring Meeting - Scientific Programme

THE overall meeting theme of In situ and Non-ambient Crystallography will be addressed in the four plenary lectures that open the meeting, and this theme is strongly evident in many of the parallel sessions, for example In situ Diffraction, Phase Transitions, and Photocrystallography. A session on Modern Techniques in Crystal Structure Refinement will be accompanied by a hands-on CRYSTALS Workshop, and other parallel sessions will explore High-throughput Crystallography, Non-ambient Pharmaceutical Studies, processes and structures At and in the Membrane, and Crystallography in Industry. Throughout the meeting, we will be joined by the X-ray fluorescence community with a parallel programme of talks that should provide something of interest to us all. We also welcome members of the RSC Solid State Chemistry Group, who have been involved in the planning of several of the sessions.

This year's meeting includes the BCA Prize Lecture, given by a crystallographer in honour of an eminent colleague: the Prize Lecturer will be announced later. With the prizewinner also to be announced at the meeting itself, the CCDC Prize Lecture will also be given in plenary session. An innovation this year is an Exhibitors' Forum; this will provide an arena for exhibitors at the meeting to present their non-ambient, *In situ* and other offerings to us. Following the successful teaching sessions last year, there will be a Tutorial Session to introduce the Phase Transitions sessions. There will also be a hands-on CCP14 Workshop.

There will be the usual Commercial Exhibition running from Tuesday to Thursday, and, of course, a poster session. The posters and commercial exhibition will take place in the same area, with a café in the corner of the exhibition hall to aid interactions with and between exhibitors, poster presenters, and participants generally.

Several Satellite meetings will run on the day before and the first morning of the main BCA meeting. Two all day workshops, one on White Beam Techniques, and a hands on computer-based CCP4 Workshop, will run on Monday 11th April. The Monday afternoon will also see ISIS and Daresbury crystallography user meetings, while a further innovation this year is a Joint Facilities User Meeting on the Tuesday morning where issues of common interest to users of the major central facilities will be discussed. If you want to attend any of these satellite events, just tick in the relevant box on the main meeting registration form.

By the time you read this, the Scientific Programme will be complete, and available on the main BCA Webpage at **www.crystallography.co.uk** (for the X-Ray Fluorescence programme at **bca.cryst.bbk.ac.uk/bca/ig/meet5xrf.htm**). Most of the talks have however already been fixed, as set out in the following pages. It's particularly pleasing to see a good number of eminent scientists from outside the UK – this really will be an international meeting.

Plenary Session

In situ and Non-ambient Crystallography

Phil Coppens (SUNY Buffalo, USA)
X,Y,Z and time: introducing the time dimension in crystallographic research.

Malcolm McMahon (Edinburgh)
Pressure induced complexity in the elements.

Herbert Pöllmann (Halle, Germany)
XRD, XRF and in-situ investigations on anhydrous and hydrous cementitious materials - some examples.

John Rafferty (Sheffield)
Structural studies of DNA Holliday junction resolvases.

BCA Prize Lecture
Prize Lecturer to be announced

Plenary Session

CCDC Prize Lecture
Prize Lecturer to be announced

Exhibitors' forum:
Talks by both Crystallographic and X-Ray Fluorescence Exhibitors

Parallel Sessions

***In situ* diffraction**
Co-chairs: **John Evans,** Durham; **Andrew Harrison,** Edinburgh; **Paul Raithby,** Bath; **Jeremy Cockroft,** UCL; **Steve Norval,** ICI.

Matt Rosseinsky (Liverpool)
In situ diffraction in inorganic materials discovery and processing

Poul Norby (Oslo)
In situ synchrotron studies probing the synthesis/application of inorganic materials

Roger Davey (UMIST)
Using x-rays for the *In situ* study of crystallisation processes.

Pam Thomas (Warwick)
Synchrotron X-ray studies of ferroelectrics under applied electric fields

Mark Smith (Warwick)
The use of *In situ* diffraction to probe the processing of amorphous silicate-based materials from gelation to reaction with biofluids

Rudolf Winter (Aberystwyth)
In situ small angle X-ray scattering study of interface morphology in sintered nano-ceramics

Amber Thompson (Durham)
In situ diffraction studies of spin crossover coordination polymers

Andy Dent (Diamond)
In situ monitoring of oxide-supported metal catalysts by energy dispersive EXAFS, infra-red and mass spectroscopy

Simon Redfern (Cambridge)
How P modifies high-T disorder in oxides: observations with neutrons

In situ processing in industry

Co-chairs: **Jeremy Cockroft,** UCL; **Steve Norval,** ICI.

Gordon Tiddy (Manchester)
Surfactant formulation

Geoff Moggridge (Cambridge)
Processing block co-polymers for nano-pores

Simon Jacques (UCL)
In situ crystallisation studies of pharmaceutical materials

Non-ambient Pharmaceutical Studies

Co-chairs: **Anne Kavanagh,** AstraZeneca; **Roy Copley,** GlaxoSmithKline

Jeremy Cockcroft (UCL)
Obtaining accurate non-ambient laboratory PXRD data for pharmaceutical studies

Steve Cosgrove (AstraZeneca R & D)
Probing (de)hydration behaviour by high resolution X-ray powder diffraction

Francesca Fabbiani (Edinburgh)
High pressure studies of pharmaceutical compounds

Angus Forster (GlaxoSmithKline R & D)
The use of X-ray diffraction in the pharmaceutical development of a dihydrate API

Jonathan Burley (Cambridge)
Crystal Structure and Intermolecular Forces from Variable Temperature XRPD

At and in the membrane

Co-chairs: **Neil Isaacs,** Glasgow; **Steve Prince,** Manchester

Bob Stroud (UCSF, USA)
Title TBA

Piet Gros (Utrecht, The Netherlands)
Translocation unit of autotransporter NalP from *N. meningitides*

Steve Baldwin (Leeds)
Membrane protein expression in the genomic era

Crystallography in industry

Co-chairs: **Judith Shackleton,** Manchester; **Mark Farnworth,** Pilkington; **Richard Morris,** Huntsman; **Martin Gill,** Natural History Museum

Peter Laggner (Graz, Austria)
Bridging the nano-gap: simultaneous SAXS and XPD on nanomaterials

Michael Preuss (Manchester)
Residual Stresses in friction welded aeroengine components

Tony Fry (National Physical Laboratory)
Improving methods for analysis of residual stress

Martijn Fransen (PANalytical)
Title TBA

Modern techniques for crystal structure refinement

Co-chairs: **Simon Parsons,** Edinburgh; **Charlie Bond,** Dundee

Richard Cooper (Oxford)
Advanced techniques in structure refinement

Thomas Schneider (Milan)
Refinement of proteins as large small molecules using SHELXL

Garib Murshudov (York):
REFMAC: Recent developments towards automatic refinement

Charlie Bond (Dundee):
What's that blob? Identifying metal ions in protein crystal structures.

Bill David (ISIS)
Beyond least squares

Alan Coelho (ISIS)
TOPAS-Academic, programming ideas

Phase Transitions Tutorial Session

Mike Glazer (Oxford)
Introduction to the science of phase transitions

Phase Transitions

Co-chairs: **Pam Thomas,** Warwick; **Kevin Knight,** ISIS

Jens Kreisel (Grenoble)
Pressure-induced phase transitions in piezoelectric lead-based perovskites

Julien Haines (Montpellier)
Stability of the crystal structures of alpha quartz homeotypes at high temperature and at high pressure

Michael Carpenter (Cambridge)
The role of protons in ferroelectric, ferroelastic and coelastic phase transitions in lawsonite, $CaAl_2Si_2O_7(OH)_2.H_2O$

Laurent Chapon (ISIS)
Magnetic phase transitions

Ivana Evans (Durham)
Structural origin of the oxide ion migration pathway in $La_2Mo_2O_9$

Michael Morris (Cork, Ireland)
In-situ studies of order – disorder phenomena in the synthesis of mesoporous silica

Photocrystallography

Co-chairs: **Paul Raithby,** Bath; **John Helliwell,** Manchester

Jacqui Cole (Cambridge)
Single-crystal X-ray diffraction studies of photo-induced molecular species

Judith Howard (Durham)
Spin cross-over complexes: structures and photomagnetism of high spin, low spin and metastable states and the LIESST effect

Eric Collet (Rennes, France)
The key role of X-ray diffraction for the investigation of photo-induced phase transitions

Beatrice Vallone (Rome, Italy)
Protein structural dynamics observed by time resolved crystallography

John Helliwell (Manchester)
The 15K neutron structure of saccharide-free concanavalin A

High-throughput crystallography: more biology and new drugs

Co-chairs: **Jim Naismith,** St Andrews; **Charlie Bond,** Dundee

Stephen Burley (Structural GenomiX, USA)
Structure-guided fragment based drug discovery

Samar Hasnain (SRS Daresbury)
Combined X-ray approach for studying metalloproteins function/misfunction: A powerful approach to Metallogenomics

X-ray Fluorescence

Co-chairs: **David Beveridge,** Ilford: **Dave Taylor,** BCA

Introducing XRF

Dave Taylor (BCA)
Introducing XRF – what is it and what can it do?

Phil Russell (PANalytical)
What XRF for which job?

Liquid samples

Siân Shore (Shell Global Solutions)
Overcoming cobalt interference in sulphur analysis

Al Martin (RigakuMSC)
Ultra Carry filter, allowing ppb detection levels by WDXRF

Gaetan Deshais (BrukerAXS)
Film 2005. A review of thin films used in XRF analysis of liquid samples.

Steve Davis (PANalytical)
The elemental analysis of grease and the preparation of a suitable specimen for measurement.

WDXRF Applications

David Beveridge (ILFORD Imaging UK Ltd)
Determination of sulphur and chlorine in organic compounds by XRF

Michel Davidts (Socachim-XRF Scientific)
Fusion for better analytical results in XRF analysis

Rainer Schramm (FLUXANA)
Fusion technology for XRF sample preparation

Al Martin (RigakuMSC)
Light element analysis - the benefits of using a 30 micron tube window for B – O

Graham Oliver (CTE, Ceram.)
Status of WDXRF in ceramic analysis

Standards & Calibration

Margaret West (West X-ray Solutions Ltd)
Setting the standards for calibrations

Neil Eatherington (British Geological Survey)
An improved analytical methodology using synthetic standards, fused beads and X-ray fluorescence spectrometry for cements and associated materials

Continued on page 22 >>>

BCA 2005 Spring Meeting 12 - 14 April 2005

	Monday 11 April			Tuesday 12 April		Wednesday	
	SATELLITE MEETINGS						
08.30hrs				SATELLITE MEETING Joint Facilities User Meeting		In situ diffraction General (1)	Photocrystallography 1
10.00hrs				Coffee & Registration		Coffee & Exhibition 1	
10.30hrs						In Situ diffraction Processing in industry	Photocrystallography 2
10.45 hrs	White beam workshop	CCP4 Workshop		Opening Ceremony 10.45			
11.00 hrs				Plenary session 1			
12.00 hrs						AGM: Chemical Crystallography Group	Lunch & Exhibition 12.
12.30 hrs	Workshop/User Mtg lunch			Lunch & Exhibition 12.30 - 13.30 hrs			
13.00 hrs						AGM: Physical Crystallography Group	Crystallography in Industry 1
13.30 hrs	White beam workshop	CCP4 Workshop	ISIS CRY Use Meeting	Plenary session 2		In situ diffraction General (2)	
14.00 hrs							
14.30 hrs							Tea/Exhibi
14.45 hrs							
15.00 hrs				Tea/Exhibition: 15.00 hrs - 15.30 hrs		Tea/Exhibition: 15.00 hrs - 15.30 hrs	Crystallography in Industry 2 15.00 - 16.00
15.30 hrs	White beam workshop: tea & discussion	Tea		CCDC Prize Lecture		In Situ diffraction Central Facilities	
16.00 hrs	Daresbury XRD User Meeting	CCP4 Workshop	ISIS CRY User Meeting	Exhibitors' Forum Crystallography	Exhibitors' Forum XRF		AGM:Industrial Group 16.00 hrs - 16.30 hrs
16.30 hrs							BCA AGM: 16.35 h
17.00 hrs							
17.30 hrs							Prize Lec 17.30 hrs - 1
18.00 hrs							
18.30 hrs	Buffet for Workshops/ User Meetings/Council			Posters & Exhibition 18.30 - 22.00 hrs Buffet & Wine Reception 19.00 hrs			Conference 19.30 h
20.00 hrs							

Loughborough University Timetable of Events

13 April		Thursday 14 April			
At and in the membrane	XRF: Liquid samples	Phase transitions 1 (Workshop)	High-throughput crystallography 1	Non-ambient pharmaceutical studies 1	XRF: Standards & calibration
0.00 - 10.30 hrs		Coffee/Exhibition 10.00 hrs - 10.30 hrs			
Modern techniques for crystal structure refinement 1	XRF Workshop: Awkward samples	Phase transitions 2	High-throughput crystallography 2	Non-ambient pharmaceutical studies 2	XRF: EDXRF applications
00 hrs - 13.00 hrs		Lunch & Exhibition: 12.00 hrs - 13.00 hrs			
Modern techniques for crystal structure refinement 2	XRF: WDXRF applications	Phase transitions 3	CCP14 workshop (hands-on session)		XRF: Combined XRF/XRD applications
AGM: Biol Structs Group					
tion: 14.30 hrs - 15.00 hrs		Tea: 14.30 hrs - 15.30 hrs			
Modern techniques for crystal structure refinement: CRYSTALS WORKSHOP	XRF: Light element analysis				
rs - 17.20 hrs					
ture: 8.30 hrs					
Dinner: rs					

Prior to the Spring Meeting itself, there will be a series of facilities User Meetings, including the SRS XRD and ISIS Crystallography User Groups. A Joint Facilities User Meeting is also planned, with involvement from ILL and ESRF as well as the UK-based Facilities.

SRS XRD User Meeting (11th April)
Organiser: **Mina Golshan,** Daresbury

This meeting will focus on discussion of issues of interest to SRS X-ray diffraction users.

ISIS CRY User Meeting (11th April)
Organiser: **Richard Ibberson,** ISIS

The programme will include reviews by **Steve Wakefield** on ISIS and the TS2 project and **Paolo Radaelli** on ISIS instruments. There will also be presentations on new instruments and instrument upgrades (WISH, HRPD, POLARIS, SXD optics and TS2 instruments), as well as a number of science presentations by users. The meeting will conclude with an open discussion, suggested topics being beamtime access modes, sample environment and software.

<<< Continued from page 19

Ken Field (Oxford Instruments Analytical)
Use of disparate materials for the calibration of an EDXRF spectrometer for the analysis of waste packaging material.

EDXRF – Applications

Leian Grimsley (British Geological Survey)
How does mobile XRFS measure up to contaminated land assessment?

Stanislaw Piorek (R&D Niton, LLC)
Field portable XRF for on-site screening and analysis of prohibited substances in plastics

Martin Teasdale (GlaxoSmithKline)
EDXRF applications in the pharmaceutical industry

Simon Fitzgerald (HORIBA Jobin Yvon Ltd)
Micro-EDXRF and its applications - non-destructive elemental mapping

Combined XRF/XRD applications

Noel Thomas (WBB Minerals, Germany)
Combining XRF, powder XRD and structural modelling techniques: application to plastic clays and kaolins

In addition to the above sessions, there will also be a Workshop on Awkward Samples. The sessions will wind up with an informal discussion session which will allow you to ask all the questions that haven't been answered so far in the sessions. Finally, we will seek your views on the future of XRF within the BCA.

Workshops

CRYSTALS
Organisers: **David Watkin** and **Richard Cooper,** Oxford

This 90 minute workshop complements the Modern techniques for crystal structure refinement session and will include an opportunity to try hands-on examples of difficult data sets that may be encountered from time-to-time.

CCP14
Organisers: **Richard Cooper,** Oxford;
Richard Stephenson, UCL

There will be two hands-on sessions in this workshop. Richard Cooper will provide material for a CRYSTALS session, and Louis Farrugia will put on a WinGX show.

Satellite Meetings

White Beam Techniques
Organiser: **Mina Golshan,** SRS Daresbury

Paul Barnes and **Jeremy Cockroft** (UCL)
Introduction to energy dispersive synchrotron radiation

Simon Jacques (UCL)
Energy dispersive data analysis

Alexander Korsunsky (Oxford)
Engineering applications

Phil Withers (Manchester)
Tomography with white beam

Bob Cernik (Daresbury/ Manchester)
RAPID TEDDI

Shamus Husheer (Cambridge/Daresbury)
Small molecule crystallography with white beam

David Laundy (Daresbury)
Detector statistics in white-beam diffraction experiments

John Helliwell (Manchester)
White beams of SR X-rays and neutrons for Laue protein crystal structure analysis

The Workshop will end with an open discussion.

CCP4 Workshop
Organiser: **Martyn Winn,** CCP4, Daresbury

This will be a hands-on workshop. Tutors include:
Harry Powell (MRC-LMB)
Data processing with Mosflm

Liz Potterton or **Stuart McNicholas** (York)
The CCP4 Molecular Graphics project

Paul Emsley (York)
Coot

Eleanor Dodson (York)
CCP4

Airlie McCoy (Cambridge)
Molecular replacement with Phaser

Phil Evans (MRC-LMB)
CCP4

Martyn Winn (Daresbury)
CCP4

Full workshop details are at: **www.ccp4.ac.uk/courses/BCA2005/BCA_2005_register.html**

Obituaries

Francis Crick 1916-2004

FRANCIS HARRY COMPTON CRICK, who shared the 1962 Nobel Prize in physiology or medicine with James Watson and Maurice Wilkins for discovering the structure of DNA, died July 28th after a long battle with colon cancer. He was 88.

To those who knew him best, it was Crick's insatiable curiosity about life and the creativity of his mind that set up him apart from others. In recent years, he put these qualities to work in an attempt to find the neural correlate of consciousness, a problem he defined as the search for the link between the mind and the brain. Although he was a pathfinder in this young field, he knew that it would take younger minds than his to one day untangle the myriad mysteries of the human brain. When asked what he hoped his future contributions would be, Francis said, "To excite younger people to study the problem of consciousness." Christof Koch, a professor of neuroscience at Caltech and one of Crick's collaborators said "Francis delighted in playing the important role of devil's advocate for several generations of young researchers."

Born in Northampton, England, on June 8, 1916, Francis Crick showed an early curiosity for all things, but for science in particular. To help answer his many questions, his parents Harry Crick and Annie Elizabeth Wilkins bought their young son a Children's Encyclopedia that covered a vast range of topics, from history and music to science. But the subjects that intrigued him the most centered on things like the nature of the galaxy, chemistry and how things were made of atoms. Later, Crick studied physics at University College in London, where he received a bachelor of science degree in 1937. He began studying for his Ph.D., but this work was interrupted by the outbreak of war in 1939. During World War II, he worked as a scientist for the British Admiralty, helping to design magnetic and acoustic mines.

When the war ended, however, Crick found himself less interested in physics and somewhat vague about what he wanted to do with his future. "I still didn't know much about anything so I could go into whatever I wanted," Crick recalled in 1997 during an honors seminar lecture at Rutgers University. "I used what I call the Gossip Test to decide what I wanted to do," he said. "The gossip test is simply that whatever you find yourself gossiping about is what you're really interested in. I had found that my two main interests which I discussed the most were what today would be called molecular biology, what I referred to as the borderline between living and the nonliving, and the workings of the brain."

In 1947, Crick turned to studies in biological research at the Strangeways Laboratory in Cambridge, At that time, Crick knew little biology and practically no organic chemistry or crystallography, however he soon went beyond the fundamentals in each of these areas. In 1949, he joined the Medical Research Council (MRC), and in 1951 met James Watson, a young American graduate student. Two years later the two men used their respective knowledge of genetics and x-ray diffraction, along with x-ray images from Rosalind Franklin and Maurice Wilkins, to determine the structure of DNA. Crick and Watson subsequently suggested a general theory for the structure of small viruses. Later, in research with Sydney Brenner, Crick developed ideas about protein synthesis (the adaptor hypothesis) and the genetic code.

By 1966, sensing that the foundation for molecular biology was adequately set, Crick turned his attention to embryology. Then, in 1976, he joined the Salk Institute for a sabbatical year away from the MRC. The following year, he left the UK for the Salk Institute in La Jolla, CA, where he pursued his interests in understanding the brain and the nature of consciousness.

In the epilogue of his book What Mad Pursuit: A Personal View of Scientific Discovery, Crick says that the brain sciences today are reminiscent of the state of molecular biology and embryology in the 1920s and 1930s. "The brain sciences still have a very long way to go," he writes. "But the fascination of the subject and the importance of the answers will inevitably carry it forward. It is essential to understand our brains in some detail if we are to assess correctly our place in this vast and complicated universe we see all around us." A new Center for Computational and Theoretical Biology at the Salk Institute will bear Francis Crick's name.

Aside from more than 130 published papers in his life, Crick also wrote several books including Molecules and Men (1966), Life Itself (1981), The Astonishing Hypothesis, and The Scientific Search for the Soul (1994). In addition to the Nobel Prize, his honors included the Lasker Award, the Award of Merit from the Gairdner Foundation, and the Prix Charles Leopold Meyer of the French Academy of Sciences. He was a member of the U.S. National Academy of Sciences, the Royal Society, the French Academy of Sciences and the Irish Academy.

Crick is survived by his wife, the artist Odile Speed; two daughters by this marriage, Gabrielle A. Crick and Jacqueline M-T Nichols, both residing in England; a son by a previous marriage, Michael F.C. Crick of Seattle, and six grandchildren. Crick was divorced from his first wife, Ruth Doreen Dodd, in 1947.

Connie Chidester *(reprinted by permission from the ACA Newsletter)*
Photograph by Marc Lieberman/Salk Institute

An historical memoir in honour of Maurice Wilkins 1916-2004

MAURICE (HUGH FREDERICK) WILKINS was born in Wellington, New Zealand on December 15, 1916. His father had moved there from Dublin in 1913 to practice medicine and the family did not return until 1923 thereby missing the horrors of World War I and the coincidental troubles in Ireland during and after the war.

Maurice died on October 5, 2004 at Blackheath, London where he had resided for the last half of his long life. In between there was a good education at King Edward's School in Birmingham and at St John's College, Cambridge where he did not get a good enough degree to be invited to stay on to do research in Physics as he might have wished. The personal and professional consequences were profound. Exploiting his St John's network he got a place at Birmingham where his old tutor, Mark Oliphant, had recently (1937) become Professor and J. T. Randall, newly arrived with his Warren Research Fellowship of the Royal Society, was looking for recruits to do research on the luminescence of solids. The Oliphant connection led to Maurice's wartime participation in the Manhattan Project (1944-5) and his brief first marriage. The Randall connection provided lifelong scientific patronage on a munificent scale as Sir John moved on from his co-invention at Birmingham of the radar-stabilising cavity magnetron to the Chair of Natural Philosophy at St Andrews, then the Wheatstone Chair of Physics at King's College London and the simultaneous Directorship of the MRC Biophysics Unit there. Randall, the abrasive impresario, had to build and develop two new departments (Biophysics as well as Physics) during his time at King's and throughout used Maurice as an emollient deputy, a congenial and important role that he resented only occasionally as he progressed from assistant to deputy director of the MRC Unit, the Chair of Molecular Biology, and eventually succession to the directorship on Randall's retirement (1970).

Along the way something far more exciting happened: Maurice encountered DNA, played a key role in unveiling and establishing its double helical structures and the related ones of some RNAs. For these achievements he was elected to the Royal Society (1959), received the 1960 Albert Lasker award (made to Wilkins, Crick and Watson in that order), and finally in 1962 shared (also with Watson and Crick) the Nobel Prize for Physiology and Medicine. By this time Maurice had re-married and with his new and growing family might have lived happily ever after had not Jim Watson published a provocative, best-seller about the provenance of the DNA double helix. This spawned other hopeful literary monsters in which Maurice, the unassertive third man of the double helix, became a convenient vaudeville villain for those seeking posthumous recognition of another King's physical scientist, R.E.Franklin, who also had contributed to X-ray diffraction studies of DNA.

It has to be understood that the MRC Biophysics Unit at King's was not intended to study macromolecular structures. Its chosen tools would be physical (optical and electron microscopy and spectroscopy), but the targets of its investigations would be supra-molecular (chromosomes, cells and tissues, and motile elements like cilia and flagella). Consequently there was no early investment in X-ray diffraction equipment or personnel. The Wheatstone Laboratory's diffraction expert, A.R. Stokes, was very much a physicist and not a chemical crystallographer. In fact it is not unfair to say that there was a pervasive suspicion of crystals. These were tombs for dead molecules but physicists who had become biophysicists preferred to be seen to be studying more vital systems. It says a great deal for Maurice Wilkins' insight that he was not only one of the first to accept that DNA was indeed the genetic material but on discovering that its gels could be ordered at the molecular level he at once decided to abandon his optical microscopes for the higher resolution probe of X-ray diffraction.

Despite the local practical difficulties, he and R. G. Gosling were able to produce by the summer of 1950 a well-oriented and polycrystalline specimen of what we now call A-DNA. It was an early version of its diffraction pattern (Fig.1) shown by Maurice at a meeting in Naples in the Spring of 1951 that so excited J. D. Watson with the prospect that gene structures might be simple and crystallisable. Stokes and Gosling determined the unit cell dimensions of A-DNA (a=22, b=40, c=28Å, β=97^{o}) and accurately assigned the monoclinic space group *C*2. These dimensions imply that in projection down the fibre axis the polymer molecules are packed on an approximately hexagonal net of spacing ~22A and the space group symmetry implies that the evenly spaced molecules would have to consist of pairs of chains related by diad axes in the plane of the net. In retrospect it is difficult to imagine a committed and well-trained crystallographer looking at space group no.5 in International Tables and not concluding that the A-DNA unit cell would contain 4 quasi-identical polynucleotide chains, diadically paired and packed like a bundle of cylinders of 22Å diameter. Of course the bundled chains could not be cylinders exactly but spirals with 11-fold screw symmetry as indicated by the absence of meridional X-ray reflexions until the appearance of the diagnostic 0,0,11 reflexion that is so prominent at the top of Fig.1. As every crystallographer would know: an 11-fold screw axis could not be a crystal symmetry and therefore it would have to be a molecular property!

If DNA was indeed the genetic material, then the information it contained would have to be complex at some level of resolution, but here again classical crystallographers should not have been dismayed by the apparent simplicity of the A-DNA crystal structure. Crystalline minerals excited much attention both before and after the discovery of X-ray diffraction. The bewildering complexity of their chemical compositions was a challenge until it could be shown by X-ray crystallography that relatively few three-dimensional structural motifs of alumina and silica could accommodate a wide variety of chemical variation. DNA presented an analogous challenge: how might the constituents of

chemically diverse polynucleotides form isomorphous components that might vicariously replace one another in a simple regular structure like a helix. This was the problem addressed directly by the biologist J.D.Watson and solved by his discovery of base-pairing after some crucial advice about tautomerism from the chemical crystallographer Jerry Donahue. Of course a demonstration model had to be built to show that Watson's base-pairs could be accommodated in a double helical cage with the correct overall dimensions but it is fair to say that such niceties would be of little interest to molecular biologists for whom the duplex nature of DNA and the complementary base pairing would be the key revelations.

All this happened at Cambridge while the London DNA effort was taken on a bizarre detour into the desert of crystallographic orthodoxy by recruitment of R.E. Franklin, a physical chemist with just enough X-ray diffraction education obtained while studying coal and coke to be full of wise saws and modern instances concerning X-ray structure determination in general. Pre-war methods were out. Too often these had used heuristic methods to produce preliminary models of unit cell contents from which were obtained a preliminary set of X-ray phases that were slowly improved by a succession of Fourier syntheses of electron density and sometimes the introduction of yet more chemical insights. By 1950 X-ray crystallography was on the threshold of its robotic, triumphalist stage: with better computational methods and more sophisticated diffraction theorems, number-crunching of the intensities alone would solve the phase problem and produce structures needing no further authentication because no chemical prejudices had tainted their genesis. More experienced experimentalists might prefer to retain a choice of horses for courses and and give priority to getting the right answer rather than to the use of currently correct methods. This kind of thinking was now anathema at King's.

Another unhelpful contribution involved a second allomorph of DNA, B, which can also be uniaxially oriented and persuaded to be polycrystalline in fibers (Fig.2) which have the appropriate combination of hydration and retained salts. Preliminary experiments by Franklin suggested that A-DNA was a 'dry' form although later polymer studies and current oligonucleotide crystal structures show that A-DNA-like structures are just as hydrated as B-like duplexes. But at the time the erroneous 1950s conclusion caused A-DNA with its straightforward crystal symmetry to be relegated to the role of a laboratory artefact while much energy was diverted to crystallizing B-DNA, the 'wet' and therefore more 'biological' form. Only when RNA duplexes were discovered to have A-like conformations (Fig.3) was A-DNA rehabilitated as a canonical structure.

The Watson and Crick eureka at Cambridge must have disappointed Maurice at the time but no one who knew him well would have expected him to be other than pleased with the outcome. He certainly was more committed to getting the right answer than to following fashionable procedures. It was ironic therefore that his next role in the DNA saga was the problem of authenticating the

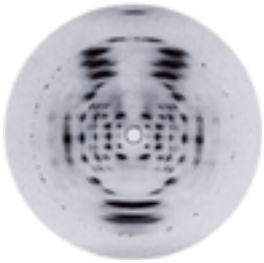


Fig.1. *A-DNA diffraction with the fiber tipped into the X-ray beam to record the 0,0,11 reflexion dignostic of the 11-fold screw symmetry of the molecules.*

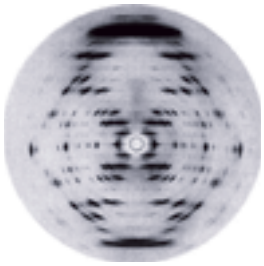


Fig.2. *B-DNA diffraction indicating 10-fold screw symmetry and an overall structure very different in detail from that of A-DNA.*

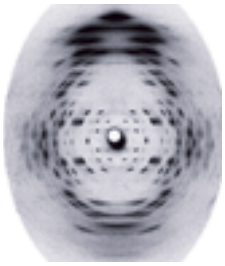


Fig.3. *Diffraction from a fiber containing 12-fold RNA helices with conformations similar to A-DNA.*

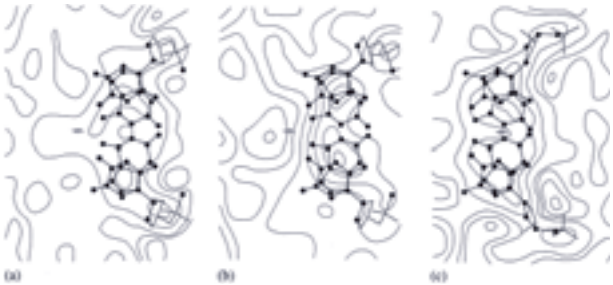


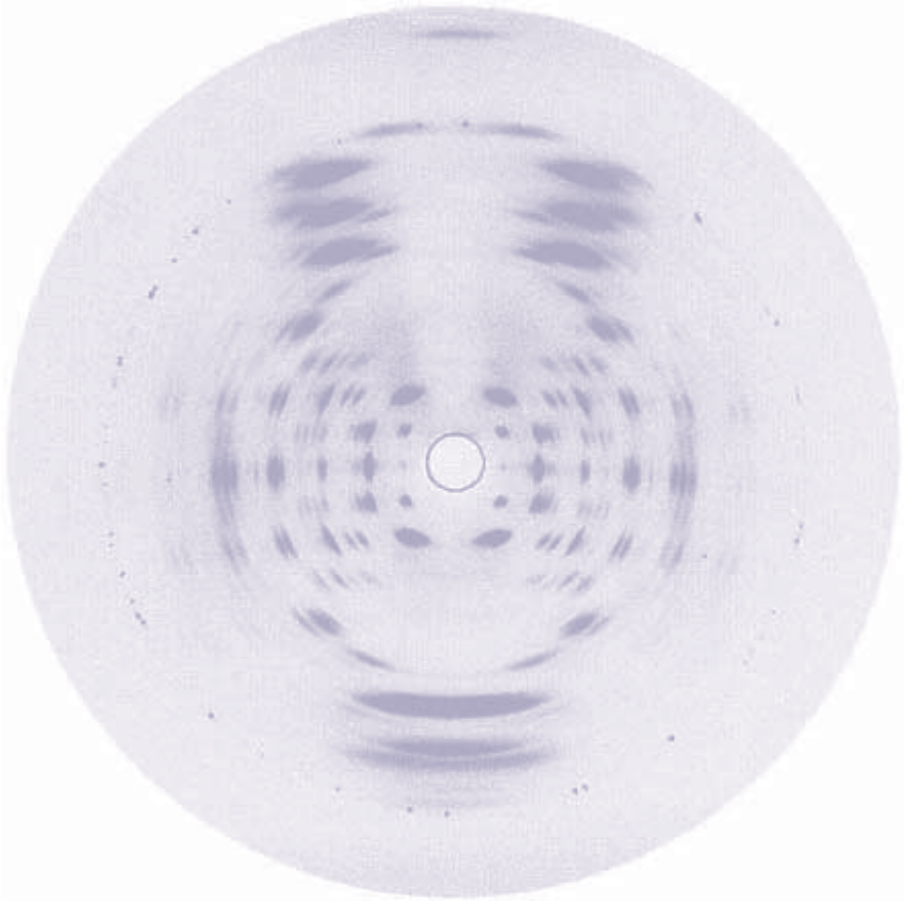
Fig.4.(a) *The electron density distribution in the plane of an (average) Watson–Crick base-pair obtained with diffraction amplitudes for B-DNA and phase angles calculated from the original Crick-Watson demonstration model. The image shows not only the (expected) low resolution but also a poor fit with the model.* ***(b)*** *The corresponding difference map reveals the major geometrical flaw in the model is the position of the base-pairs relative to the helix axis.* ***(c)*** *A model with the correct deoxyribose conformations and other refinements shows a better fit with the new electron density map.*

Watson-Crick hypothesis, and doubly ironic that a subtle property of A-DNA was the ghost in the machine. The stereochemically reasonable model that Crick and Watson built to reinforce the plausibility of their conjecture was designed to be a model of B-DNA. Such was their attention to precise detail that the 5-membered deoxyribose rings in their model not only had accurate bond lengths and angles but they also were puckered and not planar as observed in Furberg's pioneering crystal structure of the nucleoside cytidine at Birkbeck. There are essentially two ways in which deoxyribose rings can be puckered, C3'-endo and C2'-endo. Both are observed in polynucleotide duplexes; the former in A-like structures, the latter in B-like structures. The macroscopic consequences of these local conformational differences are quite profound. A-type structures have their base-pairs about 4Å nearer the surface of their double helices than B-type structures and therefore have a deep groove and a shallow groove in contrast to B-DNA's more similar grooves. None of this was fully and explicitly understood until many years later so it was especially unfortunate that Furberg's cytidine had the C3'-endo-puckered rings appropriate for A-DNA but not for B!

Thus in 1953, Franklin having left King's for Birkbeck, Maurice Wilkins was once again in sole possession of the DNA diffraction problem but with a new and agonizing twist. There now existed a stereochemically entirely plausible structure for B-DNA that rationalized a great many biochemical observations and clearly suggested how nucleic acids might function biologically, yet this attractive structure provides X-ray intensities profoundly at odds with those observed. The R = 90% discrepancy was nearly twice as bad as that which textbook theory predicted for a completely wrong structure. Such a discordance was too provocative to be ignored but it was to take nearly a decade of improvements in computation, in preparing well-oriented and polycrystalline specimens, in perfecting X-ray cameras for the special needs of fiber diffraction, and in developing new methods of structure refinement before the structures of DNA were fully refined and brought into concordance with all the diffraction data. There was however an additional dividend from Maurice's investment: there could now be rapid analyses not only of fibrous DNAs but also of RNAs and many other spiral structures found with peptide and carbohydrate polymers that did not form single crystals but were of biological or industrial importance.

Maurice Wilkins' early acceptance of DNA as the genetic material and his recognition that it had structures that could and should be tackled by X-ray diffraction analyses, not necessarily under his exclusive control, was important in ensuring that the essence of DNA's structure was discovered as early as it was. His success in resolving patiently and effectively all the technical problems, great and small, that arose unpredictably in the course of his own work on DNA and RNA was substantial. His pacific acceptance of the slings and arrows that unjustly assail those involved in momentous enterprises was typical and showed a life that had a certain style as well as much substance.

Struther Arnott



Books

The Science and Technology of Undulators and Wigglers

James A. Clarke
Oxford Series on Synchrotron Radiation, 4;
Oxford Science Publications, 2004
Price: £85.00 (hardback)
ISBN 0198508557

SYNCHROTRON RADIATION is produced when an electron beam in a storage ring is deflected, and hence accelerated, by some type of magnetic insertion device, such as an undulator or a wiggler.

This two hundred and thirty page text, number 4 in the Oxford Series on Synchrotron Radiation, starts at a level appropriate to a complete novice, explaining the history and outlining the physics behind such insertion devices in a clear manner. However it swiftly shifts up a gear mathematically, considering the form of synchrotron radiation from a bending magnet (Chapter 2), multipole wiggler (Chapter 3) and undulator (Chapter 4). These are not chapters for the faint hearted, but the explanations start at an appropriately simple (undergraduate) level, and can readily be followed by the more mathematically intrepid. In fact, with graphs given of all the key results, the essentials of the form of the photon flux shape, critical energy, brightness and power generated in each of these cases is readily accessible to all. This is expanded upon in Chapter 5, where a variety of numerical calculations are used to look at the flux obtainable in a range of cases.

The emphasis of the book then shifts into more practical areas. Some of the different insertion devices are introduced in Chapter 6, which uses a mixture of theoretical work and discussion to investigate the types of polarised light which can be produced from each. Chapters 7 to 9 look at the actual construction and installation of these devices. Firstly the advantages and engineering difficulties of using permanent magnets (Chapter 7) or electro-magnets (Chapter 8) are discussed, with many references to undulators and wigglers in use at various synchrotron sources. Chapter 9 considers the different methods for measuring the magnetic fields from both insertion devices and their component blocks, and, building on an earlier section on end design, shows how such results can be used to minimise any disruption to the electron beam and to provide the best possible flux. The effects of insertion devices on the electron beam are considered in more detail in Chapter 10. The fact that this chapter assumes a certain level of knowledge makes it less suitable for the interested novice, although again figures are used to illustrate all of the major points.

Chapter 11 briefly covers the role of undulators in free electron lasers. The book concludes by looking at less standard insertion devices that have been tried, together with some ideas for future devices.

The text has a reasonably useful index, and a helpful number of references. The author has tried, and largely succeeded, to avoid using jargon or terms without defining them. However the nature of the material means that there is not a single natural route through the text, and a glossary might have been useful to enable the more casual reader to dip into the book.

This fact-packed book covers the wide breadth of science underpinning the design and installation of undulators and wigglers in synchrotron radiation sources, and provides an invaluable source for those working in this field. Its direct value for the average crystallographer is less clear, as it concentrates on the devices themselves, rather than why their particular properties are useful in the design and execution of instruments and experiments.

C.C Wilson and **V.M. Nield**

X-Ray and Electron Diffraction Studies in Materials Science

D J Dyson
Maney 2004 368 pages
Price: £78 (hardback)
ISBN 1902653742

IT is good to see a new book on x-ray and electron diffraction aimed at the less experienced analyst working in a materials laboratory that will also find use as an undergraduate learning aid.

Supplying the units in formulae throughout the text is welcomed and will assist more detailed calculations. The author draws on his 40 years experience in the steel industry to add a wealth of real examples to illustrate the subject. The text covers a wide range of topics including useful sections on texture and electron diffraction which add to a balanced overview of the subject and its everyday application to Phase ID, quantitative and size strain analysis. The book is well supported with photographs and clear diagrams which complement the text as do comprehensive references.

The first half of the book has sections on; real space, crystal chemistry, intensity of diffraction, stereographic projection, instrument consideration and line profiles which provide a good grounding in the basics of crystallography and the theory of diffraction. The first chapter (p1-44) on Real Space gives a very clear introduction, through symmetry, lattices, space groups to Bragg's law, of the basic crystallographic concepts needed for a full understanding of diffraction.

The second chapter (p45-76) on Crystal Chemistry encompasses the packing of atoms within the crystal structure, building up from simple to complex inorganic systems and covering interstitial phases, metallic glasses and silicates. The next chapter on Intensity of Diffraction (p77-98) covers the factors which influence the intensity of a reflection and the equations needed to calculate its intensity, focussing particularly on the cubic system. The fourth chapter provides a useful explanation of Stereographic Projection (p99 -114) underpinning its use in later chapters. The next chapter on Instrument Considerations (p115 - 135) covers just the basics for x-ray diffraction and offers simple practical information on instrument parameters. The sixth chapter is devoted to Line Profiles (p136 – 160) and explains the factors which affect the size and shape of diffraction peaks and offers useful advice on the use of peak fitting routines.

Chapter 7 sees a move into applications and covers Phase Identification (p161 - 189). It starts with peak location and associated errors, moves on to intensity and then identification. It has sections on precision, reference materials and the figures of merit used to scale database searches. The next chapter covers Quantitative Analysis (p191 - 234) and starts with validation which is becoming increasingly important as we strive for standardisation. It covers sampling and preparation, instrument considerations specific to quantitative work and the various procedural methods. Particular cases are studied including: airborne dusts, glassy phase, metals and clay minerals. This chapter is supported by 44 references, more than any other. Chapter 9 covers Crystallite Size Analysis (p235-248) and offers practical advice on the various methods and their application. The next chapter covers the specialised field of Thin Layers (p249-271) and introduces the use of high resolution equipment and is followed by Crystallographic Texture (p273 - 317) which is well supported with useful pictures and diagrams which help put across what is often a difficult subject in a comprehensible way. A section on Electron Backscatter leads on to the final chapter on Electron Diffraction and its Relation to XRD (p319 - 354). Here theoretical aspects including the reciprocal lattice are interspersed with practical explanations and comparisons to provide a useful grounding in understanding the complementary nature of the two disciplines.

All laboratories working on the everyday applications of x-ray and electron diffraction will find this book a useful addition to their bookshelf.

Dave Taylor

International Tables for Crystallography

Volume A1: Symmetry relations between space groups

Hans Wondratschek and **Ulrich Müller,** Editors
Published for the International Union of Crystallography by Kluwer Academic Publishers: Dordrecht/Boston/London, 2004
Price £155, Euro240, $250 (institutions/libraries) half-price for personal use.
ISBN 1-4020-2355-3, 731 + xii pages

THIS extensive supplement to Volume A of International Tables has now appeared, and is almost as long as the volume itself.

As it is an extension of the tables of sub- and supergroups in Volume A, it might be assumed to be for a very small number of specialists. In fact, it should be useful for a wide variety of crystallographers. The book is divided into three parts. The first is a historical and mathematical introduction to the tables (40 pages). The second goes through the 2- and 3-dimensional space groups in tables similar in format to those in Volume A, giving tables of maximal subgroups and minimal supergroups, with a useful set of graphs (290 pages). The final part is again a table of space groups, this time relating the Wykoff positions of sub- and supergrpoups (295 pages). The two sets of tables are illustrated, the first inside the front and the second inside the back cover, with helpful short guides. As with all volumes, the typesetting is clear and attractive, and the explanations, though demanding, are full and worth reading!

Fundamental to the organisation of the tables is the distinction between t-groups and k-groups, (here invariably given their full German names with an inflexional "e" on the end). In the first, the unit cells of the two groups are the same, while in the second, the crystal classes are the same, and a maximal subgroup or minimal supergroup must be one or the other.

With the rapid rise in the number of crystal structures determined, chemical crystallographers will increasingly need to compare structures whose similarities are masked by different space groups. For example, recently I had to compare two very similar structures in $P2_12_12_1$ and $P2_1/n$. The relationship became clear when it was seen that these are both maximal t-subgroups of *Pnma.* The tables proved very useful, as they neatly relate the origin shifts and alteration in vectors required.

While this book is certainly not light reading in any sense, it will prove a valuable tool to a wide range of crystallographers.

Bob Gould

Mathematical Techniques in Crystallography and Materials Science

Edward Prince
Springer-Verlag, Berlin, Heidelberg and New York. 3rd Edition, 2004
Price: £30.50 (paperback).
ISBN 354021111X , 224 pages.

PRINCE'S book, Mathematical Techniques in Crystallography and Materials Science, is something of a 'Desert Island' book for crystallographers, and is amongst the most important texts available in computational crystallography. Springer have now released a Third Edition, though there seem to be few, if any, differences between this and the Second Edition published in 1994. However, the book is now available in paperback costing about £30, instead of over £60 for previous hardback editions.

The book starts with a revision chapter on matrix algebra; rotations of axes, Euler angles and the metric tensor are also discussed. Chapters 2 and 3 are about symmetry, covering point groups and then developing the concepts to repeated patterns and space groups. The basics of vector algebra are covered in Chapter 4.

The material in Chapters 1-4 is mostly also available in other text-books, including for example, Giacovazzo's Fundamentals of Crystallography. Prince's book is indispensable because of what is presented in the later chapters. Chapter 5 covers tensors. More exhaustive treatments of tensor methods, with all the ramifications of co- and contra-variance, are available elsewhere, particularly in Sands' Vectors and Tensors in Crystallography. However, Prince's development of the concept of the normal distribution into a discussion of anisotropic thermal motion is particularly lucid; the discussion is developed to include higher-order models of thermal motion. Rigid body motion and the TLS model is also covered, and also extended to cover higher order terms.

Chapter 6 is entitled Data Fitting, and starts with a justification for the use of least squares. The concepts of robustness and resistance and their implementation in crystallographic weighting schemes are very clearly described, though it would have been nice at this point to have included an example or two to illustrate the effect of a robust-resistant weight-modifier on a refinement, or even to have included a reference to the author's own work in this area. Indeed, this is a more general criticism of the book, which would greatly benefit from more numerical examples and literature citations. The value of numerical illustration is evident in the following section on minimisation, in which a linear least squares example is given. The same example is developed in later chapters in sections on estimation of uncertainty (Chapter 7), correlation and the projection matrix, greatly enhancing the clarity of the text.

Chapter 8, entitled Significance and Accuracy, contains a superb discussion of correlation and methods for treating correlated refinements. It also contains a section on the projection matrix, and a description of a method for finding out which reflections are most influential for determining the precision of selected parameters. Chapter 9 deals with constraints in refinement, and includes a section on the use of rigid body constraints on thermal motion. The latter reflects Prince's work in application of the TLS model during refinement. The final chapter concerns fast Fourier transforms. There are, in addition, a number of useful appendices including listings of matrices for generating sub- and superlattices, symmetry constraints on tensor components and some useful computer subroutines. It would have been useful for the last of these to have been made available electronically.

Prince has written one of the finest accounts available of crystallographic least squares, and every graduate student should own a copy. The book makes no claim to be exhaustive in other areas of mathematical methods, however, and techniques such as simulated annealing, crystallographic uses of spherical harmonics or uses of quaternions are not discussed. Since these (and numerous other) techniques have become quite common in software, there might be scope for including some of them in future editions of this excellent book.

Simon Parsons

News from the Groups

PCG Winter Meeting

Neutron Scattering from Biological Systems

The winter meeting, hosted at Cosener's House, Abingdon, on 13-14 December, 2004, gave a broad overview of the contribution of neutrons to biology, with particular emphasis on neutron protein crystallography, neutron fibre diffraction.

It dealt with small-angle neuton scattering (SANS) and reflectometry from systems such as enzymes, amyloids, membranes, proteins absorbed on surfaces, drug delivery vehicles, biosensors and many more. Nine talks were given by a series of expert speakers, and there were many beautiful posters throughout the meeting. These topics were quite specific and very useful to me, a beginner who has only used SANS once before. They gave me many ideas of how neutron scattering techniques could be used in biological systems. The first talk, 'The structure of troponin from skeletal muscle' was very interesting, **Peter Timmins** talked about Biology and the Millennium program at ILL first, and then introduced his work on using SAXS and SANS to investigate the structures and interactions of Troponin.

The lecture 'Supramolecular architectures in matrix biological tissues' given by **Tim Wess** was one of the most interesting and useful talks I found in the whole meeting, for it was closely related to my project. Some of his work on fibrillin, cellulose and collagen inspired me especially, as I may do some research on these materials later. 'Neutron reflectivity studies on DNA-membrane interactions' presented by **Jayne Lawrence** was another topic I was interested in, she chose zwitterionic lipids as ideal nonviral gene delivery vectors, and used Raman spectroscopy and neutron reflectivity to probe the interactions of DNA and phospholipids monolayer with and without Ca^{2+}, these interactions between DNA and the artificial bio membrane are being studied to investigate the fate of DNA in the cell. The talk 'Recent Results from LA(ue)DI(ffractometer)' by **Matthew Blakeley** was also very good, he gave some introduction to neutron crystallography and LADI and then described the work on saccharide-free concanavalin A at 15 K using neutron diffraction.

The material in some of the talks was challenging; overall the conference was very instructive, stimulating and successful.

Yuan Wang
University of Bristol

The 62nd Annual General Meeting

of the Physical Crystallography Group of the British Crystallographic Association and Structural Condensed Matter Group of the Institute of Physics

13:00 Wednesday 13th April 2005, Loughborough

1. Apologies for absence
2. Minutes from the 61st AGM held at UMIST, 7th April 2004
3. Matters arising from minutes
4. Chairman's report
5. IOP matters
6. BCA matters
7. Secretary/Treasurer's report
8. Elections to PCG/SCMP committee
9. Future Meetings
10. New Activities
11. Any other business

Elections to Committee

There are vacancies arising for Chairman, Vice-Chairman, Honorary Secretary and Ordinary Members. The committee will seek the approval of the AGM to co-opt the Secretary/Treasurer for a further 12 months to provide continuity amongst the officers. Nominations (with name of seconder and note of acceptance from the nominee) for any of these positions should be sent to the Honorary Secretary (**john.evans@durham.ac.uk**) by April 1st, or communicated to him in person at the 2005 BCA Spring Meeting.

Current Committee

Title	Name	Grade	Since
Dr	**Pam Thomas**	Chairman	2002
Prof	**Paolo Radaelli**	Vice Chairman	2002
Dr	**John Evans**	Honorary Secretary/ Treasurer	2002
Dr	**Jeremy Cockcroft**	Ordinary Member	1999
Dr	**Jon Wasse**	Ordinary Member	2002
Dr	**Jon Loveday**	Ordinary Member	2003
Dr	**Tom Lyford**	Ordinary Member	2003
Dr	**Mina Golshon**	Ordinary Member	2004
Dr	**Andrew Wills**	Ordinary Member	2004
Dr	**Jonathan Wright**	Ordinary Member	2004

Minutes of the 61st Annual General Meeting

of the Physical Crystallography Group of the British Crystallographic Association and Structural Condensed Matter Group of the Institute of Physics

14:30 Wednesday 7th April 2004, UMIST

There were 16 members present. Committee members present: **Pam Thomas, Paolo Radaelli, John Evans, Tom Lyford, Dave Allan**

1. **Formal apologies** for absence were received from **Steve Collins, Jon Wasse, Jon Loveday** & **Jeremy Cockcroft.** Informal apologies were later received from many group members who had been unable to attend the meeting due to an unfortunate timetable clash with other scientific sessions.

2. **Minutes** from the 60th AGM held at Nottingham were circulated and accepted.

3. There were no **matters arising** from the minutes.

4. **Chairman's report:**
   a. Autumn meeting on "Probing Structure at the Nanoscale" organised by **Jon Wasse** and **Paolo Radaelli** had been extremely successful and well attended and was written up in Crystallography News.

   b. Scientific sessions at the BCA spring meeting on incommensurate structures had also been extremely well attended.

   c. As discussed during the 60th AGM at York, the group had focussed in 2003-4 on teaching activities by organising sessions on symmetry at the BCA spring meeting and a residential Rietveld refinement school on 16th/17th April at Birkbeck College.

   d. There had been strong competition for the Panalytical Physical Crystallography prize which was awarded to **Dr Andrew Wills** for his work on the symmetry aspects of magnetic structures.

   e. It was proposed that in future the Physical Crystallography prize would be awarded every two years and would be sponsored by the PCG/SCMP. The prize will be increased to £750. This proposal was agreed unanimously.

   f. A proposal was made to instigate a £500 annual prize for the best Ph.D. thesis featuring physical crystallography. This proposal was agreed unanimously. Final details of the submission procedure and eligibility will be decided by the committee. Panalytical have agreed to fund this prize. Action: PCG/SCMP committee.

   g. The issue of SCMP members receiving a £3 discount when joining the BCA was discussed. The meeting felt strongly that this should be retained. Action: JSOE/PT to raise with council. [a course of action whereby the PCG/SCMP block pay the BCA the £3 discount was later agreed with the BCA treasurer and ratified by council]

5. **IOP matters**
   a. Paolo Radaelli has been nominated by the PCG/SCMP committee to serve on IOP Conference Committee.

   b. Financial issues/budget capping in 2003 were discussed.

   c. Paolo Radaelli was unanimously voted to represent the group at CMMP division level.

   d. Possibility of increasing interactions with the neutron scattering group of the IOP via a joint meeting on neutrons in biology was discussed.

   e. There was no other IOP business.

6. **BCA matters**
   a. BCA subscription mechanism/rate for IOP SCMP member were discussed during the chairman's report.

   b. The committee will nominate honorary members of BCA.

   c. There were no matters arising from BCA council.

7. **Secretary/Treasurer's report**
   a. Accounts were presented and accepted by the meeting (Proposed: **Mike Glazer;** Seconded: **Tom Lyford)**.

8. The chairman expressed a strong vote of thanks to **Dave Allan** and **Steve Collins** for their contributions to the PCG/SCMP during their terms of office and for organising several meetings and scientific sessions on behalf of the group. **Jon Goff** was also thanked for his contributions. New members elected to the committee were:

   Mina Golshan, Proposed: Steve Collins; Seconded:Pam Thomas

   Jon Wright, Proposed: Paolo Radaelli; Seconded: John Evans

   Andrew Wills, Proposed: Jeremy Cockcroft; Seconded: Dave Allan

9. **Future Meetings**
   a. 34 students have registered for the SCMP/PCG/CMSD co-sponsored workshop on Rietveld refinement to be held April 16th at Birkbeck. Tutors: **Jeremy Cockcroft, John Evans, Ivana Evans, Kevin Knight.**

   b. Autumn/Winter meeting 2004 proposed topic: proteins/neutrons/biophysics. Action: PGR.

   c. BCA 2005 theme will be "*in situ*/non-ambient". Proposed PCG/SCMP activities to include a session of phase transitions; *in situ* with solid state chemists; light/field induced with CCG. Action: JSOE/PT to attend planning meeting

   d. Tom Lyford will consider the possibility of a diffuse scatter/thin films workshop for a future meeting (possibly in collaboration with the Industrial Group). Action: TL.

   e. A second magnetic Rietveld workshop for winter 2004/spring 2005. Action: PGR/AW?

10. **New Activities** were discussed under Chairman's Report/Future Meetings.

11. **Any other business**
   a. The issue of speakers for IUCr 2005 was discussed and later raised at the BCA AGM. Suggestions to **Bill David** (**W.I.F.David@rl.ac.uk**).

   b. The completeness of PCG/SCMP mailing lists was raised. Action: JSOE to check current lists.

Industrial Group Autumn Meeting: DIY Crystallography

FORTY delegates from UK Universities, Commercial and Industrial institutions attended this one-day meeting, organised by the Industrial Group of the BCA at Birkbeck College on 4 November 2004. The meeting was organised into two main sections – Hardware and Software. The speakers addressed the Do-It-Yourself aspects of crystallography which are widespread in the field due to the specialised nature of many activities which are not easily catered for in commercial instruments and software.

The hardware group: *Chiu Tang, Olivier Leynaud, Ellen Heeley, Mark Farnworth and Jamie Nelson.*

The software group: *David Beveridge, Christopher Hall, Ron Ghesh, Richard Stephenson, Robin Shirley and Richard Cooper.*

Building a High-Resolution Powder Diffractometer

(Chiu Tang, DIAMOND)

The synchrotron will have a 'medium' electron beam energy of 3.0GeV. The storage ring has a diameter of 561.6M and it has more than 20 bending magnets. Chiu showed a number of photographs obtained by a colleague flying a model helicopter containing a camera over the site! With 3 diffraction circles its design is highly versatile. The sample chamber is large (40x40x40 cm^3) and there is a high precision, heavy-duty, xyz table.

Oscillating a sample for in-situ furnace studies

(Olivier Leynaud, Birkbeck College, UCL)

The project is focussed on in-situ experiments using gasses or vacuum at high temperatures. The furnace needs to be able to heat up to 950C and needs to accommodate capillaries with diameters up to 2mm. Different types of oscillating systems were investigated to oscillate, backwards and forwards, capillaries in the furnace: polarity, piston, wheel-like and it was the latter that was selected. Olivier showed some photographs of the completed device. The device oscillates at 68rpm with a 12V battery.

Industrial Polymer Processing Studies using Combined SAXS/WAXS Techniques

(Ellen Heeley, Polymer Centre, University of Sheffield).

Ellen began by saying that there is extensive use of polymer films in packaging. Texture is developed during processing but the nucleation in crystallisation is still largely a mystery. Ellen can record Small Angle X-ray Scattering (SAXS) and Wide-Angle X-ray Scattering (WAXS) data at the same time, which can be combined with rheology studies. The main areas for research are quiescent (slow processes) and sheer induced crystallisation / orientation.

Multiple Sample Holders

(Mark Farnworth, Pilkington plc).

Mark described two multi-sample holders for the PANalytical Materials Research Diffractometer that he had designed and then had fabricated out of aluminium plate. Use is made of the batch programming software in X'Pert Data Collector. Sample *x, y,* and *z* values and the name of the data acquisition program are entered into the 'batch' program. *Z*-values for each sample are determined in the conventional manner, using the dial contact gauge. Mark explained that the plate dimensions had to be carefully calculated to avoid contact with the primary optics and the sample stage.

A Multi-Sample X-ray Diffractometer with Photographic and Counter Recording

(Jamie Nelson, Gemmological Instruments).

Jamie described the work that he had carried out on the Debye-Scherrer photographic camera. His passion for tinkering with the camera, attaching items such as proportional counters, eventually led to him to receive Fellowship of the Institute of Physics. Jamie described several aspects of diffractometry hardware and used, for a relatively younger audience, unfamiliar terms such as Hole, Slot and Plane mounting or the 'Kelvin Mount'.

MATLAB: A Software Tool for Quick Data Analysis

(Christopher Hall, University of Edinburgh)

Christopher described his use of MATLAB 7. He finds several features particularly useful. These include good data input/output, built in utilities and functions, scripting (the stitching together of MATLAB commands into small programs) and a good graphic environment for reports and producing a common 'house' style. Christopher has built up a collection of scripts and utilities for handling synchrotron diffraction data – called XMAT.

Sharing Software Toolkits (Ron Ghosh, ILL)

Ron explained that over the last thirty to forty years there have been numerous computer languages from 'Plot 10' in the 1960's to modern day 'Windows'. Many of the packages have individual scripting languages and so this, and other complications, often deter the 'novice' from getting involved. He gave a simple demonstration of the use of Fortran for data display, plotting and filtering routines. Individual peaks can be selected for analysis e.g. line broadening. Ron finished the presentation by giving a number of useful internet links (see web version of report).

DIY Single Crystal Structure Analysis

(Richard Cooper, University of Oxford)

Richard described the use of the 'Crystals' package for the analysis of single and twinned X-ray/Neutron Diffraction data. There are three main areas, Guidance, Validation Criteria and Tools. The Guidance step covers data collection (initial *hkl* analyses), early refinement, getting a complete model, later refinement, weightings and publication. The script language can access any crystal data or results. The Cambridge Structural Database (CSD) can be used to validate chemical geometry.

CCP14 Developments

(Richard Stephenson, UCL, Birkbeck College)

The CCP14 website at **www.ccp14.ac.uk** contains freely available software, including state of the art algorithms and utilities. There is a concentration on crystallography. User feedback optimises the direction of the project. CCP14 contains multiple single crystal suites and multiple powder indexing programs and suites. It has 60GB of software and help files and has 35,000 monthly hits. It has a 'wiki' component (!) by which users can add comments that can be edited by any other user. Thus, the quality of the data is continually refined and improved.

Making do without the JCPDS

(David Beveridge, Ilford).

David gave a series of steps that could be used to identify a diffraction pattern without the use of the JCPDS database. A good prior understanding of the sample would be ideal since this could drastically reduce the number of options for identification. A local library of patterns from reference materials can then be used for the search. A good understanding of the crystalline components in common materials would also be helpful. For example, paints contain rutile and anatase titania, kettle fur, soil and building dust contain calcium carbonate

(calcite) whereas plaster contains hydrated calcium sulphate (gypsum).

CRYSFIRE Update (Robin Shirley, University of Surrey)
Indexing a powder pattern may only be a 6-parameter problem, but can still be a challenge. While methods of treating data have improved greatly, there is still great reliance on high data quality. Robin described the new CRYSFIRE, which now includes ten indexing programs with different approaches, and gives figures of merit for 10 or more indexing patterns. The newest version works with Windows XP.

Mark Farnworth
Pilkington European Technical Centre

Industrial Group AGM

THE 22nd ANNUAL GENERAL MEETING of the Industrial Group will be held at Loughborough University.

There is one vacant post on the Committee to serve for three years from April 2005.

Nominations, which shall be proposed by not less than two members of the Group and shall be accompanied by the written consent of the nominee, shall be sent to reach the Honorary Secretary of the Group not later than seven days before the Annual General Meeting.

A nomination has been received & seconded for **Dr Royson Copley** of GlaxoSmithKline R & D Ltd.

If you wish to nominate a candidate for the Committee, or raise an item on the agenda, please contact,

Judith Shackleton,
Secretary Treasurer BCA Industrial Group,
Materials Science Centre,
Grosvenor Street,
University of Manchester,
Manchester, M1 7HS.
0161 200 3581.
Judith.shackleton@manchester.ac.uk

Proposed changes to BCA Industrial Group Constitution for the 2005 AGM

Introduction:
There is an ever-increasing trend for Industrial Crystallography to be carried out in collaboration with Academic Institutions. In recognition of this fact, and as suggested by the membership at the last AGM, the committee of the Industrial Group proposes to change the wording of rules 11 and 15 of the BCA Industrial Group Constitution as follows:

Current version:
11 COMMITTEE. The affairs of the Group shall be managed by a Committee consisting of the Officers of the Group together with no more than six Ordinary Members of Committee. Not more than three Officers or Members of the Committee shall be from Academic Institutions. The BCA representative to the ICDD shall be a member of the committee ex officio. Additional members may be co-opted from time to time under Rule 13. The Committee shall be broadly based, with no one field or discipline unduly favoured. Only members of the Group shall be eligible for Membership of the committee.

15 NOMINATIONS FOR OFFICERS AND COMMITTEE. Vacancies for Officers and Ordinary Members of the Committee shall be filled by election at the Annual General Meeting of the Group. Nominations, which shall be proposed by not less than two members of the Group and shall be accompanied by the written consent of the nominee, shall be sent to reach the Honorary Secretary of the Group not later than seven days before the Annual General Meeting.

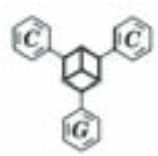
Proposed revision:
11 COMMITTEE. The affairs of the Group shall be managed by a Committee consisting of the Officers of the Group together with no more than six Ordinary Members of Committee. The BCA representative to the ICDD shall be a member of the committee ex officio. Additional members may be co-opted from time to time under Rule 13. The Committee shall be broadly based, with no one field, discipline or type of institution unduly favoured. Only members of the Group shall be eligible for Membership of the committee.

15 NOMINATIONS FOR OFFICERS AND COMMITTEE. Vacancies for Officers and Ordinary Members of the Committee shall be filled by election at the Annual General Meeting of the Group. Nominations, which shall be proposed by not less than two members of the Group and shall be accompanied by (a) a brief statement demonstrating the nominee's experience in the application of crystallography to industrial research; and (b) the written consent of the nominee, shall be sent to reach the Honorary Secretary of the Group not later than seven days before the Annual General Meeting.

These proposed changes will be put to the membership for discussion and approval at the AGM.

Jeremy Cockcroft

Annual General Meeting of the Chemical Crystallography Group



THE AGM will be held on Wednesday 13 April 2005 during the BCA Spring Meeting in Loughborough, starting at 12 noon

Final details of the agenda and venue will be published on the CCG website: **http://crystallography.org.uk/CCG/ccg.html**

Items for inclusion in the agenda should be sent to the secretary of the CCG, **Dr Georgina Rosair** and received no later than Wednesday 6 April 2005.

Call for nominations

Elections will be held for the post of Chairman, Deputy Chairman and three ordinary members of the committee. The Deputy Chairman takes over the post of Chairman. The present post holders Chairman: **Dr Sandy Blake,** Deputy Chairman: **Dr Simon Parsons,** ordinary members of the committee: **Dr Richard Cooper, Dr Michaele Hardie, Dr Simon Teat,** are not eligible for re-election to the same posts (see rules 12 and 15 of the constitution).

The deadline for nominations is Wednesday 6 April 2005. Nominations may be sent in by email, they must be supported by no fewer than two members of the CCG and should be accompanied by the written consent of the nominee.

Current Officers

Chairman, Dr Sandy Blake (2003-2005)
Deputy Chairman, Dr Simon Parsons (2003 – 2005)
Secretary Treasurer, Dr Georgina Rosair (2004-2008)

Committee

Dr Andrew Bond (2004 - 2007)
Dr Richard Cooper (2002 - 2005)
Dr Michaele Hardie (2002 - 2005)
Dr Mary Mahon (2003 - 2006)
Dr Andy Parkin (2004 - 2007)
Dr Simon J Teat (2002 - 2005)
Ms Katherine Bowes
(co-opted student representative)(2003 - 2005)
Dr Carl Schwalbe (co-opted local organizer Autumn Meeting 2004) (2004 - 2005)

Dr Georgina Rosair

Secretary Treasurer of the Chemical Crystallography Group

Email: G.M.Rosair@hw.ac.uk
Phone: 0131 451 8036 **Fax:** 0131 451 3180
William Perkin Building, School of Engineering & Physical Sciences, Heriot Watt University, Edinburgh EH14 4AS.

CCG Autumn Meeting on In situ Crystallography

THE autumn meeting of the CCG was held at Aston University in Birmingham the on 17th November 2004. The topic for the day was "*In situ* crystallography", and around 70 delegates attended from around the UK.

Dermot O'Hare from Oxford University started proceedings with a talk on Studying solid state reactions using time-resolved X-Ray and neutron diffraction. His talk highlighted how powder diffraction techniques can be used for studying the kinetics of solid state reactions, and to monitor *in situ* the formation of materials synthesised by hydrothermal techniques. The reversible insertion of LiCl into γ-Al(OH)$_3$ was shown to occur through lamellar diffusion with the insertion of the anions being the rate determining process. Studies of the kinetics of intercalation of pharmaceuticals were also presented which is important for drug delivery systems. Applications in separations science were discussed with the separation of benzenedicarboxylates, where changes on intercalation of the host d-spacings were monitored. A kinetic product was observed to form before the final thermodynamic product, due to intercalation of different benzenedicarboxylate isomers. The outcomes of hydrothermal syntheses are very difficult to predict, hence kinetic studies of hydrothermal crystallisations have been undertaken at Daresbury station 16.4 using a teflon-lined autoclave. A study of the formation of microporous gallium phosphate, for instance, showed that there were no intermediate products and that the reaction is complete after 1.5 hours. However if P_2O_5 is used in place of H_3PO_4 in the reaction then an intermediate product is observed. This intermediate cannot be isolated and its existence would not be known without these kinetic studies.

Richard Ibberson from ISIS spoke on Molecular crystal structures by neutron powder diffraction - the highs and lows of parametric studies. He described a number of parametric studies on well known molecular crystals such as sulfur and adamantane, and *in situ* formation of low-melting powders such as CD_4. CD_4 has three phases and the presumed tetragonal phase III was shown to be orthorhombic with an ordered structure. Libration of atoms in a powdered sample of adamantane was studied, and the carbon atoms librate around the centre of the molecule and the deuterium atoms follow the carbon libration.

After a lunch break **John Warren** from the SRS gave a talk on Single crystal, powder, liquid, spotty rings, star wars: *in situ* diffraction at the SRS. He described a number of the types of *in situ* diffraction experiments being undertaken at station 9.8 at Daresbury. These include the development of an environmental gas cell where single crystals can be put under vacuum or exposed to a gas during X-ray data collection. Initial experiments looking at the SO_2 uptake by "Chinese Lantern Complexes" were described. Experiments using variable temperature (volcano), high

pressure (spotty rings) or photo-crystallography (star wars) were also discussed. In particular the development of a chopper to use for diffraction experiments of photo-excited single crystals was presented.

Andrew Bond from the University of Southern Denmark spoke on *In situ* crystallisation and co-crystallisation. He described the flash freezing and annealing process required to obtain single crystals of compounds that are liquids at room temperature. The heating/annealing stage often uses an expensive IR laser, but Andrew described an alternative method that was developed by **J. E. Davies** in Cambridge. In the Davies method, the sample in a capillary is mounted on the diffractometer at a chi of 90° and flash frozen. The cryostream temperature is raised to just below the sample's melting point and the goniometer head height manually adjusted to allow for melting and refreezing of the sample until a single crystal is obtained. The phase obtained will be in equilibrium with the melt. Interestingly the two annealing methods seem complementary and for compounds such as decane where the IR laser method has not been successful the Davies method has been, whereas for azetidine the IR laser method worked while the Davies method did not. A range of *n*-alkyl carboxylic acids (C_6 to C_{15}) were studied using the Davies method and the hitherto unexplained alternating trends in melting point were matched by alternating trends in D_{calc} for the crystal structures.

David Allen from the University of Edinburgh spoke on Crystal growth from the melt or from solution at high pressure: generating new small-molecule polymorphs. He discussed the use of diamond anvil cells for determining crystal structures at high pressures. In many cases the crystals being studied were grown *in situ* inside the diamond anvil cell. A liquid sample can be placed under pressure which will induce crystallisation and single crystals can then be obtained by heating so that the sample melts and only one crystallite is left which nucleates the growth of a single crystal on cooling. A number of mono-alcohols were studied using this technique. High pressure induces a more symmetric structure, in, for instance, cyclobutanol. One problem with this method for high pressure crystal growth is that compounds may decompose before melting and this is exacerbated by pressure. Another *in situ* crystal growth technique that circumvents this problem has the pressure cell loaded with a solution and crystallisation is induced by pressure when the lattice energy overcomes the solvation energy. This technique has been used to study drug polymorphs.

Katherine Bowes from the University of Cambridge spoke on Studying photo-induced isomerism of $[Ru(NH_3)_4(H_2O)(SO_2)](tosylate)_2$ by X-ray diffraction. She described the difficulties in studying photo-excited states which requires exciting a crystal by irradiation without destroying it, and synchronising the light source and X-ray source. It is easier to look at compounds that have a metastable state with lifetimes of several minutes such as $[Ru(NH_3)_4(H_2O)(SO_2)](tosylate)_2$ which, on irradiation with soft light, can transform from a ground state with an S-donor SO_2 ligand to a metastable chelating SO-donor ligand. This was studied at Daresbury station 9.8. Refinement of the data indicated that there was still a large portion of the complex in the ground state, though the excited state η^2-SO_2 ligand was found in the difference map and appeared to be positionally disordered. There was also small movement of the NH_3 ligands and the counter-anion positions were different in the excited state compared with the ground state structure.

Jamie Bickley from the University of Liverpool was the final speaker for the day, and his topic was *In-situ* re-crystallisation of an amorphous solid into single crystals. He is studying hydrogen bonding networks and coordination polymers of derivatised triazatriphosphorines and described some 2D and chain coordination polymers. Reaction of $AgClO_4$ with an allyl functionalised triazatriphosphorine ligand gives an amorphous precipitate. When methanol and a catalytic amount of $AgClO_4$ are added to the powder then single crystals are grown, and this crystal growth can be monitored by diffraction techniques. These crystals show a chain polymeric structure.

Many people must be thanked for their contributions to a highly enjoyable, informative and successful day. Special thanks must go to the local organiser **Carl Schwalbe,** to the session chairs, to all the speakers and to the organising committee. Extra thanks must also go to Bruker-AXS for generous sponsorship and to Pfizer Ltd for sponsorship that allowed for free registration of student participants.

Michaele Hardie

The Winter Meeting of the Biological Structures Group

Imperial College, 17 December 2004

THE winter meeting of the BCA Biological Structures Group proved an ideal vehicle to honour the memory of David Blow.

His many friends and colleagues (and his son Julian) gathered at Imperial College, where David worked, to enjoy an exciting programme put together by **Peter Brick, Katy Brown** and **Peter Moody. Richard Henderson** (MRC Cambridge, and David's third student) began the day with a biographical overview that highlighted (1) David's analysis of the errors in isomorphous replacement that has formed the basis of MIR phasing, (2) his work on molecular replacement with **Michael Rossmann** that has become the phasing method of choice in all protein crystallography laboratories

because of the now ready availability of suitable search models, and (3) David's enormously personable qualities: his keen scientific mind, his friendliness, his generosity and above all, his modesty. Richard showed some delightful slides, including a marvellous packing model David had constructed using 16 left dolls' shoes (which David had to go and buy – leaving the right counterparts in a pile in the office for a long time) and also lovely slides of "David on the river" which certainly gave the impression that David enjoyed his time in Cambridge.

David on the River Cam with some of his group.
Photo taken by Jens Birktoft.

Michael Rossmann (Purdue), who shared the Cambridge office with David (and the pile of shoes), described how detailed studies of the T4 bacteriophage had been facilitated by combining EM projections using mathematical methods developed by **Tony Crowther** (MRC Cambridge and David's second student). The phage genome consists of 168 kbp and encodes around 300 open reading frames with 40 of these known to code for structural proteins. Michael described how the phage tail is assembled from 6 'wedges' packed around a central 'hub', and how the head is formed from two proteins, gp23 (the main capsid protein) and the homologous gp24 (which form the 5-fold vertices of the capsid). He then described how the X-ray structure of gp24 had been modelled into images of the phage capsid obtained by cryo-EM. After reporting the capsid structure of another phage, Φ29, Michael returned to T4, describing the structure and function of the tail proteins. He described the cryo-EM imaging of the virus following DNA injection into the host cell and how the sheath surrounding the tail contracts by a helical motion of the viral capsid caused by changes in the relative positions of the tail proteins. The story was summarised in an impressive computer-generated movie, starring the spidery bacteriophage as a chillingly efficient infection machine (not for the mildly arachnophobic).

Brian Matthews (Oregon), who overlapped in Cambridge for three months with Michael Rossmann (and pointed out that Michael had failed to interest him in taking over his house), gave a fascinating lecture concerned with the physics of flash cooling crystals. The topic arose, albeit some 35 years later, from his time working in David's lab and the independence given him there to publish his own work: it was a referee challenge on guessing the number of molecules per asymmetric unit in a chymotrypsin crystallisation paper that lead to a subsequent (and highly-cited) paper on the Matthews' coefficient. Brian spoke of how cryo-cooling commonly causes shrinkage in unit cell volume of some 5 - 8 % and how, with some proteins, this change is reversible on returning the crystal to room temperature. His group had found the surface areas involved in crystal contacts increases on freezing. Analysis of β-galactosidase, as well as other proteins in the PDB, showed increased lattice contacts could be largely attributed to Arg, Gln and Glu residues, with lysine rarely being involved in lattice contacts (and hence a good candidate for surface mutation to improve crystallisation). Brian showed that contraction of the solvent region on freezing is affected by the amount of cryoprotectant, and that the optimal freezing parameters are those that will match the lattice contraction with solvent region contraction. During the questions, Brian had a single slip-of-the-tongue when lysozyme emerged – the audience welcomed the L-word as heartily as a beloved rendition of an old song.

Tom Steitz (Yale) had requested a post-doc with David Blow on Hilary Muirhead's recommendation. He said that despite his interest in isoleucine tRNA synthetase, David had convinced him to work on chymotrypsin. Tom began by reminiscing on this work, noting the excitement at discovering the transition-state stabilisation afforded by the 'oxyanion hole'. He continued with his synthetase interest that has led naturally to the mechanism of protein biosynthesis. The audience was given an overview of the structure of the ribosome as deduced by a combination of X-ray crystallography of isolated subunits and electron microscopy of the whole particle. He then zoomed in on the mechanistic studies of amino acid transfer from tRNA to growing polypeptide that also required oxyanion-type stabilisation. He mentioned that something had happened which he had not foreseen in the chymotrypsin days: his work on the ribosome had actually become "useful" in that it was being exploited for antibiotic design. Precisely at the time his lecture was scheduled to finish, his rapid description of the analysis of numerous antibiotic complexes was truncated by some projection gremlin, no doubt with an eye on lunch!

The gathering for David's 70th birthday. *Katy Brown, Silvia Onesti, Gerard Bricogne, Alice Vrielink, Richard Henderson, Phil Rodgers, David Blow, Alan Wonacott, Tony Crowther, Lesley Haire, Jonathan Goldberg, Emmanuel Saridakis, David Matthews, Siân Rowsell, Oliver Smart. Alan Wonacott, a former colleague, is the only one who was not one of David's students.*

The afternoon programme had six shorter presentations starting with **Jonathan Goldberg** (Sloan-Kettering, New York), one of David's more recent students, describing his work on the COP-II complex in sorting. Jonathan commented it was pleasing to see so many of David's more recent PhD students (e.g. **Lesley Haire, Katy Brown, Siân Rowsell**) at the meeting.

Murray Stewart (MRC Cambridge, but with no direct connection to David Blow) gave an entertaining breakneck tour of nuclear trafficking with stroboscopic slide-changing, ending up with a description of the Cse1:Kap60p:RanGTP complex at 2 Å resolution. Murray related how he was treated with suspicion after he lectured on nuclear trafficking to a group of North Korean parliamentarians. He described an interesting "spring-loaded" transport model where a complex upon reaching its destination would disassemble readily despite extensive surface interactions. **Dave Stuart** (Oxford) presented a "fatty virus" lecture covering his work on the phage PRD1 which is considered to be a plausible model for many human viruses. The crystals were so fragile that freezing conditions were never found and data collection to ~ 4 Å resolution required around 2000 crystals. Phasing used a combination of electron microscopy and 'small molecule crystallography' with the structures of known capsid protein structures. Although a teacup used by David Blow as an irregular object to illustrate molecular replacement was referred to, at least one picture of PRD1 shown had more in common with a lidded beer stein. The resulting structure showed a clear protein coat, the lipid bilayer and the layers of DNA in the core.

The final three talks were from London-based people with **David Barford** (ICR) discussing the insights afforded into RNA silencing by the structure of the PIWI domain from *Archaeoglobus fulgidus* an archaeon whose argonaute protein contains only the one domain. **So Iwata** (Imperial), complete with neck tie, used the title "Membrane-proteins: The Last Frontier" to describe his work on photosystem II, pointing out that a good 30% of the proteins coded by the human genome are membrane-bound, as are about 70% of current drug targets. He briefly described the structure and then guided us through details of the cofactor binding sites, concentrating on the unusual manganese cluster in the oxygen-evolving centre. The cubane-like structure has 3 Mn and 1 Ca atoms bridged by oxygens. A fourth Mn is linked to the cluster which with the Ca forms the site of the H_2O to O_2 conversion. It is now possible to relate the catalytic cycle to the protein structure. So mentioned how his work had been covered on the CNN website using as illustration not his beautiful structure but a picture of George Bush, interested in obtaining hydrogen from water. The last scientific talk of the afternoon was given by **Dale Wigley** (Cancer Research UK) who described the structure of the recBCD complex that is able to rectify errors in replication. The three proteins that comprise the complex have distinct activities; two of which, recB and recD, are helicases, while the third, recC, recognises a chi site on the DNA, binds tightly to this such that the 3'-5' activity of recB can no longer occur, allowing the 5'-3' activity of recD to become dominant. The presence of a β-hairpin 'pin' on recC that separates the two strands like a breakwater, allows the strands to be processed independently. Surprisingly, recC has the same fold as PcrA helicase despite there being essentially no sequence identity. Fortunately, Dale had found an acceptable prop to illustrate how these enzymes act along DNA: perhaps he was not wearing a belt this day. Precisely at the scheduled finishing time, the same inconsiderate projector gremlin disrupted this talk too.

Guy Dodson (York) rounded off the proceedings with a couple of delightful anecdotes about David's dedication and support of younger researchers that could lead to some gentle rule-breaking: he spoke up during **Katy Brown's** viva, for which Guy was external examiner. Guy recalled that he had had to convince a sceptical grant panel that one of David's applications was unquestionably deserving of support. Apparently, Guy's support of the case was itself considered a masterpiece, and the panel commented, 'Are you chaps all super-bright, or just good friends?' It is clear that in David's case, both were true.

The speakers. *Back row: Jonathan Goldberg, Dave Stuart, Murray Stewart, Tom Steitz, Brian Matthews and Dave Barford. Front row, Dale Wigley, Richard Henderson, So Iwata, Michael Rossmann and Guy Dodson. Photo taken by Harry Powell*

Jon Cooper
Richard Pauptit
Lindsay Sawyer

Members

Honorary Members elected in 2004

Professor Paul Barnes
(Birkbeck College/ University College London)
Paul Barnes' structural science has straddled many areas of industrial and materials chemistry, for example work on the applications of crystallography in materials such as cements, ceramics and zeolites. He has also been very influential in the synchrotron radiation area; being very active in detector development at the Daresbury SRS, among other major contributions to the user programme in this area. Paul has been a particular pioneer of "in situ" and "diffraction-plus" methods (measuring physical properties simultaneously with diffraction measurements), and a major player in the application of high energy techniques in studying systems under change. This area is high profile (and indeed forms the theme for the 2005 Spring Meeting Review Symposium) and Paul was without doubt one of its pioneers.

Paul has been a BCA member for many years and has supported the organisation in a range of areas; he also delivered the inaugural Alun Bowen Memorial lecture in 1997. Perhaps most notably he was Exhibitions Convenor throughout most of the 1990s, carrying the load of this important role until Northern Networking were brought on board.

Professor Mike Glazer
(University of Oxford)
Mike Glazer's work has straddled the areas of symmetry, phase transitions, perovskite and other inorganic structures, optical properties of crystals, and hence many of the major areas of physical crystallography. He is the author of many distinguished publications in the field of crystallography, including numerous contributions to the field of perovskite science, including the famous "Glazer tilt notation". "Firsts" in synchrotron science, together with **Joan Bordas,** included energy-dispersive diffraction (using a solid state detector), the first study of a phase transition by white beam topography, and the first high-resolution energy-dispersive diffraction experiment. In addition it was members of his research group, **Paul Thompson, Ian Wood** and **Judie Matthewman** who gave the first demonstration of the use of the Laue technique to refine crystal structures. In addition to his scientific achievements Mike has been highly influential in the area of sample environment; the Cryostream device he designed and marketed with John Cosier through Oxford Cryosystems and which has helped revolutionise the area of low temperature chemical and protein crystallography.

Mike is a past editor of the Journal of Applied Crystallography and of Phase Transitions, and is an influential and respected BCA member. He was BCA President from 1996-2000 and remains very active in the organisation, notably in developing teaching and education.

Professor George Sheldrick
(University of Göttingen)
George Sheldrick's work has for many years embraced structure solution methods, impinging initially on small molecule structures - the interest area of the Chemical Crystallography Group. More recently, George's work, and that of others in the structure solution field, has moved towards the application of structure solution in the macromolecular area, hence impacting on the interest area of the Biological Structures Group. The program SHELX, developed originally by George while in Cambridge in the 1970s, and subsequently much enhanced and extended, is perhaps the most widely used piece of crystallographic software world-wide. There can hardly be a crystallographer world-wide who has not used one or more of George's programs.

George has been for many years a regular attender at BCA meetings, and a regularly invited speaker at these. He delivered the Dorothy Hodgkin Prize Lecture in 2004, and was awarded the ECA Maz Perutz prize, also last year in 2004, and has received many other chemical and crystallographic awards worldwide. He is without doubt one of the UKs most prominent crystallographic alumni, a Fellow of the Royal Society among many other recognitions of his distinguished achievements.

Chick Wilson

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.

3-11 March 2005
LANCSE 2nd Annual Winter Neutron School on Applications to Structural Mechanics - LANSCE, NM, USA.
www.iucr.org/cww-top/mtg.lancse.html

7-11 March, 2005
International School on Crystal Growth: Fundamentals, methods and applications to biological and nano crystals, Puebla, Mexico
www.ifuap.buap.mx/ISCG05/school.html

14-17 March 2005
BRASS Rietveld Workshop University of Bremen, Germany.
www.brass.uni-bremen.de/RW2005/RW2005>.

4-12 April 2005
10th BCA/CCG Intensive Course in X-ray Structural Analysis, University of Durham
Please contact claire.wilson@nottingham.ac.uk.

5-6 avril 2005
CCN2005, Colloque annuel du GFCC, La Croissance Cristalline dans les Nanosciences, Valpré (Lyon), France
www.crmcn.univ-mrs.fr/confs/ccn2005

10 -14 April 2005
Physics, a century after Einstein, University of Warwick
www.physics2005.iop.org

10-15 April 2005
RapiData 2005 - The 7th annual data collection and structure solving course at NSLS, Brookhaven National Lab, NY, USA
www.px.nsls.bnl.gov/RapiData2005/

12-14 April 2005
BCA Spring meeting and X-Ray Fluorescence Meeting, Loughborough crystallography.org.uk

24-29 April 2005
NESE Neutron Conference - European Geosciences Union General Assembly 2005, Vienna, Austria
www.iucr.org/cww-top/mtg.nese2.pdf

2-6 May 2005
Practical X-ray Fluorescence, International Centre for Diffraction Data,Newton Square PA, USA www.icdd.com/education

12-22 May 2005
Evolving Methods in Macromolecular Crystallography, 37th crystallographic meeting at Erice and a EuroSummerSchool, Erice, Italy
crystalerice.org/futuremeet.htm

16-20 May 2005
PAC05: 2005 Particle Accelerator Conference, Knoxville, TN, USA www.sns.gov/pac05/

22-26 May 2005
9th EMAS European Workshop on Modern Developments and Applications in Microbeam Analysis/3rd Meeting of the International Union of Microbeam Analysis Societies, Florence, Italy
www.emas-web.net/EMAS-2005/IUMAS-3

23-25 May 2005
2005 NSLS Users' Meeting, Upton, NY, USA
www.nsls.bnl.gov/users/meeting.

26-28 May 2005.
Conference on EPSRC-ILL Millennium Projects - Institut Laue-Langevin, Grenoble, France. www.ill.fr/dif/epsrc/

28 May 2005
Powder diffraction software workshop (Satellite of ACA),Walt Disney World, Florida, USA www.chem.tamu.edu/xray/acawork/acaworkshop.html

28 May-2 June 2005
ACA Annual Meeting, Walt Disney World, Florida, USA hwi.buffalo.edu/ACA/

31 May 31 - 3 June 2005
E-MRS 2005 Spring meeting - Current Trends in Optical and X-Ray Metrology of Advanced Materials for Nanoscale Devices. Strasbourg, France www.iucr.org/cww-top/mtg.anc1.pdf

5-10 June 2005.
7th International Workshop on the Physical Characterization of Pharmaceutical Solids, Kona, Hawaii. www.assainternational.com/workshops/iwpcps_7/iwpcps_7.cfm

6-10 June 2005
Fundamentals of X-ray Powder Diffraction, International Centre for Diffraction Data, Newton Square PA USA
www.icdd.com/education

13-17 June 2005
Advanced Methods in X-ray Powder Diffraction, International Centre for Diffraction Data,Newton Square PA, USA
www.icdd.com/education

15-17 June 2005
14th Croatian-Slovenian Crystallographic meeting, Vrsar, Croatia
www.hazu.hr/kristalografi/vrsar05.htm

14-15 June 2005
CHESS 2005 Users' Meeting Cornell High Energy Synchrotron Source, Ithaca, NY, USA
www.chess.cornell.edu/Meetings/

17-22 June 2005
Molecular Crystal Engineering EuroConference on Evaluations and Predictions of Solid State Materials Properties, Helsinki, Finland
www.esf.org/conferences/pc05191

19-28 June 2005
7th EMU School: Mineral Behaviour at Extreme Conditions. Heidelberg, Germany
www.univie.ac.at/Mineralogie/EMU_School-7/

20-24 June 2005
International School on Mathematical and Theoretical Crystallography, Nancy, France
lcm3b.uhp-nancy.fr/mathcryst/nancy2005.htm

27 June – 1 July 2005
Joint 20th AIRAPT and 43rd EHPRG: International Conference on High Pressure Science and Technology, Karlsruhe, Germany
www.air-ehprg-2005.de

3-7 July 2005
12th Convention of the Royal Australian Chemistry Institute (RACI), Sydney, Australia
www.pco.com.au/connect2005

4-7 July 2005
IWORID-7: 7th International Workshops on Radiation Imaging Detectors, Grenoble, France.
www.esrf.fr/News/FrontNews/IWORID7/

4-8 July 2005
X05: The 20th International Conference on X-ray and Inner-Shell Processes, Melbourne, Australia. www.chemistry.unimelb.edu.au/news/X05/X05.html

27-30 July 2005
2005 TRENDS IN MICROCALORIMETRY, Boston, MA, USA
www.microcalorimetry.com/index.php?id=271

18-23 August 2005
IUCr Computing School (prior to the Florence 2005 congress), Siena, Italy
iucr.ac.uk/iucr-top/comm/ccom/siena2005

21-26 August 2005
27th International Free Electron Laser Conference, Stanford, CA, USA
www.ssrl.slac.stanford.edu/lcls/fel2005/

23-31 August 2005
XX Congress of the International Union of Crystallography, Florence, Italy
iucr2005.it

2-8 September 2005
Electron Crystallography School 2005 - ELCRYST 2005, Brussels, Belgium
www.elcryst2005.de

4-6 September 2005
Annual Conference, British Association for Crystal Growth, Sheffield www.bacg.org.uk

6-7October 2005
Watching the Action: Powder Diffraction at non-ambient conditions, Max-Planck-Institute for Solid State Research, Stuttgart, Germany
www.fkf.mpg.de/xray/

27 November – 2 December 2005
International Conference on Neutron Scattering 2005, Sydney, Australia
sct.gu.edu.au/icns2005

2006

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

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

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