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NEXT ISSUE OF CRYSTALLOGRAPHY NEWS

CRYSTALLOGRAPHY NEWS is Published quarterly (March, June, September and December) by the British Crystallographic Association. Submissions on any subject related to crystallography are most welcome. If possible, please send text electronically without special formatting. Pictures are most welcome, but should be sent as separate, graphic files. Items for inclusion in the **December 2003** issue should reach the Editor by **25 October 2003.**

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E-mail: gould@ed.ac.uk

The British Crystallographic Association is a Registered Charity (#284718)

COVER PICTURES

1. Not just girls are diamond's best friends!

2. And the point group of this castle is....

3. 50 years of snakes and ladders?

4. Getting ready for the BCA 2004

5. Hard at work in Durham

Contents

President's Remarks

It is always a pleasure to start a column like this with good news, and my good news on this occasion is the appointment of four new Honorary Members of the BCA. This accolade is awarded to distinguished crystallographers who have made outstanding contributions to crystallographic science and to the BCA. I am delighted to announce that the four new Honorary BCA Members are David Blow, Durward Cruickshank, Mike Hart and Judith Howard. Council aim to consider nominations for Honorary Membership each year; these are welcome at any time from any member, or from the subject groups.

On the subject of nominations, at next year's Spring Meeting in Manchester, the Hodgkin Prize and Lecture will be awarded and delivered. As announced elsewhere in this issue, nominations for the Hodgkin Prize are invited. Also at Manchester, a slot has been earmarked for the Bragg Lecture which we are delighted to host on behalf of the Bragg Lecture Committee.

The Spring Meeting programme itself is coming together, with the Plenary Session theme in 2004 being "Catalysis: from Metals to Macromolecules" which I think meets very well the aim of providing a unifying session in which all strands of interest within the BCA can participate. I am certainly looking forward to it. One of the most pleasing things for me at the programme committee meeting was the range of excellent topics proposed – by no means all of these could be included in the programme.

Of course, with a packed programme in our current model of a 3-day Spring Meeting, it is impossible to include everything, and we are looking at ways of increasing the flexibility. The day preceding the SM has occasionally in the past been used for Workshops (particularly of the hands-on variety), and this is a trend we can encourage, offering Workshops a more flexible timeframe in which to operate. We are also looking at ideas for a Young Scientists' day, so watch out, you young scientists I have spoken to on this subject – you have not heard the last from me!

As I write this, the summer conference season is in full swing and I am in Cincinnati at the ACA meeting. It is good to see a strong UK presence here and hopefully this will also be reflected at the forthcoming ECM-21 in Durban - I know how hard the locals there have worked to put the meeting together. On the subject of international meetings, it is good to be able to note that the contribution made by the BCA towards providing bursaries for the Geneva (IJerusalem) IUCr meeting is now back with us as hoped. This fund, provided by the Glasgow 1999 organisation headed by Chris Gilmore and Judith Howard, is intended to be an ongoing commitment to provide underpinning support for IUCr meetings. After currency exchange, the amount we will now be able to offer Florence 2005 is slightly below the original £25k fund, but we hope it will still be a substantial aid to that meeting.

By the time you read this, the summer will be in the past and we will be looking forward to the new academic year. From my personal perspective this means new challenges, as I have taken up a new appointment, based equally between the University of Glasgow and RAL. After spending much of my career to date in a Facility environment at ISIS, it will be good now to see things also from another angle and I am looking forward to it. Contacting me, with comments you may have about BCA issues, will be much the same as before, but with the option of getting me at either the Department of Chemistry in Glasgow (C.C.Wilson@chem.gla.ac.uk) or as before at ISIS (C.C.Wilson@rl.ac.uk). Or of course, the opportunity of missing me in two places rather than just one!

Chick Wilson

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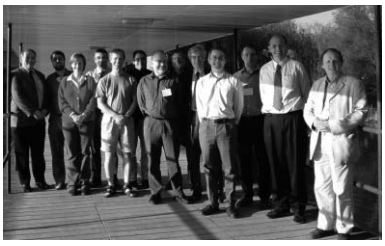
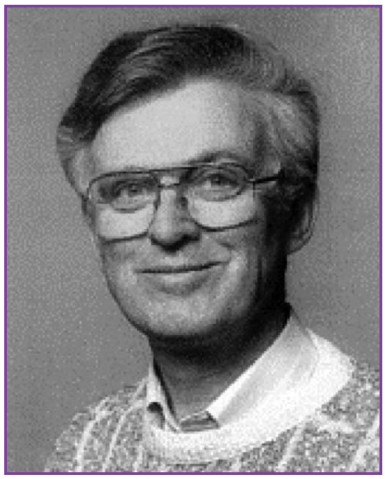
ACKNOWLEDGEMENTS:
BCA Sponsors

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



Editor's Remarks



As the President says, it is always a pleasure to start with good news, and what we can do is to fill out his modest statement about himself. He is now Regius Professor of Chemistry at Glasgow, occupying a chair with an excellent crystallographic history, as it was held by both J.M. Robertson and George Sim. Welcome back to the other end of the Forth and Clyde Canal!

More good news is that the last issue of Crystallography News did not make a financial deficit. For the time being, we are trying to restrict the central pages of each issue to 32, and we apologise to those of you who wrote articles for June which are only appearing now. They do help to complete an issue which has to be got ready too early to take in much from the major summer meetings. The ACA has just ended and Durban is still in the future as we go to press.

In the jubilee year of the DNA structure, we have our bit to offer in this issue, thanks to Kate Crennell. She also points out a recent letter to the Times (July 30) from Lord May, President of the Royal Society, in which he suggests that a sculpture based on the DNA structure might be commissioned for that vacant fourth plinth in Trafalgar Square. He continues, "The double helix structure of the DNA molecule has great aesthetic beauty and could be incorporated by any of the six short-listed artists into a novel and eye-catching design. What could be better than to create something that highlights, and stimulates public interest in, the best of both modern art and science?" One hopes that the "snakes-and-ladders" design on the postage stamp will not be used as a starting point!

In this issue we have put news from the groups into a more clearly defined single section, which we hope will encourage more cross-fertilisation. In order to save space – and discourage copies being mutilated – application forms for Group Meetings are not being printed. These are generally conveniently printed from the Group websites, which are given at the top of each item. Also a couple of very good reports from Arnold Beevers bursars have been included.

Let us know what you think! Please note that the editorial E-mail address has been changed to **gould@ed.ac.uk**

Bob Gould

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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 at the annual Spring Meeting.
- Free insert in the annual Spring Meeting delegate bag.
- Two free full registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly BCA Newsletter.
- Corporate Members will be listed in every BCA Newsletter and on the BCA Web Site with links to your corporate site.

The cost of this membership is £600.00 per annum

To apply for Corporate Membership, or if you have any enquiries, please contact:

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From Professor Dolding-Beedle and others

Dear Sir,

I wish to declare my affrontation at encountering yet another ostensibly "scientific" paper in the literature which heralds a new crystal structure that has "self assembled". I may be out of date, but I thought that was rather normal behaviour for a crystal? Have these authors discovered that normal crystals do not self assemble? - that standard, everyday crystal growth is actually the responsibility of little workmen, with little hard hats? - that typical crystal growth rates can be explained by the number of these little workmen who are working versus those that are drinking little cups of tea, while reading little tabloid newspapers in little wheelbarrows? - and that size, mosaicity and crystal quality can usually be predicted by carrying out suitable QA procedures on the workforce? If such be the case, we can only be grateful to those who have discovered new materials that actually do behave in the way we had always thought to be normal.

And don't get me started on all those other unnecessary neologisms, such as: "nano"; "femto"; "biomaterials" or "clean energy source"; with the associated hyperbolic aura marking a half-formed idea in search of generous funding!

In the eyes of the public, we are often considered lowly enough. Must we allow our meaningless drivel to drag us down further to the level of charlatans to the eventual degradation of science?

Yours sincerely,

P. Dolding-Beedle
Egregious and Regal Professor of Honesty in Science.
International Centre of Excellence in Environmentally Clean Self-Assembling Femtosecond Ultra-Nano Biomaterial Innovation
(and Name-and-address-supplied)

From Dr Tamzin Lafford

Dear Mr. Gould,

I noticed in the June edition of Crystallography News (page 28) the verbose variation on "Twinkle, twinkle, little star". I had seen a very similar version before:

Scintillate, scintillate, globule aurific,
Fain would I fathom thy nature specific,
Loftily poised in the ether capacious,
Strongly resembling a gem carbonaceous.
This was quoted by Robert Barrass in "Scientists Must Write" (Chapman and Hall, 1978) as an example against using unnecessarily long and complicated words when explaining something. He says it is anonymous. "Aurific" would relate to golden properties, while "vivific" in your earlier correspondence relates to "enduing life".

Best regards,

Tamzin Lafford
Senior Applications Scientist
tamzin.lafford@bede.co.uk

WANTED

Out of print textbook: 'Principles of Nucleic Acid Structure' by W. Saenger

I am starting a new EPSRC-funded project on liquid-crystalline DNA, and would like to purchase a copy of the out-of-print textbook 'Principles of Nucleic Acid Structure' by W. Saenger, Springer Verlag, Berlin, 1984, ISBN: 3540907610. If you have a copy you would be willing to sell, please contact:

Prof. John M. Seddon
Department of Chemistry,
Imperial College London
Email: j.seddon@imperial.ac.uk
Tel: 020-7594-5797, giving an indication of the condition and the price.

Home for old copies of Acta B

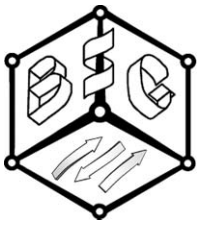
I'm hoping you or someone in BCA may be able to help me find a home for 10 years of Acta Cryst B: Volumes B27 (1971) to B36 (1980) inclusive. The 10-year run is complete though the indexes may not all be there. I seem to remember an appeal from someone in Crystallography News a year or two ago for old journals to go to either Eastern Europe or developing countries. These journals emerged during a clear out at home, still in their boxes from when I changed jobs in 1990, and if they haven't been used for that long, it's time to dispose of them. It seems a shame to just throw them out when they might be useful to someone somewhere. If it helps. I may be able to arrange transport by twisting the arm of the lab's driver.

Jim Chisholm
Minerals and Fibres Section
Health and Safety Laboratory
Broad Lane, SHEFFIELD S3 7HQ

News and meeting announcements from the Groups

Biological Structures Group

http://bca.cryst.bbk.ac.uk/bca/bsg/welcome.htm



Arnold Beevers Bursary Fund

The Biological Structures Group has made a small contribution to this BCA bursary fund, and intends to make this a yearly contribution. Remember that as members of the BCA, BSG members are entitled to apply for bursaries to attend meetings from this fund. See the BCA website for details. Remember to use gift aid to enable the BCA to reclaim tax on your subscription - the money reclaimed in this way is also paid into the Bursary Fund.

BSG AGM

Nominations are sought for the position of Vice-Chairman which is vacant. There will be an extraordinary General Meeting at the BSG winter meeting this year where the election for this post will be held. Please send nominations for this post to Andrea Hadfield along with additional agenda items to the Secretary by 31st November (a.t.hadfield@bris.ac.uk).

Twenty-first Annual General Meeting

To be held on Friday 19th December during the BSG 2003 Winter Meeting at New Lecture Theatre 2, Birkbeck College

Provisional Agenda

- *Minutes of 2003 annual meeting (York)*
- *Matters arising on the minutes*
- *Chairman's Report - Dr. Richard Pauptit*
- *Secretary/Treasurer's report - Dr. Andrea Hadfield*
- *Committee Membership and Officers (2003-2004)*
- *Future Annual General Meetings*
- *Any Other Business*

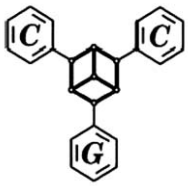
Biological Structures Group Winter Meeting 2003

The BSG winter meeting will be held on 19th December in London this year. Organiser: Richard Pickersgill. Details will follow (Time of writing: July 26th 2003). These will be posted on the BSG Website as they become available.

Andrea Hadfield

Chemical Crystallography Group

http://bca.cryst.bbk.ac.uk/BCA/CCG/ccg.html



CCG Autumn Meeting

Autumn Meeting 2003 - Beyond Refinement; What Happens Next? Sponsored by Rigaku/MSC and Accelrys

The CCG Autumn Meeting 2003 will take place at the Accelrys Center of Excellence, Cambridge, which is located on the Milton Road Science Park on Wednesday November 12, 2003. The local organizer is Vanessa Hoy.
So far, the following have agreed to speak:

Frank Allen, CCDC: The future of Crystallographic Publication

Kirsty Anderson, RSC: Publishing crystallography in chemical journals

Richard Cooper, Oxford: Validation-as-you-go?

John Davies, Cambridge: Unpublished structures

Tony Linden, University of Zurich: Validation

Peter Murray-Rust, Cambridge: e-Science and CIF/XML

Offers of short presentations (up to 30 minutes) should be sent to the program organizer, Dr Simon Parsons, Department of Chemistry, University of Edinburgh, Edinburgh, EH9 3JJ
Tel: (0131) 650 5804
E-Mail: S.Parsons@ed.ac.uk

Registration forms are available as PDFs and in MS-Word 97 (Mac Word 98) Format (as e-forms) on the CCG home page (http://bca.cryst.bbk.ac.uk/BCA/CCG/ccg.html) and should be sent to Dr Harry Powell. Address and e-mail on page 3.

Registration is £15 for members and £27 for non-members, but will be free for bona-fide student members of the BCA and also for retired members.

There is extremely limited car parking available on site, but the Cowley Road Park and Ride site (which has free supervised parking) is a short walk from the Science Park.

Harry Powell

Industrial Group

http://bca.cryst.bbk.ac.uk/bca/ig/ig.htm

Industrial Crystallography Forum II will be held at Birkbeck College, London on 13 and 14 November. The Meeting fee is £50 (£25 concessions); non-member supplements apply.
The draft programme is:

THURSDAY 13TH NOVEMBER

10.00. . . . . Registration

10.30. . . . . Coffee

11.00-12.30. . Crystallography in Industry - Non Ambient

11.00. . . . . In situ diffraction from materials and macromolecules under microwave irradiation. *Andrew Harrison, University of Edinburgh*

11.30. . . . . To be announced

12.00. . . . . To be announced

12.30. . . . . LUNCH – a buffet lunch will be provided

14.00-15.15 . PARALLEL SESSIONS

A. Pharmaceuticals - Non Ambient applications

14.00 . . . . . To be announced

14.25 . . . . . To be announced

14.50 . . . . . To be announced

B. Crystallography in Materials Science

14.00 . . . . . To be announced

14.25 . . . . . To be announced

14.50 . . . . . To be announced

15:15. . . . . Tea

15.45-17:00. . PARALLEL SESSIONS

A. Pharmaceuticals - Polymorphism & Case Studies

15:45 . . . . . To be announced

16:10 . . . . . To be announced

16:35 . . . . . To be announced

B. Non Ambient Applications

15:45 . . . . . To be announced

16:10 . . . . . To be announced

16:35 . . . . . Catalysts: *Steve Norval, ICI plc*

17:00. . . . . Adjourn for Evening programme

17:45. . . . . Introduction to Ron Jenkins Memorial Lecture- *Dave Taylor*

18:00. . . . . Ron Jenkins Memorial Lecture

FRIDAY 14TH NOVEMBER

9.30 . . . . . Industrial Group Award Lecture – *Colin Small, Rolls-Royce plc*

10:30 . . . . . Coffee

11.00 - 12.30 PARALLEL SESSIONS

A. Pharmaceuticals - Amorphous Materials

11.00. . . . . To be announced

11.30. . . . . To be announced

12.00. . . . . To be announced

B. Industrial Applications

11.00. . . . . To be announced

11.30. . . . . To be announced

12.00. . . . . To be announced – *Phil Holdway, QinetiQ*

12.30. . . . . LUNCH – a buffet lunch will be provided

14:00 -15:30 Instrumentation - Past present and future

14.00 . . . . . Past

14.30 . . . . . Present – *Judith Shackleton, Manchester Materials Science Centre.*

15.00 . . . . . Future - *Alun Bowen Lecture*

15.30. . . . . Tea & Close

Please keep an eye on the Industrial Group Web site: http://bca.cryst.bbk.ac.uk/bca/ig/ig.htm for links to the latest programme information, details of local hotels and to download a registration form.

David Taylor

Physical Crystallography Group

http://bca.cryst.bbk.ac.uk/bca/pcg/meetings.htm

PCG Autumn Meeting

The autumn meeting to be held on Monday 8 and Tuesday 9 December at Cosener's House, Abingdon, Oxon. The theme of the meeting is "disordered materials". We have a working title of "Probing Structure at the Nanoscale - Fact, Fiction or Hype?". The philosophy of the meeting concerns the range of approaches/techniques used in studying the "disordered" systems of interest, in particular the development of analytical techniques used in extracting the scientific information. The level of the presentations should appeal to beginners and experts alike. For those interested in attending this meeting, further details will be available at the PCG website: (http://bca.cryst.bbk.ac.uk/bca/pcg/meetings.htm).

Information can also be obtained from me at j.wasse@ucl.ac.uk.

Jonathan Wasse

BCA

Spring Meeting 2004
6-8 April

UMIST

Dorothy Hogdkin Prize 2004

Call for Nominations

Nominations are invited for the fifth award of this prize, which will be presented at the BCA Spring meeting in April 2004 at UMIST. The Dorothy Hodgkin prize of the BCA was instituted on the occasion of her 80th birthday in recognition of her great contribution to science in general and to crystallography in particular. Nominations for the 2004 prize are welcomed from any part of the crystallographic community and should be sent to the President of the BCA, to reach him by 31 October 2003. E-mailed nominations are encouraged.Nominations should be presented on not more than 2 pages and should include the minimum of essential biographical data and the full supporting case for the nominee including up to 6 suitable publications as references. Eligibility for this triennial award is not subject to any restrictions of age, nationality, or past and present places of work. It is anticipated that the next recipient's name will be announced with the details of the Prize lecture in the March 2004 issue of BCA Crystallography News. Previous recipients are:
1991 D. W. J.Cruickshank
1994 G. Bricogne
1997 M. M. Woolfson
2000 U. Arndt

Chick Wilson

General Information

THE BCA SPRING MEETING will take place at UMIST from Tuesday 6 April to Thursday 8 April 2004. The Spring Meeting will follow the same format as the 2003 meeting and will run for 3 full days. We will again be offering one-day registrations.

The Spring Meeting will take place in the Renold Building, part of the Manchester Conference Centre at UMIST. The conference facilities at UMIST are excellent for both delegates and exhibitors. The facilities are centrally located and are easily accessible by both public transport and by car. Car parking for 700 vehicles is available on-site. All scientific sessions, poster sessions and a commercial exhibition will take place in the Renold Building. Both en-suite and standard accommodation is of a high quality and is a short walk from the conference venue.

Euan Woodward

Scientific Sessions

The scientific sessions for the 2004 BCA Meeting will again concentrate on "hot-topics" in the field of crystallography. The main theme and Plenary Session is **Catalysis: from Metals to Macromolecules;** this will lead into a sub-theme on **Molecules in Medicine** covering both chemical and biological aspects. There will be sessions on **Small Angle X-ray Scattering,** which will be preceded by a workshop on the subject, thus offering a good introduction to this subject and an indication of the state-of-the-art. Similarly, **Incommensurate Structures** will be covered with sessions and a workshop. Another topic of importance to all crystallographers is **The Use of International Tables.** The emphasis will be on symmetry, which will be a plenary session and for those interested in a deeper insight; this will be followed by a session on **Advanced Aspects of Symmetry.** There will be other more specialized sessions including **Non-Bonded Interactions** and **Public Domain Software** as well as workshops on the CRYSTALS and CCP4 software suites. There will also be a Special Interest Group session on **DIAMOND** that should be of interest to a large proportion of the crystallographic community.

The **Bragg Lecture** will be incorporated into the UMIST BCA as well as the **Dorothy Hodgkin Prize Lecture.** The **Prize Lectures** for the Physical and Chemical Crystallography Groups will take place as usual, as well as the general **Poster Sessions.**

Paul Fewster

Crystallisation of Polymers (Second Edition) Vol. 1 Equilibrium Concepts

Leo Mandelkern,
Florida State University
Cambridge University Press, 2002
Price: £75.00 (hardback)
ISBN 0521816815; xiii + 433 pages.

Polymer crystallisation has been studied from both an academic and an industrial point of view for well over 50 years. It is still an active field with different schools of thought, surprises turning up and a general acknowledgement that certain aspects are still not well understood. Thus the publication of the first volume of the second edition of Mandlekern's 'Crystallisation of Polymers' is to be welcomed. The first edition, published in 1964, is now hard to find and obviously needs updating. The expansion in the field is such that this new edition comes in three volumes: 1 – Equilibrium Concepts, 2 – Kinetics and Mechanisms and 3 – Structure, Morphology and Properties.

Only a person like Professor Mandelkern who has worked in this field most of his life could undertake such a task. He brings together underlying principles, illustrated by numerous examples and comments on both theoretical and experimental limitations.

The first volume makes it clear that although kinetic factors often dominate the observed structure one must begin with an understanding of equilibrium concepts. Each chapter starts with an introduction and some theory progressing into more detail illustrated by examples from the literature. In the theory sections relationships between different approaches are explained and the limits of applicability are noted. Examples are drawn from a comprehensive range of polymers, predominately synthetic polymers (not just polyolefins as sometimes happens) but biological polymers such as proteins are also included. On average there are over 100 references per chapter covering a wide spread of authors and publications. With many people now relying on electronic literature searches it is helpful to have older classic references together with more recent ones.

The chapter headings describe the scope of this book: introduction, fusion of homopolymers, polymer-diluent mixtures, polymer-polymer mixtures, fusion of copolymers, thermodynamic quantities, fusion of cross-linked polymers, and oriented crystallisation and contractility. There are useful tables of thermodynamic properties determined by a variety of different techniques but it is unfortunate that the pages containing these large tables are unnumbered. Otherwise the book is well indexed.

This (together with the next 2 volumes) will be an important reference book for scientists and engineers working in the field of polymer crystallisation.

Mary Vickers

PUZZLE

This month's puzzle is similar to the "trackword" in the Radio Times. The solution is a highly significant crystallographic nine-letter word obtained by using all the letters in the diagram in turn, passing horizontally, vertically or diagonally from each letter to the next. Try to find as many shorter words as possible formed in the same way. If a tie breaker be needed, it will be the largest number of such credible (in the Editor's estimation) words found!

O	M	P
Y	R	H
L	O	P

Solution for June puzzle. This was won outright by Jim Trotter this time! He looked up the IUCr Commission's report on the web, and got each one spot on. He also found many other ways of categorizing friezes, the most fun being the Conway notation: John Conway uses the print of a left foot pointing along the direction of the frieze as an asymmetric unit; if you do this, you should be able to derive the origins of the names he uses. For more information check out:

http://www.joma.org/vol1-2/framecss/rintel/Math/seven.html

	Int. Tabs	Conway
1) ppppppp	*p*1	hop
2) xxxxxxx	*p*2mm	spring jump
3) pqpqpqpq	*p*1m1	sidle
4) pqbdpqbd	*p*2mg	spinning sidle
5) ccccccc	*p*11m	jump
6) pdpdpdpd	*p*211	spinning hop
7) pbpbpbpb	*p*11g	step

BCA/CCG Ninth Intensive Course in X-ray Structure Analysis

Trevelyan College, University of Durham, 7–15 April 2003

The Ninth Course generally followed the successful format of its predecessors, but it continues to evolve to reflect developments in single crystal structure analysis. This year we increased the number of lecturers from four to five, with Simon Parsons the new recruit. We also had several new members of the tutoring staff. As in previous years the course was oversubscribed, even with an extra tutor group this year. This continued high demand shows how highly the Course is regarded by the crystallographic community both here and overseas.

Who said mirror symmetry makes for inefficient packing?

The Course is based around lectures interspersed with tutorials in small groups of eight students: this time we had ten groups, a total of 80 students. The students came from a wide range of places, fields of study and backgrounds, and had a similarly wide range of experience of single crystal structure determination. Many of them were from overseas, including from Portugal, Denmark, Yugoslavia, France, Armenia, India, Finland and Ireland, and many other overseas students already working in the UK. This gave the Course its typically strong international character. All lecturers and tutors are present for the duration of the Course, and available for informal questions or discussions: it is common to see tutors devote all or part of their coffee breaks to helping students with particular problems or queries. The immense skill, effort and commitment by the group tutors in engendering cooperation and collaborative working is a distinctive and vital part of the Course and, judging by student feedback, one of the most appreciated. This time we aimed to provide more support in the form of late-afternoon surgeries: it was intended that the lecturers provide these, but they were largely (and very effectively) used by students working within their own tutor groups.

The Course began on the first afternoon with some gentle introductions, including a reminder by David Watkin about some essential mathematics in the so-called "Matrix Mixer". The Course continued for a further seven days with one much needed afternoon and evening off: it is intensive for everyone involved, but particularly for the students and tutors.

The Course covers all aspects of structure determination, including fundamental concepts of symmetry, diffraction, Fourier synthesis, direct methods, least-squares refinement and their application to solving and interpreting structures. The more practical aspects covered in lectures included topics such as crystal growth techniques, data collection, structure solution, refinement techniques and structural interpretation. The Course finished with two lectures given by staff of the Cambridge Crystallographic Data Centre: Owen Johnson on their new CIF editor, enCIFer, and Lucy Purkis on Mogul, the new knowledge-based library of intramolecular geometries derived from the CSD.

Undivided attention at an evening session

The evenings were given over not only to the Matrix Mixer, but also to sessions on crystallisation, a (partly crystallographic) bar quiz, an expert panel and student presentations. In the last of these, each tutorial group worked to produce a science-based presentation, i.e a 'performance' of spoken word, singing or actions and these were all of a very high standard, hugely entertaining and surprisingly informative. One evening session was the Ceilidh, where dancing skills are optional. The Course Dinner took place on the final evening, where those responsible for making the Course a success – sponsors, organisers, lecturers, tutors, students and local staff – were all thanked for their efforts and everyone has a chance to relax after a very busy week.

The Course was clearly much appreciated by the students, who provided us with valuable feedback which will inform the content and structure of the next

Course in 2005. There continue to be particular challenges in the wide range of previous experience of mathematics and crystallography. We are considering a number of ways to provide more support for the mathematical aspects of the Course. This year Peter Main kindly ran an impromptu session on essential mathematics, but in 2005 this should be a formal part of the introduction to the Course.

A book based on the Course, written by one past and three current lecturers and entitled "Crystal Structure Analysis: Principles and Practice" was published by OUP in late 2001 and has been very favourably reviewed. See Crystallography News, December 2002, page 33.

Tutorial group hard at work

The venue was again a highly successful element of the Course. Trevelyan College offers lecture facilities in close proximity to accommodation, catering and social amenities, so that different aspects of the Course can be smoothly integrated.

The number of scientists who depend on crystallographic structure determination continues to grow, as does the demand for structural results: it is an essential technique but one where they must acquire expertise quickly and alongside other methods. The Intensive Course is a unique resource, offering concentrated study and learning support not available elsewhere. Computational black boxes abound in crystallography. In many cases these work reasonably well with their default settings, but only by really appreciating how they work can difficult or non-routine problems be solved: developing this understanding is a prime objective of the Course. The Tenth Course is currently being planned, and will take place in Durham in April 2005.

Special thanks are due to organisations which generously provided financial support for the Course: EPSRC, IUCr, ICDD, Chemical Computing Group Inc, Bruker-Nonius AXS, Pfizer Ltd, Oxford CryoSystems and Rigaku MSC.

Sandy Blake
Course Director 2003

7th International School on the Crystallography of Biological Macromolecules

Villa Olmo, Como,
Italy May 10 - 14, 2003

The conference was set in the beautiful surroundings of the Villa Olmo, on Lake Como. The Villa was built in 1797 and was visited by Napoleon Bonaparte in the same year. Since 1982 the Villa has been the home of the 'Alessandro Volta' Centre of Scientific Culture and has hosted many international events. Lunch was served daily at the villa, and refreshments were provided in the grounds. The ballroom served as the lecture room, with magnificent, ornate frescos and the adjoining equally magnificent rooms were used for the poster sessions. Unfortunately the formal gardens to the front of the Villa that run to the edge of the Lake were closed off for renovation work.

Villa Olmo

The conference began at 3pm on Saturday the 10th May with a few introductory words from the organizer Kristina Djinovic-Carugo. This was followed by the opening lecture 'From DNA sequence to Protein Structure' by Terry Brown (UMIST, UK). The lecture set out the historical road from Mendel's theories to DNA structure, which was appropriate in this 50th anniversary year. It then proceeded to genomics, proteomics and metabolomics. The talk raised the disadvantages of these 'omics' techniques, referring to them as 'stamp collecting' methods. The speaker pointed out the place that structural biological crystallography would have in this century and that it would provide insight into the functions of the gene products. Three talks followed regarding the expression of recombinant proteins and assessment of their quality. One talk of interest was that of Imri Sinning (Heidelberg, Germany) who talked about use of transgenic Drosophila in the expression of membrane proteins,

expressing them in the insect eye. Apparently the freezing of the flies in liquid nitrogen and a shake and sieve method rapidly purifies the heads of the flies away from their other components!

The structure of the spindle checkpoint complex Mad1-Mad2 important in the cell cycle was reported by Andrea Musacchio (European Institute of Oncology, Milan) on day one. Wolfgang Baumeister (Max-Planck Inst. Germany) gave the last lecture of the day describing a different structural approach using electron tomography to provide 3D images of the cells entire proteome. The day was brought to a close with a wine reception held at the Villa. The reception was intended to be outside, but the onset of rain saw it moved to a veranda.

Day two saw a number of lectures on data collection, structure solution and refinement. These ranged from talks about how to obtain better data and maximize 'in-house' data collection, improving diffraction quality of crystals and designing the diffraction experiment. The detector requirements were discussed along with data processing strategies and measures of quality. The next session included talks about MAD phasing and maximum likelihood molecular replacement was discussed by Airlie McCoy (Cambridge, UK) using an imaginary dice game!

After lunch at the Villa there was the first of two poster sessions, held in two more of the Villa's ornately decorated rooms. Some 53 posters were presented on structural research topics from a diverse array of organisms, covering enzymes, receptors, signalling proteins, glycoproteins, DNA, complexes and both NMR and X-Ray methods. The final session of talks for day two were on software, validation and high resolution structures. Garib Murshudov (York, UK) talked about the principles of macromolecular refinement and Alwyn Jones (Uppsala, Sweden) talked about interactive electron density map interpretation using the program '0', demonstrating some of the new tools available in the program. Alwyn provided much entertainment in his talk by having an apparent amazement with the 'slide-changing' abilities of Microsoft PowerPoint! Gerard Kleywegt (Uppsala, Sweden) discussed the limitations and uncertainties in experimentally determined structures and ligands and the requirement for structure factors to be made available for the calculation of the electron density maps, thereby allowing the viewer/reader to validate the structural information presented to them. The last lecture of the day by Claude Lecomte (Vandoevre-les-Nancy) covered ultra high resolution and the possibility of calculation electrostatic potentials and protein ligand interaction energy.

The sessions on Monday were dedicated to high through put methods and techniques. The day opened with a lecture by Dimitrij Frishman (Neuherberg, Germany) on target selection for high through put projects. He discussed the ways in which groups had selected a target area and the ways in which this target area was further reduced by the removal of typically difficult proteins, such as membrane bound proteins. Par Nordlund (Stockholm, Sweden) followed this with a talk about strategies for HTP protein production. Valerie Campanacci (Marseille, France) gave an example of laboratory scale structural genomics, highlighting the bottlenecks and success rate so far. The major bottleneck is obtaining high yields of soluble recombinant protein and the success rates so far appear to be low. The target strategy in this case was to aim for the 'low-hanging' fruit, so one might have hoped for a higher success rate. Jan Lowe (Cambridge, UK) also talked about the HTP strategy and estimated that each crystallization experiment cost 10 pence and with around 400,000 experiments done and only 35 structures solved it is still very expensive with relatively low success, given the target selection procedures. All of the HTP strategies appear to use the vapour diffusion method of crystallization and there appear to be some issues with the success of the dish sealing robots and protein wastage. Julie Wilson (York, UK) talked of the progress being made at crystal image recognition and the success she is having and Anne Poupon (Gif-Sur-Yvette, France) talked about HalX, an electronic lab-book, putting an emphasis on the importance of recording all negative experimental results alongside the positive.

Victor Larnzin (DESY, Hamburg, Germany) provided a 'musical' movie of the automated beamline equipment as DESY, set to a tune by Shania Twain, with a finale robotics 'dance' to Blur! He also provided statistical trends in the data collected at DESY in the last year, discussing what they may imply for the future. On the tunable beamline BW7A only 38% of structures are being solved

within I month and SAD experiments are dominant on this tuneable beamine. There seems to be a trend towards smaller crystals and larger proteins, with larger unit cells becoming more common. He also talked about the program BEST being developed by Gleb Bourenkov and Alexander Popov (Max-Planck, Germany). The program provides an automated experiment strategy for data collection. Ed Mitchell (ESRF, Grenoble, France) also provided and insight into the automated set up at ESRF, discussing the 'Fed-Ex' type of experiment already in use by some industrial users. Gerard Bricogne (Cambridge, UK) and George Sheldrick (Göttingen, Germany) discussed experimental phase information and how progress was being made towards dealing with phasing in a HTP world. Anastassis Perrakis (Amsterdam, Netherlands) provided insight into the program ARP/wARP, towards automated model building and Udo Heinemann (Berlin, Germany) talked about BESSY at the Protein Structure Factory in Berlin. He discussed their target strategy, protein production and automation. Again, success rates seemed low, out of 600 targets only 163 were expressed as soluble proteins and only 115 were in high yield quantities, giving a success rate at the protein production point of about 20%. Of the 163 proteins produced to date, only 60 had been purified to date. David Stuart (Oxford, UK) talked about 'SPINE' (structural proteomics in Europe), again highlighting the difficulties in obtaining soluble recombinant proteins. The day was closed with a lecture from Eric Hovestreydt (Broker, Netherlands) about detectors, with particular reference to the use of CCD detectors with 'in-house' X-Ray sources.

Tuesday morning began with a lecture from Ulrich Gohlke (London, UK) on the structural analysis of proteins by transmission electron microscopy and its use with larger proteins. This talk was followed by Werner Kuehlbrandt (Frankfurt, Germany) discussing electron microscopy of membrane and transport proteins. Dimitri Svergun (DEST, Hamburg, Germany) finished the session by talking about small angle X-Ray scattering and neutron solution scattering, providing shape information and techniques that can be used to improve the information acquired by these methods. The rest of the talks for the day were presentations on structures obtained, which were as varied a selection as the poster session.

Day 3 also saw the second poster session where a further 53 posters were presented. The structure talks were of high quality, providing many insights into structure function relationships, complex formation and DNA binding. Almost all of the speakers provided an animation of their protein structures, with some providing ambitious 'morphs', demonstrating domain movements. It seems that a new 'minimum' level of animation had been set for talks!

Day 4 saw a continuation of the structure talks. The final lecture came from Kim Hendrick (EBI, UK) about EBI-MSD (The European Bioinformatics Institute Macromolecular Structure Database). The emphasis was on the newly developed search tools on the database and the flexibility this had for users. The conference was closed with a few words from Phil Evans (Cambridge, UK). He commented on the previous 6 schools held in the past and on how wet and cold they had been and that we had been very lucky with the hot weather we had experienced. He mentioned the crystallography 'underworld' who organize these events, implicating the absent organizer Keith Wilson (York, UK) as the 'Godfather', clearly demonstrated with photographic evidence! After thanking the organizers, secretariat and support staff he proceed to show some pictures of the sun-bathing delegates in the grounds of the Villa and, keeping to the animation standards set, proceeded to show a movie of the diggers in the fenced off Villa garden, with the promise that a good percentage of the student delegates get invited back to speak!

The conference provided many insights into the future of protein crystallography and allowed the delegates the opportunity to hear how some of the new high through put areas are progressing. For the student delegates this has emphasized the career openings in the field and allowed us to see our own work in a broader scale. We had the opportunity to put faces to many of the renowned names in the field and to speak to them.

Having met fellow students from all over Europe, the overwhelming feeling that I came away with was that we are all equally enthusiastic about the field we have chosen to go into and that this promises a strong future for biological macromolecular crystallography in Europe.

Kirsty Line
University of Exeter

Diamond - First User Meeting,19 May 2003 in RAL

Gerd Materlik welcomed users to the meeting held to inform them on the Status of the Diamond Project, Phases 1 and 2 of the Beam line selection process and get feedback on their needs. He reported that Diamond Light Source Ltd (DLS) now had 60 staff and expected to have 100 by the end of 2003. He anticipates that the main construction challenge will be the small source size and maintenance of the floor stability to less than 1 Micrometer during the time of an experiment.

PLANNED TIMETABLE
March 2003 Begin enabling works

May 2003 Pile driving begins to stabilise the machine foundations.
October 2003 Begin the main building works

Removing the old concrete from the former RAF runway in warm dry weather caused much dust. The concrete was broken up and used in other foundations

September 2004 Begin machine installation and construction of Office Block due for completion in August 2005. Hope for a beam in the storage ring by January 2006, to start beam line commissioning in June allowing the first users in January 2007.

Pile drivers in action in July

Finally he announced that ***Richard Nelmes*** had just been made a Fellow of the Royal Society in the list of new Fellows for this summer, presented him with a celebratory bottle of champagne and asked the audience to join him in offering Richard our congratulations.

Richard Walker, Technical Director, then described the status of the machine and office building. The machine design has a large capacity for insertion beam line devices with 24 'cells' arranged with a 6 fold symmetry. They are hoping for an initial beam current of 300mA and eventually hope to reach 500mA.

The 3 floor Office building will be linked by a covered bridge over the machine perimeter road to the machine building. The offices will be a mixture of Open Plan in the central part with cellular offices on the outside.

Providing stable ground conditions for the machine is difficult because of the variation in soil properties across the site and because the underlying rock is chalk with a seasonal variation of the water table. Only a solution based on piles will give suitable stability, with a compromise between static and dynamic parameters. The piles will be unsleeved, with a 600mm disc, 11 metres deep and 3 meters separation. There will be a void between the ground surface and the 600mm thick experimental hall floor. The floor under the storage ring will be 850mm thick.

A 'turnkey' contract will be let for the construction of the injector, a 100Mev Linac with a maximum frequency of 5Hz. The booster magnets are designed; a 'Call for Tender' for 'magnet and vacuum girder assemblies' will be issued shortly. These will be installed and commissioned by DLS staff.

There will be 7 insertion devices in Phase 1; a vacuum undulator based on an ESRF design with gap taper mechanism should allow possible installation of a smaller side station later. The storage ring air conditioning system is planned to be similar to the Swiss Light Source with variation of ± 0.5° C. The temperature of the lower 4m of the experimental Hall will be controlled to ±1°C on a given day, with a seasonal variation of 5°C.

Colin Norris described the Science Program. 7 beamlines are planned for development by 2007 in Phase 1; in Phase 2 14 more beamlines should be available by 2011. The beamlines are grouped in a 'Village Philosophy' with those for 'Life Sciences' together and 'Surface Science', 'Nanostructures' and 'Extreme Conditions' near to 'Magnetism and Materials' and other possible spectroscopy beamlines. During construction each beamline will have 2 Beamline scientists and a technician; they will collaborate with other laboratories, sharing the best practice with the SRS at Daresbury, with Soleil and the ESRF in France and the Swiss Light Source. Beamlines for all possible experiments will not be provided at Diamond, instead the 3 source

scenario outlined in the original Woolfson report is assumed with separate accelerators offering a range of complementary energies. For example some facilities will be at Soleil, but notable absences at the moment for Diamond are: single crystal X-ray diffraction, small angle scattering, surfaces and interfaces and soft X-rays.

There will be new experimental opportunities; for example combining synchrotron radiation and lasers and new communities developing in areas such as materials processing, pharmaceuticals and engineering.

They are still working on getting funding for the Phase 2 construction; meanwhile the Scientific Advisory Committee (SAC) will be discussing 8 proposals tomorrow, (20 May 2003) only 4 of which are likely to be in the final proposals for Phase 2. The deadline for submission of proposals for further Beam lines is **1st October 2003.**

Jim Naismith, St Andrews, spoke on opportunities for the Life Sciences, highlighting a personal selection of the main activities in the crystallography of protein complexes. Some structural work gives useful information on medical conditions, for example, DNA damage signalling is important in cancer research and insulin signalling will become important in future as more of our obese population develop diabetes. Other topics include studies of large assemblies, drug design, chemistry, circular diochroism and small angle Xray scattering.

John Evans, DLS, explained how Diamond features including brilliance, polarisation and a user friendly control system will be useful to the physical sciences in materials, environmental science and process problems in engineering. Catalysis studies are applicable to the development of greener fuels, pharmaceuticals and artificial fragrances. The beam tunability is important in modelling 'in situ' catalysis experiments on flowing systems. He discussed plans for the development of 'Research Hotels' to provide each community of users with space for meetings, laboratories and other specific equipment for their speciality.

Mike Henderson, University of Manchester, discussed details of the migration of user programmes from the SRS to Diamond just before the audience adjourned to the Exhibition area for a buffet lunch and Posters.
After lunch users split into 6 groups, each with a leader and a DLS employee as Secretary to discuss the following questions until tea at 15.30:

- *Is the current portfolio of beamlines (Year 1 and Year 2) a good match with the needs of the community?*
- *If not, what areas should be considered (bearing in mind the proposals for future beamlines to be considers at the Open SAC meeting on Tuesday 20th May)?*
- *What steps can be taken to ensure a smooth migration of User programmes from SRS to Diamond?*
- *What are the implications for Diamond of the future operations of Soleil and possibly 4GLS?*
- *How can Diamond broaden its provision to attract users who are currently perhaps not aware of the possibilities of synchrotron use?*
- *How should Diamond keep the user community informed of progress on the project?*

All groups then met together to hear Phil Woodruff describe the function of the Diamond Scientific Advisory Committee, SAC, which was to meet the next day.
Colin Norris then chaired an Open Discussion session with each group reporting back to the meeting, and in conclusion, he summarised this discussion before the meeting broke up for more informal chats around the buffet.
Kate Crennell

Further details are available on the web site, **http://www.diamond.ac.uk** or from Sue Gill, Science Co-ordinator, Tel: (01235) 446516 email: **s.m.gill@diamond.ac.uk**

Left to right, Elspeth Garman, newly elected BCA Council member in discussion with Chick Wilson, BCA President, and Christine Cardin, BCA Secretary.

Crystallisation 2003

6-9 July, Sheffield, UK

The Seventh International Symposium on Crystallisation in Glasses and Liquids was held this year at the University of Sheffield, UK. Starting in the United States in 1960 this is a major conference with a long tradition. With growing interest in glasses and glass-ceramics science and technology, this conference focuses on bridging the gap between the scientific understanding of nucleation and growth in glasses, and the industrial applications of glass-ceramics. This truly was an international arena, with representatives from Brazil, Argentina, Russia, Japan, Saudi Arabia, USA, and many European countries.

For me this was an opportunity to attend my first major international conference. I presented my paper in the Crystallisation of Metallic Glasses session with a talk entitled "The kinetics of crystallisation in $Y_{67}Fe_{33}$". In my talk, I explained how by using the Avrami-Johnson-Mehl equation, we could successfully model the kinetics of phase formation of a novel Y-Fe phase from amorphous $Y_{67}Fe_{33}$, studied using real-time neutron diffraction.

Conference proceeding started with an address from the chairman, Professor Peter James (University of Sheffield), paying homage to Michael Weinberg (deceased 30 December 2002). The first paper presentation of the conference (Michael Weinberg Memorial session) was a lively talk by Professor Edgar Zanotto (University São Carlos, Brazil) on homogeneous nucleation in supercooled liquids. Fundamental arguments such as the relevance of Turnbull's equations and classical nucleation theory were discussed.

In three packed days, papers were presented in sessions ranging from theory and modelling, experimental studies, and metallic glasses, to commercial systems and vitreous waste forms. However, by far the largest contribution came from the bioceramics and glasses community. Bioceramics, and bioactive materials applications in medicine and dentistry has gained wide interest over recent years. It is a subject relevant to everyone as we all benefit from this research through our hospitals and dental surgeries.

Dr. David Wood (Dental Institute, University of Leeds) gave the first talk from this field in which he discussed the crystallisation of barium fluormica based glass-ceramics following one and two stage heat treatments. The purpose of this study was to optimise mechanical properties and machinability of these micas for dental application (crowns, bridges etc.). Dr. Wood and colleagues used kinetic neutron diffraction, to observe the formation of mica phases in real time at the Institute Laue Langevin, Grenoble, France. He explained how by using neutron diffraction they could penetrate the bulk of the sample with data collection times of 2 to 3 minutes. This allowed them to observe a clear different in the phases present in the two distinct routes (unseen using XRD). For their study, this could explain the differences in mechanical properties observed in the two final products.

Dr. Robert Hill and Dr. Artemis Stambolis (Imperial College) presented papers on crystallisation in barium fluorphlogopite glass-ceramics, and apatite-mullite glass-ceramics respectively. Using magic angle spinning nuclear magnetic resonance (MAS-NMR), Dr. Hill observed a large broad peak in the ^{27}Al spectrum that he assigned to four-coordinated aluminium with no five or six coordinated Al seen (in contrast to other similar materials). Using ^{19}F MAS-NMR they were able to detect any fluorine-containing precursor crystal phases, and from differential scanning calorimetry (DSC) measurements during crystallisation, they detected three particles sizes formed from volume and surface nucleation. From these studies, they hope to develop machinable glass-ceramics from novel materials.

Jennifer Bibby (University of Manchester) presented her paper on fluorapatite-mullite coatings. These bioactive coatings are used on bone implant materials to encourage the fixture of implants in patients, and thus reduce the post-operative recovery time of patients. She introduced her novel technique of electrophoretic deposition (EPD) of these coatings with sintering to improve adhesion. It has been possible to coat titanium alloys using EPD which is cheap and can coat complex geometries.

From industry, Wolfram Hölland (Ivoclar Vivadent, AG, Lichtenstein) presented his paper on glass crystallisation in dental materials. His emphasis was on surface crystallisation in opal leucite glass-ceramics and volume crystallisation in apatite glass-ceramics. He highlighted

translucency, opalescence, chemical durability and good mechanical properties as the main issues in choosing appropriate restorative biomaterials for inlays, veneers, crowns or bridges. By controlled surface-volume crystallisation of composite leucite-apatite glass-ceramics he has shown, using high temperature XRD, that two different crystal phases can be produced in one material enhancing the overall properties of the dental material.

In the last talk of the bioceramics and glasses sessions, Professor Ric van Noort (University of Sheffield) provided a comprehensive overview of dental glass-ceramic applications including the development of biocompatible dental materials; improved dental adhesives; and maxillofacial reconstruction. He challenged the audience to come up with a "perfect" material that resolves all the issues in bioceramic development.

There were many other enjoyable presentations from other fields, such as Professor Lindsay Greer's (University of Cambridge) paper on multilayered metallic glasses grown by sputtering and studied by speculative XRD.

Big names in the glasses industry such as George Beall (Corning), Wolfgand Panhorst (Schott Glas), and Wolfram Hölland (Ivoclar Vivadent) provided insight into the main issues in the applications of crystallisation of glasses technology both in terms of products (kitchenware, dinnerware, telescope mirrors, dental restoration) and safe waste disposal (nuclear and municipal wastes).

All refereed and accepted papers will be published in the Society of Glass Technology journals, 'Physics and Chemistry of Glasses' and 'Glass Technology'.

The wide range of techniques used in the study of crystallisation of glasses and liquids was very apparent from the diverse papers presented at this conference. The large number of countries represented at this conference provided a diverse yet informal atmosphere in which it was possible to discuss this growing area of research and technology.

I thoroughly enjoyed my three days in Sheffield attending Crystallisation 2003 and I would like to thank the organisers of the conference for inviting me to present my paper. I would also like to express my gratitude towards the Physical Crystallography Group of the Institute of Physics and the British Crystallographic Association for providing me with a generous bursary, without which it would not have been possible for me to attend the conference.

Maisoon Al-Jawad
University of Leeds

RSC Chemical Landmark: The Braggs at Leeds University, 1912-1914

Although the Nobel Prize won by father and son W.H. and W.L. Bragg in 1915 was in Physics, X-ray crystal structure analysis, which the Braggs founded, has been enormously influential across a range of sciences from mineralogy to medicine. During World War 2, WLB played a leading role in setting up the X-Ray Analysis Group, a precursor of the BCA and, in 1946, he helped host what was effectively the zeroth IUCr Congress, followed by a symposium at Leeds, which had four separate X-ray crystallographic groups.

On 1 July, 2003 (the anniversary of WLB's death), the Royal Society of Chemistry (RSC) marked the contribution to chemistry of the joint research by the Braggs 1912-14 at Leeds by making the site a National Historic Chemical Landmark. At the ceremony, RSC chief executive David Giacherdi noted that the Braggs' achievement underpinned several other RSC landmarks, including those for Dorothy Hodgkin at Oxford and for DNA at Leicester and Kings College London. Conscious of contemporary fears about the survival of University Chemistry Departments, the Vice-Chancellor, Sir Alan Wilson, reaffirmed Leeds University's commitment to research in the

physical sciences. Memorabilia selected from the extensive Bragg archives at the Royal Institution were brought by Dr Frank James to display alongside an original Bragg notebook from the Leeds period. There were also messages from the RSC president, the University Chancellor (an unrelated Bragg) and the M.P., Hilary Benn. Derry Jones produced for participants a pack of short biographies of the Braggs and historical summaries of their achievements, and also contacted many of the descendents of WHB and WLB, several of whom have followed successful careers in science and technology. WLB's daughter Margaret (Lady Heath) unveiled the RSC plaque in the presence of a chemist grandson of WLB, Dr Charles Bragg, appropriately (in view of the encouragement both WHB and WLB gave to research in industry) a Director of R and D. Also represented were the Pippins – X-ray crystallographers who had been doctoral candidates in Chemistry at Leeds in the 1950s under the late Sir Gordon Cox, FRS.

Professor D.W.J. Cruickshank, a former Bragg Lecturer, then gave a fascinating talk on the Braggs' work on X-rays and crystal structure 1912-15 and its continuing impact on chemistry over the succeeding 90 years. None of the five presentations that we have heard previously from DWJC has begun with his unpacking salt and sugar from supermarket bags or has contained no equations of greater complexity than $n\,\lambda = 2\,d\,\sin\,\theta$. Durward first explained how the scientific background of each Bragg prepared him for the crucial creative period at Leeds immediately after they had heard of the discovery of X-ray diffraction by Friedrich, Knipping and von Laue in 1912. The father, WHB, only took up original research in Australia at the age of 42 but had in Adelaide acquired a wealth of experimental experience of radioactivity and X-rays, research quickly recognised by an FRS in 1907, and in instrumental expertise (aided by a talented instrument maker). Arriving as Professor in Leeds in 1909, he was soon involved in controversy about the wave/particle nature of X-rays and γ-rays. The son, WLB, already at 22 a graduate of both Adelaide and Cambridge, was to begin research at the Cavendish (in poorly equipped laboratories) in another field with J.J. Thomson. However, WLB was aware of the work of W. Barlow, whose celebrated "Size doesn't matter" remark related to gloves for demonstrating RH and LH objects, and W.J. Pope on symmetry theory and how crystals might be structured internally (at a time when crystal data involved interfacial angles from optical goniometry). Following long-vacation discussions between father and son in Yorkshire, the simplifying insight of X-ray *reflections* from crystallographic planes came to WLB (at Cambridge) later in 1912, while WHB soon initiated X-ray spectroscopy. In the Christmas vacation and, even more so, in the summer of 1913, father and son worked "furiously, far into the night" with the ionisation spectrometer developed by WHB from the ionisation chamber. Many of the structures solved (and published in the journals) were gathered in the Braggs' book *X-Rays and Crystal Structures,* published in 1915, by which time each author was occupied in non-crystallographic war-work.

After World War 1, WLB succeeded Rutherford at Manchester to work on inorganic structures, especially silicates (shortly before WLB's death in 1971, moon rocks had been shown to possess analogous chains). After a time at UCL, WHB moved in 1923 to the Royal Institution, where his school tackled mainly organic structures. Durward pointed out that later in the 20th century Leeds had continued to have scientific-descendence links with the Braggs. Three of WHB's young collaborators at the RI in the 1920s, W.T. Astbury, Kathleen Lonsdale (then Yardley) and E.G. Cox, later made influential contributions to crystallography at Leeds.

W.T. Astbury began X-ray studies in Textile Physics at Leeds in 1928, investigating wool proteins and stretching transitions in wool fibres and later, in the Department of Biomolecular Structure, obtained, with Bell and Beighton, early X-ray photographs of DNA. Also, from the 1970s, the Astbury Department of Biophysics, as it became, was led by Tony North, who, a generation after Astbury, had worked at the RI under W.L Bragg's directorship. Durward felt that it was remarkable that WLB, who had determined the NaCl structure in 1913 was able in 1963 to draw the lysozyme structure (work to which Tony North contributed) in time for his 75th birthday. The successive careers of each Bragg at the RI (WLB moved there from Cambridge in 1954) exemplify the interaction between research and teaching of, especially, the general public and the young.

Left to right, Professor Durward Cruikshank, Dr Charles Bragg (grandson of WLB), Leeds Deputy Lord Mayor Alison Lowe, Dr David Ciachardi (RSC), Lady Heath (daughter of WLB), Professor Derry Jones.

Kathleen Lonsdale (who graduated at almost as early an age as WLB and was later DBE, FRS) spent a productive time (in more than one sense) at Leeds, 1927-29, establishing the planarity of the benzene ring in the structure of hexamethylbenzene.

The third of WLB's young researchers, E.G. Cox (later Sir Gordon, FRS, Secretary of the ARC) set up at Leeds in 1945 a powerful chemical crystallography group. Its aims were to utilise 3-dimensional X-ray analysis to measure as accurately as feasible the dimensions of small molecules and to establish the stereochemistry of inorganic compounds, especially those of transition metals.

Finally, Durward referred to the wide ramifications in science of crystal chemical structures, to which the Braggs laid the foundations in Leeds, 1912-14, to the magnitude of macromolecular structures that can now be solved, and to the immense contemporary productivity of structures. These all illustrate what a Swedish postage stamp succinctly credits the Braggs with: "services in the analysis of crystal structure by means of X-rays". In celebrating the Braggs, the RSC Landmark recognises what was probably the most significant work – whether in science, medicine or the arts – ever done at Leeds University. And WLB remains the youngest ever winner of the Nobel Prize.

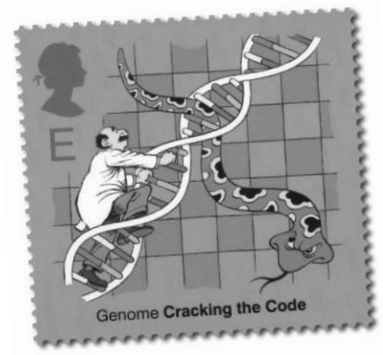
Derry W. Jones

The 50th Anniversary of the Discovery of the Structure of DNA

In April 1953 the discovery of the structure of DNA was announced in letters to 'Nature'. This event has been commemorated by many institutions world-wide.

The Institute of Physics published a special section 'Physics and DNA' in 'Physics World' March 2003. The first one is a brief history of crystallography from the research of the Braggs to that of J.D.Bernal and Max Perutz in Cambridge culminating in the discovery of the structure of DNA. This makes an excellent introduction to the subject for today's students of biological structure who may not be aware of the part played by physicists in early research. The second article is concerned with the micromechanics of DNA explaining how advances in manipulating single DNA molecules lead to better understanding of the mechanisms of repair of the double helix. The third article discusses how DNA can be used as a building block in the construction of new nanomaterials. A free single copy of the March 2003 issue of 'Physics World' can be obtained from Claire Webber, Product manager magazines, IOP Publishing Ltd, Dirac House, Temple Back, Bristol BS1 6BE email: claire.webber@iop.org

The UK Post Office issued a set of 5 commemorative stamps in February, with cartoon depictions of 5 important research topics which had been worked on during the last fifty years, as a result of the discovery of the structure. The Post office designers apparently believe these show typical scientists at work. Copies of these stamps were displayed on a Poster at the York meeting and members asked to decide whether their fellow workers on biological structures resemble these cartoon characters.



Issued for postage to Europe. Do you know any structural Biologists who look like this?

Channel 4 has broadcast a series of documentary programs on TV 'DNA: The Story of Life' the first one concerned with the discovery

of the structure of DNA itself had interviews of the most of the original research workers who are still living 50 years later.

The one who tragically died young in 1958 was Rosalind Franklin. She is represented in a new biography by Brenda Maddox, 'Rosalind Franklin. The Dark Lady of DNA', published in 2002. It had good reviews and was serialised on BBC radio 4, but at time when few working scientists would have opportunity to hear it, 9.45am. On page 61 of the February 2003 issue of 'Physics Today' there is another article on Rosalind Franklin by Lynn Elkin which is freely available on their website.

Other books include '50 years of DNA' published in association with 'Nature' in April 2003 ISBN 1-4039-1480 X and a biography of James Watson 'Watson and DNA: Making a Scientific Revolution' ISBN 0-738-203-416. 'Scientific American' April 2003 has a feature article 'A Conversation with James D Watson' which can be found on their website.

I exhibited a Poster at the BCA Annual Meeting in York 2003 and am now making a page on the BCA Website where I am collecting news of the events, and setting up links to all the events I know of so far, please look at **http://bca.cryst.bbk.ac.uk/BCA/CNews/2003/Jun03/DNA50.htm** and tell me of other publications or events.

Kate Crennell

BCA Spring Meeting: Synchrotron Radiation

The Synchrotron Radiation session was chaired by Harry Powell with speakers Simon Teat from CLRC Daresbury Laboratory, Tony Bell from the University of Manchester and Paul Raithby from the University of Bath.

Simon Teat spoke on "A Bright Way of Handling Difficult Data". He noted that the scattering efficiency of a crystal depends on both the square of the number of electrons and crystal volume, and inversely on the square of the unit cell volume. The effect of disorder is that scattering power quickly tails off, and other factors include wavelength of radiation, mosaicity and intensity of the X-ray beam. Synchrotron radiation offers an order of magnitude higher flux than a conventional X-ray source and hence is useful for weakly diffracting crystals, disordered crystals and crystals with supercells. Simon described examples of crystal structure determinations where use of synchrotron radiation allowed supercells to be determined. One example was of a microporous material where conventional X-ray data gave a disordered template molecule. The supercell solution using synchrotron data gave a solution with a fully ordered template molecule, allowing for the study of hydrogen bonding interactions.

After being presented with his fun-run T-shirt, Tony Bell spoke on "Phase Transition in Mercury Sulphides". There are a number of polymorphs of HgS including trigonal cinnabar, cubic metacinnabar and hexagonal hypercinnabar. Tony reported variable temperature EDXRD (energy dispersive X-ray diffraction) studies on a sample of synthetic HgS, where cubic metacinnabar was present at all temperatures, although it was pseudocubic at temperatures below 583 K, with a phase transition at 748 K to hypercinnabar. The high temperature phase was retained on cooling. A mineral sample of metacinnabar also showed partial transformation to hypercinnabar at high temperatures, while mineral cinnabar did not undergo a phase transition. Combined EXAFS/XRD measurements were made in situ during synthesis of HgS, where amorphous metacinnabar crystallised to the pseudocubic form before forming a poorly crystalline cubic phase.

The final speaker for the session was Paul Raithby who spoke on "The Final Frontier: Time Resolved Structural Chemistry". Normal crystal structures give a time-averaged ground state structure. However, advances in dynamic crystallography may allow us to have a better understanding of light induced processes, and they have the potential to allow us to make molecular movies of molecules going into excited states, reacting and forming products. He described powder XRD studies of photoactivated cycloaddition of coumarin 3-carboxlic acid. Single crystals may be studied by determining a low temperature ground state structure, then irradiation with laser light to excite around 20% of molecules to a metastable state, then re-determining the structure and looking for differences between the ground and excited state structures. A co-crystal of 2,2'-dihydrobenzophenone and 4,13-diaza-18-crown[6] did not show

any significant structural differences between ground and excited states. Photo-induced linkage isomerism in the complex trans-[Ru(NH_3)$_4$(SO_2)Cl]Cl was also studied. Paul finished by describing work in progress on molecules with short-lived excited states that can be studied by synchronising laser pulses with the bunch structure of synchrotron radiation.

Michaele Hardie

High Throughput, Databases and Data Mining at York

Session 1: Biology and Chemistry

The first step for the crystallographer is often the hunt for a decent single crystal, and in the macromolecular field, even this is being automated. ***Julie Wilson*** (York) on the Automatic Evaluation of High-Throughput Crystallisation Trials gave a mathematical approach to finding crystals. The wells of crystallisation plates were scanned for "interesting objects" which were evaluated according to the shape of the object's boundary. The parameters were chosen such that single well-formed crystals gave the best score, and with each well indexed, the best samples could be traced more quickly and save the crystallographer's time, eyesight and sanity.

Marek Brzozowski (York) - *Low-Cost Alternatives for Nano-Crystallisations,* told us about finding a good robot for handling tiny amounts of sample in a reproducible way. It was the Mosquito robot that came up trumps and this was also displayed in the commercial exhibition, for its ability to prevent evaporation of the sample by using injection with needles, having disposable tips and a user friendly interface for operation.

Horst Puschmann (Durham) - *DIMAS: Seamless Crystallography from Sample Submission to Archiving of Results* showed us a way of running a large small molecule lab efficiently by having both queue and file location management, for easy tracing of data after collection. It's based on an MS Access database which also acts as a link to regularly used structure solution and refinement packages, to guide the user through the process for submitting a sample to a CIF ready for deposition.

Session 2: Chemistry and Industry

David Rendle (The Forensic Science Service, London) - *Database Use in Forensic Analysis* gave a fascinating talk on how powder diffraction applied to paint and drugs can tell us why scaffolding has paint on it and also chart trends in drug abuse. We learned that when dealers stole their raw materials for amphetamine manufacture from pharmacies who had optically active forms, the chirality was apparent in the resultant drugs. Glucose monohydrate is used to cut cocaine because its particle size and free-flowing properties are best at mimicking cocaine. Scaffolding paint contains specific markers so if a builders' scaffolding gets stolen and is subsequently found, the original owner can be traced. Materials were identified using pattern recognition particularly the identification of the three strongest lines (mini-Hanawalt index) in the powder diffraction pattern. Some of the data were collected on a Debye Scherrer camera and the photos examined on a light box. The DNA database was also mentioned as a valuable source of data in the fight against crime, particularly since most crimes are committed by repeat offenders, as high as 90% for rapists.

Richard Storey (Pfizer) - *Automation of Solid Form Screening Procedures for the Pharmaceutical Industry and How to Avoid the Bottlenecks*
In the development of pharmaceutical products, reducing the time a product takes to get to the market is crucial. A change in solubility resulting from a polymorphic change is disastrous perhaps leading to the loss of patents. The complete understanding of the solid form and how to control the form made is a cornerstone of pharmaceutical development and manufacture. Powder diffraction and Raman spectroscopy are major tools used for characterisation along with DSC and HPLC. In the initial stages of screening, very small quantities are used and inspection is done manually with a hot stage microscope so not everything is automated. On a larger scale (1g) a polymorph screening robot is used. Each sample is assigned a reference code and this follows the sample, scanned by a robot, throughout the screening process so its history can be traced. High throughput powder XRD was carried out using the Bruker GADDS system which uses an area detector, thereby reducing the effects of preferred orientation. Other measurements included

birefringence employing a polarised stage requiring the well plates to be made of stainless steel and glass for viewing samples. Melting points were also measured and graticules were employed in the microscope lenses for location of crystals using image analysis. To make use of all this multi-dimensional information, pattern recognition was done in collaboration with Chris Gilmore's group in Glasgow using the polySNAP program bringing together the sample information and powder pattern. To illustrate the effectiveness of their set up, in one run, all four predicted polymorphs of a compound were detected.

Mariette Hellenbrandt (FIZ Karlsruhe) - *The Inorganic Crystal Structure Database (ICSD) - Present and Future* gave us some background on the ICSD, the database which contains structures with at least one non-metallic element which now has web interfaces for more user friendly searching. Constructing queries such as the elements of a compound and the mineral form, the powder pattern can be displayed and often the structure too. It is an Oracle database with funding mainly from Germany but also the US and France. CIF deposition is possible but they are currently working at speeding up the process of getting CIF information into the Oracle database.

Session 3: Chemistry

Frank Allen (CCDC) - *High-throughput Crystallography: The Challenge of Publishing, Storing and Using the Results* gave us much food for thought. Currently the CSD has 452, 445 entries, and yearly 33,000 are added. The predicted growth pattern of the CSD was made before the arrival of CCD's. We all know that the throughput of structures of crystallography labs has soared so why are the predictions on structures in the CSD made in the 70's correct? It should be an underestimate. Although nearly 500,000 structures sounds a lot, when you come to search for specific fragments for conformational analysis, there really aren't that many. We need more datasets. Each and every valid crystal structure contributes to knowledge and development of areas such as polymorphism and crystal engineering studies. Frank also made the point about accountability to the tax payer and funding agency as to what they get for their money. Perhaps the proviso "all data should be published" should be included. We all realise that the sheer pressure of time and the labour-intensive nature of getting structures published is a key reason for this bottleneck between structures on crystallography lab computers and the publicly searchable databases. There's also the issue of who "owns" the structure - is it the chemist and/or the crystallographer? Particularly when a valid but not very exciting chemistry paper gets rejected or the structure determination is of a compound that the chemist has no interest in. How do the journals view databases when structures are deposited as private communications? As primary or secondary source of information? – does it constitute publication in their eyes? And what constitutes publication? Could there be a direct link between lab management systems and the database to ease and speed up the transfer of crystal data, with data validation done at source. In this area enCIFer, has been made freely available for the manipulation and validation of CIF files. Some journals don't employ crystallographic referees and structures with serious mistakes have been published in prestigious journals. Sometimes the CSD has been the first referees of published crystallographic data. The issues of collaboration with chemists, journals and publication, and academic recognition will continue to be hot topics.

Steph Harris (Bristol) - *Structural Knowledge Base Development for Metal Complexes* gave us an account of building a molecular geometry library known as MOGUL, an electronic version of Guy Orpen's database comprehensive survey of metal ligand distances published in Dalton since 1989. Access to mean molecular dimensions to hand is essential for accurate refinement restraints, molecular modelling and for structural validation and comparison. The distribution of distances for these fragments needs to be unimodal and sharp, and to do this subdivision of the datasets is necessary according to metal oxidation state, co-ordination number and sometimes spin state. This requires more structures in the database to make effective subdivision possible. For ligands, a template library is being constructed with ligands grouped together according to topology, connectivity, stereochemistry and coordination mode. These groups are also part of a hierarchy ordered according to how specifically the ligand is defined. Bond types are also being classified using the bond valency state method.

Iain Oswald (Edinburgh) - *Rationalising Co-crystal Formation through Data Mining.* The drive for making non-covalent derivatives i.e. making co-crystals of pharmaceuticals is to be able to alter physical properties without changing the chemical constituents which could introduce unwanted side effects. Iain used the example of paracetamol, which has orthorhombic and monoclinic crystalline forms. The physical properties of the orthorhombic form are more attractive to the pharmaceutical industry but the monoclinic form is most prevalent. Yet both forms have very similar hydrogen bonding patterns. Perhaps different adducts can change the hydrogen bonding pattern and give a material with industry-friendly physical properties. The packing patterns of adducts such as dioxane and N-methyl morpholine were shown and for the weaker hydrogen bonds the word was "you are the weakest link – goodbye" when the incoming adduct could make a stronger hydrogen bonding link. Iain also illustrated use of the CSD relational database CSDsymmetry which can look for molecular positions in relation to symmetry operators in a space group - such as whether a solvent molecule is situated on an inversion centre or a two fold axis or general space. For dioxanes, he found that 59% of those extracted from the data base sat on a special position and of those over 80% were inversion centres.

Z'> 1 Session

Sam Motherwell (CCDC) - *Packing Energy Patterns in CSD for Z' = 2* asked can we predict when Z'>1? Can packing energy tell us what polymorphic form we will get? Not necessarily , it doesn't always follow that the most dense with the lowest packing energy will be the preferred form. Molecular shape is also a factor. In fact Van der Waals forces can be stronger in energy terms than hydrogen bonds yet in packing motifs it is the hydrogen bonds that are often focussed on. Where compounds exist in polymorphs where Z' = 1 and another where Z' = 2, there are very small energy differences. It appears that when Z'=2 the structure is trying to be in another space group with local pseudosymmetry between the two crystallographically independent molecules. Certainly it appears to be more common in some space groups such as $P\bar{1}$ and $P2_1$. Sam showed us a survey of functional groups with respect to the occurrence of Z'>1. Primary alcohols are known to have higher incidences of Z'>1 than average , yet bipyridine species also scored highly. At the other extreme, sugars with many hydroxy groups are less likely to have Z'=2.

Ton Spek (Utrecht) - *Z' Structures from a Symmetry and Molecular Geometry Viewpoint*, again using the CSD, Ton extracted about 7000 organometallic and 9000 organic crystal structures where z'=2. In some cases the two independent molecules possessed different conformations, in others they had the same conformation but were related by symmetry incompatible with the lattice symmetry. There are also structures where symmetry has been missed, with his ADDSYM (modified MISSYM) Ton found 466 missed or pseudosymmetric structures out of the 9000 organic structures. An example of missed symmetry was published in JACS last year, with just the picture of the structure and the crystallographic information relegated to the supporting information. Checkcif would have found this error. The level of crystallographic refereeing is an ongoing issue. Ton introduced us to NEWSYM which determines the space group from systematic absences in Fcalc, as extinctions in Fobs may differ from those in Fcalc with poor data. Poor data and disorder hamper detailed analysis of near symmetry as much of the crucial information is in the weak reflections.

Richard Cooper (Oxford) - Z' > 1: *just a nuisance, or something more interesting?* had also looked at the prevalence of Z'>1 with respect to functional groups and temperature of data collection. As yet the low/room temperature dataset is too small to see a definite trend, with the added complication that a form stable at a higher temperature may be frozen in at low temperature, as habitually crystals are flash frozen. When we have two independent molecules we want to see if there is anything significantly different between them and now there is a facility (MATCH) in the CRYSTALS package that enables this and even helps with numbering the structure. As to how close the fit is between the two independent molecules, and how this is related to space groups, the root mean square values were lowest in $P2_1/c$ and worst in P1.
Pseudo-symmetric relationships were found between independent molecules and whilst pseudo-inversion and two fold axes were found, mirrors were notable by their absence. More investigations on the differences between the two molecules involved separating the odd and even data on a

compound that undergoes a second order phase transition so that at 150K there are weak spots relating to a pseudo translation yet at 250K these spots disappear. Wilson plots of the odd and even data have different slopes. The even data relate to the similarities between the structures and the odd data tell us about the differences.

Georgina Rosair

High-pressure neutron diffraction and models of Titan

An account of the PANalytical prize lecture, given by John Loveday at the York BCA in April.

Saturn's largest moon, Titan, is an extremely important body. It is the only moon in the solar system to have a significant atmosphere, and this atmosphere is of considerable interest. It is composed largely of nitrogen with some methane and traces of other organic molecules, and may mimic that of the early Earth and provide insight into the origins of life. A much more comprehensive understanding of Titan's atmosphere and surface are the aims of the Huygens lander on the Cassini mission due to arrive at Saturn in November 2004.

Titan is believed to have condensed from a nebula composed of ammonia monohydrate, methane clathrate hydrate and rock (silicates and iron) at a temperature of ~120K. The standard model of accretion assumes that during the early stages, since Titan was small, gravitational heating of material falling into Titan will have been small and so the rocky and icy components remained mixed.

As Titan became larger, gravitational heating became more significant and the surface temperature increased until the melting temperature of ammonia monohydrate (~170 K) was reached and the surface melted. Material accreting after this surface temperature had been reached became differentiated on impact with the ammonia hydrates melting, the rocky component falling through the molten layer to form a carapace, and the methane hydrate thermally decomposing and losing methane to space.

At the end of accretion, Titan was then composed of an undifferentiated rock-ice core whose pressure ranged from 2-6 GPa and which contained all of Titan's methane. Overlying this was a rocky carapace, which was in turn overlaid by an ammonia water ocean and a crust of ice. After accretion, the core would have been warmed by radioactive decay until thermal expansion ruptured the carapace and initiated core overturn. Calculations suggest methane clathrate hydrate becomes unstable with respect to ice and methane at 1.2 GPa and so just prior to overturn, all of the methane in the rock-ice core is assumed to have been in the form of free methane. During core overturn, the icy components of the core would rise, and the low density of methane implies that it would rise more rapidly than water and ammonia. This rapid rise would permit methane to reach the surface of Titan without being re-enclatharated in the ammonia-water ocean.

The ~5% of methane currently observed in Titan's atmosphere was then thought to be the remnant of this pulse of methane which reached the surface early in Titan's history. But this model has problems. The pulse of methane cannot have been injected directly into the atmosphere because the rate of removal by photo-dissociation is such that all methane would be lost in a timescale much shorter than the life of the Solar System. It has instead been suggested that the atmosphere is being supplied from a methane reservoir either at or near the surface and ideas like a methane-ocean or methane in surface cracks or pores have been postulated. However, these models are complex and difficult to reconcile with the observed rotational dynamics of Titan. Furthermore, the idea of an early methane pulse is based on the calculated or assumed high-pressure behaviour for the icy components since there was until recently no experimental information on the behaviour of methane hydrate or ammonia monohydrate along the relevant P-T path.

The Paris-Edinburgh cell is ideally suited to studies under the conditions found in Titan. It can easily cover the entire P-T range needed (0-6 GPa, 100-300 K) and its open opposed-anvil geometry makes it possible to load mixtures that are unstable under ambient conditions. Furthermore, neutron diffraction is the technique of choice for structural studies of H-bonded ices.

Five new phases have been identified in the phase diagram of ammonia monohydrate as determined in our neutron

diffraction studies. As expected, pressure increases the co-ordination so that in ambient pressure phase I, the molecules are essentially four-fold co-ordinated whereas in phase VI the molecules are eight-fold co-ordinated. Fourier transforms of diffraction patterns, which reveal pair-correlation functions, suggest that the intermediate phases IV and V (whose structures still remain unknown) have intermediate co-ordinations that are more similar to phase VI than phase I. Plausible densities can only be obtained for phase IV with 8 or 9 formula units in the unit cell, and 8 formula units per cell gives a density that is almost continuous with that of phase I, which is inconsistent with evidence from the phase diagram. Accordingly, the volumes shown for phase IV are for 9 formula units per cell, and indicate that most of the ~10% increase of density certainly shown by phase VI happens as a step change from pseudo-four-fold to pseudo-eight-fold on going from phases I to IV at around 3 GPa. This is the first information on the density of ammonia monohydrate at high pressure and constrains the density of the ice component of the core prior to overturn.

From neutron diffraction patterns of methane hydrate collected on increasing pressure at room temperature, it is found that at ~0.9 GPa, methane clathrate hydrate transforms to a new form, methane hydrate II (MH-II) and ice VI appears — indicating that MH-II is richer in methane than its parent phase. At ~1.9 GPa, MH-II undergoes a further transformation to form methane hydrate III (MH-III) and more free ice appears. MH-III then remains stable up to at least 10 GPa. On decompression these changes are fully reversible and X-ray studies of hydrogenous methane hydrate reveal essentially the same behaviour. Structure solution reveals that MH-II appears to adopt the known hexagonal clathrate structure and has a 3.5:1 water methane ratio. MH-III is a dihydrate with a new H-bonded network, which is related to that ice Ih.

Before these (room temperature) conclusions can be applied to Titan, it needs to be established that the same non-dissociating behaviour is obtained along the P-T path followed by Titan's core. On compression at ~120 K the sample amorphises and this amorphous form does indeed crystallise when warmed to form MH-III and ice VII. This implies that the primordial rock ice core at the end of accretion contained no free methane but instead was composed of MH-III, ice and ammonia monohydrate.
This conclusion has important consequences for models of Titan. MH-III and ammonia hydrates have similar densities and would have ascended together after core-overturn. As the ices ascended and decompressed MH-III would have transformed back to MH-II and then to the low-pressure clathrate-I structure, taking water from the ammonia-water component. We thus estimate that after core overturn and full differentiation the ice mantle of Titan would contain a layer of methane clathrate-hydrate ~100 kilometers thick either just below or just above the ammonia-water ocean — the ocean's density is not well enough known to determine which. Such a layer is a much more plausible methane reservoir than an ocean or near surface storage in cracks and pores.

The presence of this layer may also have important consequences for the thermal history of Titan. Methane clathrate-hydrate has substantially lower conductivity than ice or ammonia hydrates and has a higher shear strength. Hence the presence of a layer of methane clathrate hydrate could strongly alter conductive and convective heat flow within the ice mantle of Titan. This could have a strong effect on the temperature of the rocky core — for example, it may be that the iron in the core is or has been molten, giving Titan a magnetic field.

These results move modelling of Titan onto new ground. Our results provide the first complete information on the density of the icy components of the core prior to overturn and need to be incorporated into modelling. Similarly the existence of the clathrate layer within the ice mantle needs to be included in models of Titan's thermal history after overturn. And new modelling is needed to explore how this layer may act as a reservoir to supply the atmosphere with methane.
We acknowledge help from D.D.Klug in preparing the samples of methane hydrate, and assistance from M.Guthrie and S.A.Belmonte with the experiments. This work is supported by funding from the EPSRC and the British Council and through access to beamtime and other resources from CLRC.

Much of this report was abridged from a paper by John Loveday and Richard Nelmes, from whom a copy may be obtained.

Pam Thomas

Education SIG at the Spring Meeting – Reports on Available Courses

1. Techniques Courses Held At Accelerators In The UK

These courses cover the production and uses of other types of radiation used to determine structure, synchrotron radiation (SR) and neutrons, and may include some experiments at the accelerator.

Summer Schools in Synchrotron Radiation Science

Bill Clegg described the course given in August 2002 on page 18 of the March 2003 issue of 'Crystallography News'. He organised it with Bob Cernik with invaluable assistance with the administration from Alison Mutch of the Daresbury Laboratory; such help is essential for a smooth running course. They obtained sponsorship from CCLRC, EPSRC, BBSRC and the EU to allow the students to attend at reduced cost; the 'students' ranged from new postgraduates to academic and central facilities staff who had little previous experience of SR. About 30 students came from different countries, mainly in Europe with some from Canada. They had a week of lectures and seminars at Chester College, then a 'social outing', some safety training and then 3 days of practical sessions at Daresbury Laboratory where station scientists supervised the students doing half-day experiments. The school covered basic fundamentals of SR (theory and operation), scientific techniques which use it and a range of applications. Informal social activities with the students are essential to maintain their interest and allow tutors to discover the weaknesses in the students' formal training. The next course will probably be held in 2004, details will be available on the Daresbury Web Site.

Training for neutron scattering; ISIS courses, and the Oxford neutron theory school

Chick Wilson then talked about Courses in the techniques of using neutrons in crystallography. The **Oxford School of neutron scattering** was established in 1989 by Terry Willis who had worked at Harwell for many years; he still directs it with help from staff at ISIS and other European Centres. The school is residential, held in Mansfield College of the University of Oxford; this year it is from 8th to 18th September. There were a few places left in March so if you want to attend this year, it may be worth looking at the details on the website **http://www.isis.rl.ac.uk/Conferences/osns2003/**

The course is intended for scientists new to the field of neutron scattering, it covers the fundamentals of neutron scattering including the concepts of scattering lengths, techniques and applications at both steady state and pulsed neutron sources. Some more recent applications to magnetism are included and students encouraged to give an overview of their own research as part of the tutorial sessions. A tour of ISIS, the pulsed neutron source at the Rutherford Appleton Laboratory, is part of the course, but otherwise this course is theoretical, consisting of lectures, seminars and social events to relieve the stress of such an intensive course.

The theory course is complemented by an **ISIS Practical Neutron Training Course,** organised by Steve Bennington, which lasts 10 days and is given approximately annually for about 40 students in response to User demand. The last course was held in January 2003. The course offers 'hands on' experience using beam time at the ISIS neutron source; it begins with a short review of the basics and then splits into 3 groups for more detailed study. There is a diffraction option; students get a thorough grounding in single crystal and powder diffraction methods, or can choose to study liquids or amorphous diffraction. Details can be found on the ISIS web site, look under the heading 'Training Courses'.

A third 'course' is the **'New Perspectives in Neutron and Muon Science Meeting'** which was inaugurated in 2000 as a satellite to the annual UK Neutron and Muon Users meeting. This is organised by young research workers from ISIS, who get experience of running meetings, for Young Researchers (defined as less than about 35) who present their own research work in a relaxed and friendly environment, to give them experience of making presentations and help them gain confidence before presenting their work to larger meetings. The most recent meeting was held in April 2003. Details of all these training events can be found starting from the ISIS web site at: **http://www.isis.rl.ac.uk** then look under the headings 'Conferences' or 'Training Courses'.

2. European Short Courses

John Helliwell gave us a British perspective on the **H E R C U L E S** training courses. The most difficult thing about the courses is probably remembering what the acronym means, **H**igher **E**uropean **R**esearch **C**ourse for **U**sers of **L**arge **E**xperimental **S**ystems. These courses are based in Grenoble but include a 1 week stay in Paris to visit the LURE SR Xray Facility and the LLB neutron Facility. They are rather longer than the British ones, lasting between 6 and 8 weeks. The most recent was held from March 2 to April 11, 2003 but usually they are held in February and March when good skiing is possible. The objectives are to provide multidisciplinary training in Biology, Chemistry, Physics and the Geosciences, optimize the use of large installations and develop a community of young European scientists around those installations. There are ~100 participants and about 70 lecturers drawn from across Europe. Funding is available from the EU for EU applicants.In addition to lectures the course includes practicals on all instrument types backed up by tutorials.

The course content is training in the use of neutrons and synchrotron radiation. There are two parts: Part I, common to all, is basic methods and instruments (35hours). There are lectures on basic notions on diffraction, small angle and diffuse scattering, X-Ray absorption spectroscopy, inelastic neutron scattering and X-Ray imaging techniques. Part II is centred around applications (45hours), this year there were two parallel sessions each lasting four weeks with 80hours of lectures, 40hours of practicals and 18hours of tutorials.

Session A : Physics and Chemistry of Condensed Matter covered synchrotron radiation, beam parameters and insertion devices, the Interaction of radiation with matter in both the elastic and inelastic case. Examples covered included Surfaces, Magnetic layers and multilayers, Vibrational spectroscopy of interfaces, Solid state and coordination chemistry, Catalysis, Earth science and Industrial applications

Session B : Biomolecular Structure and Dynamics
Challenges in structural molecular biology, proteins structure, dynamics of proteins, studies in solutions and partially ordered systems. Specials topics included crystallography of viruses and very large macromolecules, time resolved fluorescence studies, the quest for a high resolution in ribosome structure, X-ray microscopy, nuclear spin contrast variation studies on macromolecular complexes, medical imaging with synchrotron radiation, industrial applications and structural genomics.

The teaching staff and students come from mostly EU countries, but there is a mis-match between the large number of UK teaching staff and the very small number of UK students. One possible reason for this is that this course is very much longer; post graduates just starting their Ph.Ds find it difficult to get away for that length of time. With a trend towards a 4 year Ph.D there may be time in future.

The content of some of the courses have been published - some as Copublication Éditions de Physique - Springer, others by the Oxford University Press. Details can be found on the BCA webpages for courses.

Information about future HERCULES courses can be obtained from:
Marie-Claude Moissenet,
Secretariat Hercules, CNRS-Maison des Magistères, BP 166, 38042 Grenoble cedex 9, France
Tel: +33 (0)4 76.88.79.86
email: **marie-claude.moissenet@polycnrs-gre.fr**

http://www.polycnrs-gre.fr/hercules.html

There was little time for discussion of these courses at the end of the Education SIG, but discussion continued over the education posters in the 'Poster Session' held later that evening, Suggestions for future educational topics are welcome at any time. Meanwhile please send me news of further short courses to add to the BCA web site at **http://bca.cryst.bbk.ac.uk/BCA/ed/courses.htm**

Kate Crennell

ACA, Cincinnati, July 2003 - Micro symposium on Future Strategies for Successful Crystallographic Computing.

This symposium, organised by Ross Angel & David Watkin will have a wide interest. David Watkin has supplied this summary.

SP.02.01 Crystallographic Software – a Bleak Future? David Watkin & Richard Cooper

David Watkin, restricting his comments to the small molecule situation, tried to foresee developments in this field. He noted that most widely used programs come from authors in the last half of their expected careers, that past experience had shown software to fade away rapidly after their authors' retirement, and that there appeared to be no new young authors in posts that would enable them to continue to maintain programs. Although George Sheldrick was more optimistic about the emergence of new programmers, Watkin was worried that much of the wealth of experience encoded in current programs would be lost to future programmers because little of it was documented. He pinned his hope for the future on small molecule developments being made to the open-sourced structured programming now emerging from the macromolecular sector.

SP.02.02 Government Funded Central Initiatives for Encouraging Diversity of Freely Available Crystallographic Software; and the threat of Crystallographic Software Patents. Lachlan Cranswick.

Lachlan Cranswick explained the role and functioning of the EPSRC funded CCP14 project for Single Crystal and Powder Diffraction. Before Lachlan's time, this project had sought to maintain established software on multiple platforms. Developments in the World Wide Web and the reduced choice of hardware platforms meant that this was no longer necessary, and under Lachlan's stewardship CCP14 had taken on a role aimed at raising people's awareness of the available software and exposing the strong points of different programs. His mission had been to encourage people to seek out the best tool for each problem, rather than just make do with the software they were familiar with. His close interaction with users at the many workshops he has run has enabled him to provide valuable feedback to people still developing programs.

The second half of Lachlan's talk was distinctly worrying. He presented a whole catalogue of cases where ideas that were in common circulation had been successfully patented, mainly in the USA. The situation looks as if it will deteriorate further should Europe also introduce Software Patents.

SP.02.03 Hacker Vulnerability: A Major New Complication in Crystallographic Computing. Carroll Johnson.

Carroll Johnson briefly explained the methods used by hackers to gain access to private and institutional computers, and what can be done to minimise the risks of intrusion. He explained that the main risk was to machines left running on local area networks, especially home-grown networks. The principal safe guards are to use firewalls, and to run intrusion detection and logging software. He pointed out the need to verify that backup systems really would enable one to recover work after a serious hack or system crash.

SP.02.04 Crystallographic Software from the NIST Centre for Neutron Research. Brian Toby.

Brian Toby looked back over 20 years of programming, and lamented the fact that with each generation, fewer and fewer people are able to write even the simplest programs. He observed 'One thing has not changed: support for programming efforts remains lacklustre'. Brian tried to provide answers to three questions: What are the software needs within the community? How should programming efforts be organised? and What are the incentives to make these goals happen?

SP.02.05 There is No Such Thing as Free Software. Jim Pflurath, Rigaku/MSC Inc.

Jim Pflugrath painted an excellent summary of the history of software development, the similarities and differences between writing code in laboratories and in a company, and the mechanisms by which software can be funded. At the

end of the day, he pointed out, crystallographic software is generally paid for by the taxpayer, either through the salaries of university staff, through grants for individual projects or as part of the purchase of an instrument. The so-called free software is generally paid for by someone's employer (even if they don't realise it). In later discussion it emerged that software written at home in the evenings but related to what is done at work, also generally belongs to the employer!

Like Brian Toby, Jim also noted that programming skills are disappearing amongst scientists, to the point where many will not even be able to read code with any understanding. He drew parallels between writing software in a company and in a university. In particular, he noted that in both environments the programmers are also usually scientists, working in collaboration with other scientists. One common difference was the measures taken by companies to ensure some level of quality control and security.

Looking to the future, he explained that Rigaku/MSC make a point of employing scientists who can both write code, and teach other programmers the science of crystallography. 'After all', he said, 'there is more to software than 'push a button"

SP.02.06 Crystallographic Computing at Bruker Nonius. Susan Byram, Bruker Advanced X-ray Solutions.

Susan Byram showed examples of recent software products that were the result of collaborations outside of the company, and explained that interaction with the university community was vital. She took the opportunity to explain that while Bruker-Nonius did protect their investment in instrument design with patents, to date they had not patented software or algorithms. Bruker-Nonius are keenly aware that users or their funding agencies will not accept the real cost of software development. *'Frequent comments are heard that no funding is available to purchase software for more than a few hundred dollars, or to support software upgrades'.* Her response to the observation that less and less software is being developed in the public sector was to suggest that grant applications should contain an amount to cover the real cost of writing innovative software by commercial or independent developers.

SP.02.07. The CrysAlis Software Suite for Area and Point Detector Measurements: Open Source Option and User Modifications. Mathias Meyer, Oxford Diffraction, Poland Sp.

Oxford Diffraction is a relatively new player in the field, and so Mathias Meyer took the opportunity to provide an overview of their software products, and explain how they hope to encourage active interaction with the user community. The CrysAlis software is open source, so that users can examine it and make modifications. The modified code remains local to the user, but is dynamically linked to the rest of the system as a so-called plug-in. This mechanism enables enthusiastic users to try out and develop new ideas without undermining the security of the rest of the code.

SP.02.08 Developing Modern Crystallographic Libraries and Applications: PHENIX and the Computational Crystallographic Toolbox. Ralf Grosse-Kunstleve, Nigel Moriarty, Nicholas Sauter & Paul Adams.

Paul Adams explained how the need for rapid innovation in macromolecular software to meet the demands of the structural genomics efforts required a totally new approach to system development. The PHENIX project hopes to achieve this through a two-layered approach. High level applications are written in PYTHON to facilitate rapid and accurate code development, while the underlying core algorithms are written in C++, the computational crystallographic toolbox (cctbx). This toolbox is freely available under an Open Source license with the aim of fostering widespread collaborations.

David Watkin

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

1 - 4 September 2003
The XIX Conference on Applied Crystallography, Krakow, Poland
[http://crystallography.us.edu.pl/]

2-6 September 2003
ECNS 2003 European Conference on Neutron Scattering, Montpellier, France,
[http://www.sfn.asso.fr/]

3-6 September 2003
9th European Conference on Solid State Chemistry, Stuttgart, Germany
[http://www.mpi-stuttgart.mpg.de/conf/ecssc9/]

3-7 September 2003
Fifth International Conference On Molecular Structural Biology, Vienna, Austria.
[http://pharmchem.kfunigraz.ac.at/icmsb2003/]

4-7 September 2003
Summer School on Polycrystalline Structure Determination by Direct Methods, Krakow, Poland
[http://crystallography.us.edu.pl/]

7-12 September 2003
13th V.M. Goldschmidt Conference, Kurashiki, Japan
[http://www.ics-inc.co.jp/gold2003]

8-11 September 2003
Biocrystallography course: From gene to drug, Centre of Excellence in Biocrystallography of the University of Trieste, Italy.
[http://www.univ.trieste.it/~ceb/course.html]

8-13 September 2003
Aperiodic-2003,
Belo Horizonte, Brazil,
[http://www.fisica.ufmg.br/~ap2003/]

8-18 September 2003
8th Oxford School on Neutron Scattering, University of Oxford, Mansfield College
[http://www.isis.rl.ac.uk/conferences/osns2003/]

10-11 September 2003
Annual UK Synchrotron Radiation Users Meeting, Daresbury Laboratory
[http://www.srs.ac.uk/srum/index.html]

12-14 September 2003
Materials Discussion 6: Controlled Polymer Architectures - from Micro to Meso Scale, Durham, UK
[http://www.rsc.org/lap/confs/md6.htm]

14-19 September 2003
Structure Solution from Powder Diffraction Data, Stara Lesna, Slovak Republic.
[http://www.sspd-03.sav.sk]

15-19 September 2003
XV International Conference on X-ray Diffraction and Crystal Chemistry of Minerals, St Petersburg State University, Russia
[http://www.lcm3b.u-nancy.fr/cims/forthcoming.htm#STPeterburg]

18-23 September 2003
SHELX Workshop</A>, University of Goettingen, Germany
[http://shelx.uni-ac.gwdg.de/SHELX/workshop.htm]

22-25 September 2003
DyProSo XXIX conference / Elettra (Dynamical Properties of Solids),Trieste, Italy.
[http://www.elettra.trieste.it/dyproso]

22-26 September 2003
XVII International Congress on X-ray Optics and Microanalysis", Chamonix Mont Blanc, France.
[http://www.esrf.fr/Conferences/ICXOM]

23-26 September 2003
The Joint Institute for Neutron Sciences NSFCHEMBIO Workshop and SENSE Workshop, Tallahassee, Florida
[http://www.sns.gov/jins/tallahassee_workshops_2003/workshops.htm#synopsis]

2-3 October 2003
Neutron Macromolecular Crystallography at the Spallation Neutron Source - a Workshop, Argonne National Laboratory, IL, USA
[http://www.pns.anl.gov/]

6-10 October 2003
Introduction & Advanced X-Ray Diffraction For Pharmaceutical Applications, Danbury, CT, USA [http://www.assainternational.com]

8-10 October 2003
IBC,s Protein Interactions, IBC Life Sciences, San Diego, CA, USA [http://www.LifeSciencesInfo.com/protein/?source=3003-2]

9-11 October 2003
The First Fifteen Years of Reverse Monte Carlo Modelling, Budapest, Hungary. [mailto: Laszlo Pusztai <lp@szfki.hu>]

15-17 October 2003
Polymorph Screening - Techniques & Applications, Stamford, Connecticut, USA [http://www.assainternational.com]

19-21 October 2003
Sixth LANSCE User Group Meeting, Los Alamos, NM USA, [http://lansce.lanl.gov/usermtg6/]

24 October 2003
36th SRC Users' Meeting, Stoughton, WI, USA, [http://www.src.wisc.edu/meetings/SRC_UM2003/default.htm]

24-26 October 2003
Workshop on Radiation-based Analytical Techniques. Cape Town, South Africa. [http://www.medrad.tlabs.ac.za/isrp9.htm/]

27-30 October 2003
International Symposium on Pulsed Neutron Science and Instruments (IPN2003), Tsukuba, Japan [http://www.neutron.anl.gov/mailman/listinfo/neutron]

27-31 October 2003
Ninth International Symposium on Radiation Physics. Cape Town, South Africa. [http://www.medrad.tlabs.ac.za/isrp9.htm/]

31 October- 1 November 2003
UK-Japan Neutron Science Workshop (UKJ2003), Izura SPA (Pacific seaside), Japan [http://www.neutron.anl.gov/mailman/listinfo/neutron]

31 October- 1 November 2003
Neutron Detector Workshop (ND2003), Tsukuba, Japan [http://www.neutron.anl.gov/mailman/listinfo/neutron]

12-20 November 2003
A Practical Course in Molecular Microscopy, Center for Integrative Molecular Biosciences (CIMBio),
The Scripps Research Institute (TSRI), La Jolla, California [http://nramm.scripps.edu/seminars/2003/cryoem/]

3-4 December 2003
The Molecular Basis of Life: is Life Possible without Water?', The Royal Society, London [http://www.royalsoc.ac.uk/events/discussion_meetings/level_2/dec_water03.htm]

4-7 December 2003
High Pressure Structure and Reactivity: The Science of Change. Lawrence Berkeley National Laboratory, Berkeley, California. [http://www-esg.lbl.gov/esg/meetings/IUCrCHP0903/index.html]

9-13 December 2003
International School on Crystal Growth and Characterisation ,La Pedrera, Rocha, URUGUAY [http://www.iscgcha2003.fq.edu.uy/]

13-16 January 2004
Joint Meeting on Neutron Optics and Detectors, Tokyo, Japan [http://www.nop2004.jp]

14-18 February 2004
Biophysical Society 48th Annual Meeting, Baltimore, MD, USA [http://www.biophysics.org]

15 March 2004
2nd Annual Biomaterials Workshop, Cranfield University, Shrivenham [http://www.cranfield-biomaterials.com]

6-10 June 2004
American Conference on Neutron Scattering, College Park MD, USA [http://www.ncnr.nist.gov/acns]

9-20 June 2004
Electron Crystallography: Novel Approaches to Structure Determination of Nanosized Materials, Erice, Italy. [http://www.crystalerice.org/2004/ElCryst2004.htm]

9-20 June 2004
Polymorphism : Solvates and Phase Relationships. Erice, Italy, [http://www.geomin.unibo.it/orgv/erice/bernstei.html]

19-23 July 2004
20th General Conference of the Condensed Matter Division , European Physical Society, Prague, Czech Republic, [http://cmd.karlov.mff.cuni.cz/CMD/]

20-28 August 2004
32nd International Geological Congress, Florence, Italy [http://www.32igc.org/]

22-24 August 2004
Satellite meeting on "Mathematical and Symmetry Aspects" (ECM-22). Budapest, Hungary, [http://www.lcm3b.u-nancy.fr/mathcryst/satellite.htm]

25-30 August 2004
European Crystallographic Meeting: ECM22, Budapest Hungary
[website not yet known]

2-5 September 2004
EPDIC-IX, European Powder Diffraction Conference, Prague, Czech Republic, [http://www.xray.cz/epdic]

7-10 September 2004
X-TOP 2004 - 7th Biennial Conference on High Resolution X-Ray Diffraction and Imaging, Pruhonice (near Prague), Czech Republic, [http://www.xray.cz/xtop]

17-21 November 2004
SGO International Conference on Structural Genomics 2004 (ICSG 2004),Washington Hilton & Towers Hotel, Washington, DC, USA
[no website yet given]

19-29 May 2005
Evolving Methods in Macromolecular Crystallography, Ettore Majorana Centre, Erice, Italy
[http://www.crystalerice.org/futuremeet.htm]

23-31 August 2005
XX Congress of the International Union of Crystallography, Florence, Italy, [http://www.iucr2005.it]

28 November-2 December 2005
2005 International Conference on Neutron Scattering, Sydney, Australia
[A website will be up and running shortly]

9-18 June 2006
The Structure Biology of Large Molecular Assemblies, Ettore Majorana Centre, Erice, Italy. [http://www.crystalerice.org/futuremeet.htm]

7-17 June 2007
Engineering of Crystalline Materials Properties: State-of-the-Art in Modeling, Design, and Applications, Ettore Majorana Centre, Erice, Italy, [http://www.crystalerice.org/futuremeet.htm]