Crystallography News

British Crystallographic Association

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BCA Spring Meeting 2006 - Lancaster p9-16

Crystallography News March 2006

Contents

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

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

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

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

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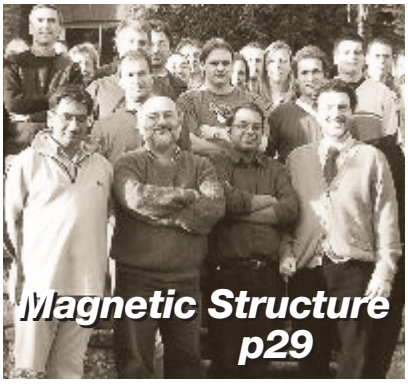

***Magnetic Structure* p29**

This month's cover: *It's back to Italy this summer for a BCA-style School. For the inset, see page 7.*

From the President

MY last column as BCA President and it is tempting to reflect. I will allow myself to do so, but only to reiterate what a pleasure and privilege it has been to lead this fantastic organisation. I feel enriched by the experience, and if my successors find the role half as rewarding as I have, then they have much to look forward to. I look back with particular pleasure at the establishment of the Young Crystallographers group, who are running a session again in Lancaster, my many interactions with colleagues in the UK and overseas in my role with the BCA, and the stimulation of being involved in busy, vibrant, exhausting but highly enjoyable Spring Meetings - and still one to go for me!

Turning to the Spring Meeting, I think you will see from the programme detailed elsewhere in this issue, an outstanding few days is on offer in Lancaster. I should repeat our pleasure at welcoming colleagues from BACG to the Spring Meeting this year, and thanks to **Paul Raithby** and the Programme Committee for bringing this excellent programme together. Again on a personal note, I am delighted to be Abstracts convenor once again in 2006 but, having been involved in this role since 1998, it is undoubtedly time to hand this task on, and I look forward to new approaches from a new Abstracts convenor - volunteers welcome.

Another significant innovation has been the increasing emphasis on distinct education/teaching content in the Spring Meeting programme, moving from the traditional Education discussion sessions to those delivering teaching content; once again we have significant such components in Lancaster, with Workshops and a Keynote Teaching lecture. The re-launched Education web-site is taking shape (www.chem.gla.ac.uk/BCAEducation) and I hope will gain additional momentum and relevance under the new President and Council. This is one of the ongoing challenges for the BCA, in securing and advancing our impact as a national Educational Charity.

Another challenge is the maintenance of sound finances, while enhancing our commitment to funding education and training initiatives such as the Young Crystallographers, and our support for teaching schools, along with launching new initiatives in this area. We can of course only do this if our income stream is secure. Growing the membership is a longer term aim, and one we continue to work towards, but we on Council have also addressed the issue of membership fees, which have remained unaltered for many years. Our reserves are sound, but in spite of cautious financial management, we have been running at a small effective deficit on turnover for several years. In order to maintain and if possible expand our spending on education, bursaries and similar vital areas, it is essential that we secure our future membership income. At the AGM in Lancaster, Council will therefore propose and recommend an increase in standard membership fees to £20 per annum, in my opinion still a modest cost for BCA membership, and in line with inflation-linked increase since the fee was last set. I hope and trust the membership will approve this, to leave the new President and Council in good shape to pursue our ongoing aims.

I would like to end by extending my thanks to all on Council during my time as President, in particular the officers, Crystallography News editor and our colleagues at Northern Networking Events, with whom it has been a pleasure to work and who have made my job easy and such a pleasure. I wish the BCA and my successor well.

Chick Wilson

BCA Council

Front Row: Christine Cardin, John Finney, Chick Wilson and Sheila Gould. Back row: Bob Gould, John Helliwell, Sandy Blake, Jeremy Cockcroft, Sheila Gover, Elspeth Garman, Georgina Rosair, John Evans and Peter Moody.

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BCA Corporate Membership

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

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

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 the Editor

ISSUE number 96 looks to our Spring Meeting, and you will find as up-to-date a programme as possible here, including several workshops and the second appearance of the highly popular Young Crystallographers Meeting.

As several readers have pointed out, I am responsible for the mis-spelling of **Sir Lawrence Bragg's** name in the last issue. I am very sorry indeed for this senior moment, and for any pain it may have caused. A further error of transcription made the date of the talk wrong. It was given on Sunday 26 August, 1945. Thanks to **Tony North** whose letter appears in this issue, and to **Geoff King** and **Harry Powell** who also wrote.

Sadly, our oldest honorary member, **Dr Robert Crispin Evans**, died on 18 December 2005 at the age of 96. We hope to have an obituary for him in the next issue. Meantime, I am grateful to his nephew, **Edward Peacock**, for sending photographs, one of which is a group photograph of the Department of Mineralogy and Petrology at Cambridge in 1938. Dr Evans and a number of others in the Crystallographic Community at the time are pictured here, and I have included it in this issue without the names, hoping that readers will write in with identities and memories of any of those present.

One of the outcomes of the IUCr meeting in Florence was the decision to hold a school in Italy next summer based on the BCA-CCG school held every other year in Durham. This is a real compliment to that school and to the education initiatives of the BCA. **Lachlan Cranswick** has contributed an article on it, as well as the best pictures we received for this issue.

Meantime, may I once again encourage everyone to consider writing something for Crystallography News. One heartfelt plea, though! Pictures are very welcome indeed, but please do not embed them in the text document! In order to put the magazine together, these have to be stripped out, and as a result lose resolution usually to the point of being unusable.

Finally, may I take this opportunity to thank our outgoing president, **Chick Wilson**, for the cheerful support he has given Crystallography News, even if he couldn't always remember what it is called! It has been great to know that there would always be one good, positive article coming in for every issue!

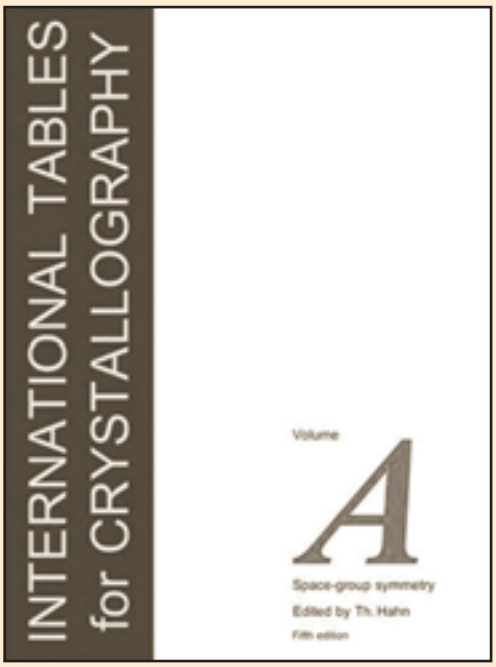
Bob Gould

Puzzle Corner

THE numbers in the following sequence all represent the total number of some category in symmetry groups in 1, 2 or 3 dimensions, as covered in International Tables A: e.g. 230 is the number of three-dimensional space groups. To how many can you assign a significance? Extra credit for getting more than one!

2, 4, 5, 7, 14, 17, 32, 65, 73, 230.

In keeping with rising costs, the prize has now been increased to a £20 book Token for 2006!



The winning (and only) entry for December was from Kate Crennell, whose reasoning follows:

1a Kindergarten child
1b Paul Klee

I recognise Klee's style and although I don't recall the name, this picture looks to be his style

2a Josef Albers
2b Kindergarten child

This 2b looks simpler than 2a, so is more likely to be by the child

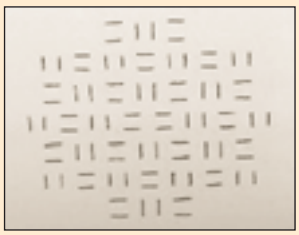
3a Kindergarten child
3b Bart van der Leck

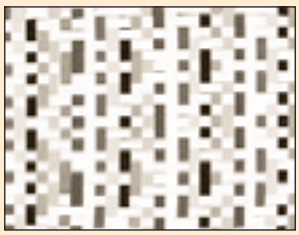
The lower picture looks too complicated to have been produced by a child

4a Kindergarten child
4b Piet Mondrian

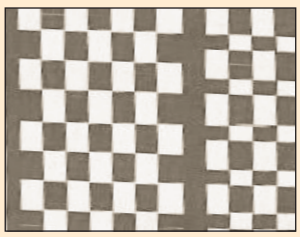
I recognise the Mondrian style, the upper picture does not have so many colours and has too many repeats compared with the lower one, so is more likely to be by the child.

An excellent effort! Well, three out of four for recognizing the child's work - in fact all the "as" were by children. Unfortunately the artists are somewhat different: 1b: Mondrian; 2b: van der Leck; 3b: Klee; 4b: Albers. Shame on the rest of you for not trying or sticking your head above the parapet. I wouldn't have done very well myself.


1a


2a


3a


4a


1b


2b


3b


4b

Letters to Ed.

From Professor Tony North

Dear Bob

First, congratulations on the latest BCA News. It gave me a mixture of amusement, puzzlement and outrage!

I am amused that my mouse pointer efforts have struck such a positive response - though I do believe that they might have some effect if the Industrial Group has really taken up the challenge to make speakers face the audience. Unfortunately I failed at a recent talk that I gave in a (Leeds) lecture theatre where keyboard, monitor and audience could not be seen simultaneously! I was surprised some time ago to hear that a quick and dirty method of empirical absorption corrections for diffractometer data that I published had become a citation classic - I doubt if my murine efforts will follow!

Puzzlement arose through your use of 'bursar' for recipients of bursaries; I had always thought a bursar was the chap who doled out the money - but 3 dictionaries tell me that it is used by Scottish universities for people who receive them; but, to use another Scottish term, I don't think it is used outwith Scotland in that sense. Anyway, never mind.

A minor source of outrage was your mis-spelling of Sir Lawrence Bragg's name with a 'u' instead of a 'w', in each reference to him. Greater outrage was caused by the road directions to Lancaster (page 17) being illustrated by a 4 X 4, aka Chelsea tractor, despite the print being green. Oh dear!

Best wishes,

Tony North

Ed. **Dear Tony,**

Thanks for your letter - I'm always pleased to hear that someone has actually READ Crystallography News. Now for your points.

1. Yes, the Industrial Group have produced some pointers, but I was at their last group meeting, and none of the speakers used them. Maybe they'll catch on! Meantime, I'm certainly one of those who have quoted North, Phillips and Williams for a very satisfactory method of absorption correction - now on a really firm footing with area detectors which measure many equivalent data.

2. Yes, our use of bursar is a Scoticism - but since like the country, the world, and, for all I know the galaxy, The BCA is run from Scotland, one forgets that furth of this realm ....

3. And yes, I'm entirely to blame for the Laurences. I knew I had got it wrong the first time and unfortunately corrected it twice, getting back to where I started. A large piece of humble pie will be eaten. The only positive feature is that I expect it did generate a lot of correspondence, and that, of course is great! As for the 4x4 - that was the imagination of our excellent typesetter, Barry Brown at Anderson's, and I like to encourage him! Presumably, anyone coming that way will load in lots of students for the journey.

Ed.

From Dr Andrew Bond

Bob,

I was interested to see your section on Nicolai Steno in the last CN. He is still remembered by the Danish research councils. I am currently funded on a "Steno Stipend" - rather like a Royal Soc. Research fellowship (but evidently much easier to get!).

Andrew Bond

From Mrs Kate Crennell

Dear Bob,
Did you read about the early closure of the 'Diamonds' exhibition in London due to rumours of some planned stealing attempts? Lucky I'd managed to see it myself.

There are some pretty photos of crystals on Fred Kruijen's site, perhaps you could find space in the next issue of 'Crystallography News' for a mention?

Kate Crennell

From Fred Kruijen

Hello,

May I introduce to you my new website about the quarry "The Wannenköpfe" in the Eiffel region of Germany, with many mineral pictures. You can find it under: http://wannenkopfe.strahlen.org I hope you'll like it.

With friendly regards,

Fred Kruijen
Email: f.kruijen@tiscali.nl

Department of Mineralogy and Petrology, University of Cambridge 1938.

Please write in if you can identify any or all of the people pictured here, one of whom is Dr R.C. Evans. The full caption will appear in the next issue.

Siena 2006

Siena 2006 : IUCr School on Basic Crystallography - modelled on the BCA Durham school

THE IUCr Teaching Commission will be holding an immersive school, focusing on the crystallographic fundamentals, from Sunday 27th August to Saturday 2nd September 2006 at the Certosa di Pontignano, Siena, Tuscany, Italy. The Certosa is a medieval monastery, now run by the University of Siena, and is an excellent venue for such a school. Due to the regression in many parts of the world in university teaching of crystallographic fundamentals, the Teaching Commission has modelled the school on the successful BCA Durham School. The Teaching Commission considers the BCA School to be the best and most appropriate of its kind available at this time, providing a week-long immersive course focusing on crystallographic fundamentals.

As would occur at a BCA Durham School, there will be a mixture of lectures and tutorials. All the tutorials are pen, paper and pocket calculator exercises, consistent with the aims of properly teaching students the fundamentals of crystallography. This is in contrast to more common styles of school or teaching workshops, which often concentrate on button pushing and the use of computers. Computer based approaches can obscure or gloss-over the contribution of crystallographic and algebraic theories, such that little fundamental appreciation is obtained by the students. With GUI based computers, it is moderately easy to attend workshops to determine which computer software buttons can be pushed; but obtaining a rigorous proper appreciation of the scientific theory behind what these buttons are doing is not so readily available. The

IUCr Teaching Commission believes it is important that more rigorous and effective “fundamentals” schools in crystallography become available; and it hopes the Siena 2006 school will help fill this gap, and promote this type of school in other regions of the world.

The total cost of the school (including board and all meals) is 500 Euros. Student bursaries are also available. Many of the Durham BCA school teachers have agreed to lecture at the Siena school and will be presenting a similar school in Durham in 2007. The Teaching Commission would like to see the basic school model exported to other regions of the world, where university based teaching of crystallographic fundamentals for academic bachelors and masters formation is in a worsening decline.

Lecturers and tutors include: **Alexander Blake**, **Gervais Chapuis**, **Jacqueline Cole**, **Giuseppe Cruciani**, **Giovanni Ferraris**, **Carmelo Giacovazzo**, **Robert Gould**, **Peter Main** and **David Watkin**. School organisers are **Paola Spadon** (Current chair of the Teaching Commission) and **Marcello Mellini**. The programme committee includes **Gervais Chapuis** (programme chair), **Alexander Blake**, **Angelo Gavezzotti**, **Robert Gould** and **Reinhard Neder**.

The school is sponsored and supported by the European Crystallographic Association (ECA) - http://www.ecanews.org/, Associazione Italiana Cristallografia (AIC) - http://www.chim.unipr.it/aic/, University of Siena - http://www.unisi.it/, and IUCr - http://www.iucr.org/.

More information is available (including travel and accompanying person information) via the Siena 2006 School website:

http://www.iucr.org/iucr-top/comm/cteach/siena2006/

Lachlan Cranswick

BCA 2006 Spring Meeting

BCA/BACG Spring Meeting 2006

Keynote Lectures

Keynote 1
Chair: **Richard Pauptit** (AstraZeneca)
Lecturer: **Larry De Lucas** (University of Alabama, USA)
Novel Protein Crystallisation Technologies

Keynote 2
Chair: **Simon Parsons** (University of Edinburgh)
Lecturer: **Mark Spackman** (University of Western Australia)
Visualizing and exploring intermolecular interactions in molecular crystals: A new toolkit for crystal engineering

Keynote 3 - Alun Bowen Lecture
Chair: **Jeremy Cockcroft** (UCL)
Lecturer: **Ulrich Griesser** (University of Innsbruck)
Relevance and Analysis of Polymorphism in Drug Development

Keynote 4 - Teaching Plenary
Chair: **Neera Borkakoti** (Medivir UK Ltd)
Lecturer: **Garry Taylor** (University of St. Andrews)
Protein Crystallography for Non-biologists

Named Lectures

The Lonsdale Lecture
Chair: **Chick Wilson** (University of Glasgow)
Lecturer: **Mike Glazer** (University of Oxford)

Parallel Sessions
Chair: **Dr David Allan** (Edinburgh)
High Pressures, Liquids and Surfaces
Lecturers:
Colin Pulham (University of Edinburgh)
Exploring crystallisation processes at high pressures

Dominic Fortes (UCL)
Crystallisation of ammonia hydrates under high pressure

Roy Wogelius (University of Manchester)
Crystallographic controls on biofilm formation

Daniel Bowron (ISIS Facility, CCLRC)
Changing the structure of water using pressure or solute species

Crystal Stories - Session 1
Chair: **Neera Borkakoti** (Medivir UK Ltd)
Lecturers:
Lesley Haire (NIMR)
A novel vapour batch method for organics

Lindsay Sawyer (Edinburgh)
Protein crystallisation - an anecdotal approach

Frank Von Delft (SGC)

Crystal Stories - Session 2
Chair: **Andrea Hadfield** (University of Bristol)
Lecturers:
William Hunter (University of Dundee)
Accidental Discoveries in Crystals of Complexes

James Murray (Vernalis)
Tales from the Crystallisation Bench

Neutron and Synchrotron Opportunities for Industrial Users
Chair: **Jeremy Cockcroft** (UCL)
Lecturers:
Alan Hewat (ILL)

Andrew Jupe (Georgia Institute of technology)

Customised Crystallisations - Session 1
Chair: **Jon Cooper**

Allan D'Arcy (Novartis)
Nucleation and Seeding in Protein Crystallisation

Jonathon Grimes (University of Oxford)
Virus Crystallisation

Topology
Chair: **Jacqui Cole** (Cambrdige)

Lecturers:
Simon Parsons (University of Edinburgh)
The Effect of High Pressure on the Topologies of Molecular Crystals

Elna Pidcock (CCDC)
The Box Model of Crystal Packing

Thomas Gelbrich (University of Southampton)

German Sastre (University of Valencia)
Ring Topology and Strain in Zeolites

Caroll Johnson (ORNL)
Orbifolded thermal motion critical net topology

Customised Crystallisations - Session 2

Chair: **Katie Brown**

Lecturers:

Paul Rowland (GSK)
Crystallisation using Free-interface Diffusion

Monika Spano
Crystallisation for Neutron Diffraction

Anne Cleasby (Astex)
Crystallisation and Crystal Handling for High Throughput Fragment Screening by Crystallography

Crystallisation and Polymorphism of Pharmaceuticals

Chair and co-chair: **Roy Copley** (GSK) and **Anne Kavanagh** (AstraZeneca)

Lecturers:

Roger Davey (University of Manchester)
Controlling nucleation of enantiomers from solutions - the chiral enrichment of mandelic acid

Sally Price (UCL)
Progress and problems in computational prediction of crystallisation and polymorphism

Terry Threlfall (University of Southampton)
Growing Crystals: Growing Polymorphs (and Some Thoughts on Crystal Growth)

Caroline Day (GSK)
Polymorph Screening by Automated Techniques

Customised Crystallisations - Session 3

Chair: **Nick Keep**

Lecturers:

So Iwata (University of London)
Current Challenges in Membrane Protein Crystallisation

Nigel Unwin (University of Cambridge)
Title tba

Charge Density

Chair: **Dr Mary Mahon** (University of Bath)

Lecturers:

Piero Macchi (University of Milan)
The XD software package for charge density analysis

Louis Farrugia (University of Glasgow)
Experimental aspects of charge density studies

Paul Popelier (University of Manchester)
Quantum chemical topology

Sebastien Pillet (Nancy)
Electron density of metastable states

Crystal Structure and Growth at the Nano-Scale (joint BACG/IG Session)

Chair and co-chair: **Kevin Roberts** (University of Leeds), **Richard Morris** (Morris Analytical X-ray Ltd)

Lecturers:

Peter Laggner (University of Gratz)
How crystals are born: novel insight from small-angle X-ray scattering

Kevin Roberts (University of Leeds)
Solution phase nucleation: cluster size & shape and its correlation with crystallisation kinetics and polymorph selection

M Lal (Liverpool University), **M Plummer** and **W Smith** (CCLRC Daresbury Laboratory)
Metal nanocrystallites in supercritical fluids - the solvation process and its impact on the nanostructure

Getting the Most Out of Your Crystals

Chair: **Richard Pauptit** (AztraZeneca)

Lecturers:

George de Titta (HWI, Buffalo)

Torsten Neufiend
Improving Diffraction with the Free Mounting system

Elspeth Garman (University of Oxford)
Freezing Crystals

Julie Wilson (University of York)
Crystal Edge Detection

Powder Diffraction in Industry

Chair and co-chair: **Judith Shackleton** (Manchester) and **David Beveridge** (Ilford)

Paul Fewster (PAnalytical) will be awarded the IG prize and will give a lecture

David Beveridge (Ilford)
The Precipitation of Pigment Red 57:1 from Homogeneous Solution for X-ray Powder Diffraction

Chris Staddon (Nottingham)

Crystal Engineering (BACG Session)

Chair and co-chair: **Nick Blagden** (University of Bradford), **Kevin Roberts** (University of Leeds)

Lecturers:

Dario Braga (University of Bologna)
Making Crystals by Reacting and Transforming Crystals

Christer Aakeröy (Kansas State University)
Constructing Co-crystals with Molecular Sense and Supramolecular Sensibility

Jonathan Steed (University of Durham)
Anion Binding Venus' Flytraps and Tweezers

Chris Gilmore (University of Glasgow)
Snap: A New Way of Analysising the Results of Cambridge Data Base Searches and a New Tool for Crystal Engineering and Structure Prediction

Chris Sumby (University of Leeds)
Crystal Engineering with Derivatives of the Molecular Host Cyclotriveratrylene

Joshua Mckinnon (University of Western Australia)
Extensions of Hirshfeld Surface-based Tools: Decomposing Fingerprint Plots

Workshops

A full day XRPD workshop on phase identification

Organisers: **John Faber** (ICDD), **David Rendle** (consultant) and **Dave Taylor** (consultant)

This is a modular workshop based on 4 distinct sessions which build to give a complete understanding of phase identification and its progression into quantitative analysis, culminating in a flexible hands on computer session to gain practical experience with real examples. The modular structure will allow delegates, on the basis of their experience, to dip in and out of sessions through the day giving the package something to offer everyone with an interest in phase identification.

Module 1: 09:00 - 10:30
History & Structure of the Powder Diffraction File (PDF)
This module will cover important background information on the Powder Diffraction File with the emphasis on gaining an understanding of the various databases and how to interpret the data from an individual entry and select the best entry to use from multiple entries of the same compound.

Module 2: 11:30 - 12:00
Phase Identification
This module will cover collecting data for phase identification (PID).
An understanding of the various manual search methods, alphabetical, Hanawalt, Fink and long 8 will underpin the knowledge required for automated search match techniques. It will cover selecting the database to use and subfile selection for particular applications.

Module 3: 13:00 - 15:00
Advanced Phase Identification and Quantitative Analysis
Here we will cover data mining, total pattern analysis and the methods of quantifying the phases detected, covering reference intensity ratio, spiking and Rietveld analysis.

Module 4: 15:30 - 17:15
Hands on computer session
This module will allow you to put into practice the techniques covered in the workshop by using practical examples of both qualitative and quantitative problems for you to solve in a dedicated computer suite.

TOPAS Academic Workshop

Organiser: **John Evans** (University of Durham), assisted by **Sarah Lister**, **Graham Stinton** and **Ivana Evans** (University of Durham).

The PCG and CCG will be running a Topas-Academic workshop on the final afternoon of the BCA spring meeting 2006 at Lancaster University. Topas-Academic is a powerful software suite written by Alan Coelho which allows the analysis of both powder diffraction and single crystal diffraction data. Data from most laboratory/central facility diffractometers can be analysed. More features of the software are detailed below. Like many other software suites used by the academic community, it is available for academic use for a nominal fee (in this case 500 Euros) to help the developer cover distribution and program support costs.

The workshop will be run along similar lines to the successful ones previously organised on packages like Jana and Crystals. A very brief overview of the software and how to operate it will be given. Attendees will then be encouraged to work through examples in their own specific areas of interest. Expert tutors will be on hand to assist with any difficulties. We will endeavour to prepare tutorials of relevance to molecular/extended systems and of interest to biologists/chemists/physicists. You can also bring your own data along to play with.

An Introduction to Protein Crystallisation

Organiser: **Tony Savill** (Molecular Dimensions Ltd)

The speakers, **Alan D'Arcy** and **Terese Bergfors**, will give a coordinated presentation on protein crystallisation for beginners.

Spring Meeting Exhibitors Forum

Following the success of the forum at the Spring Meeting last year the event will be repeated this year.

The forum will provide each exhibitor with the opportunity to present their latest developments and encourage participants along to their stands in the Commercial Exhibition. It is serious, but entertaining and enlightening, and we encourage participants to provide a good audience for this valuable session, to be held on the opening day of the main meeting.

Satellite Meetings

Young Crystallographers Meeting

Organiser: **Andrew Parkin** (University of Glasgow)

Following the great success of the Young Crystallographers Meeting that took place at the BCA Spring Meeting two years ago, the event is being repeated. It provides a showcase for Ph. D. students and post doctoral workers to present their latest results in a relaxed and enlivening atmosphere.

Synchrotron chemical crystallography for all

Organiser: **Bill Clegg** (University of Newcastle and SRSR Daresbury Laboratory)

Single-crystal "small molecule" diffraction facilities were established at Daresbury SRS about ten years ago, and a Diamond beamline is planned for 2008. Access at the SRS is for specific research projects and also, since 2001, more widely as part of the EPSRC National Crystallography Service. Users and service providers will present some results and discuss past experience and future prospects. Come and see what's in it for you.

Bill Clegg (University of Newcastle and SRS Daresbury Laboratory)
Synchrotron crystallography for all: past, present and future

John Warren (SRS Daresbury Laboratory)
Updates to SMX @ the SRS

Sandy Blake (University of Nottingham)
Some co-ordination chemistry at the SRS

Alan Kennedy (Strathclyde University)
Mony miekles mak a mucle

The Hursthouse Event

Organisers: **Paul Raithby** (University of Bath) and **Alan Welch** (Heriot-Watt University)

A symposium and dinner in honour of Mike Hursthouse to recognise the outstanding contribution that he has made to Chemical Crystallography throughout his career.

Thursday 6th April

16.30 Alan Welch (Heriot-Watt)
Supraicosahedral heteroboranes

17.00 Martin Schröder (Nottingham)
tba

17.30 Maria Carrondo and Teresa Duarte (ITQB, Lisbon, Portugal)
tba

18.00 Robert Shaw (Birkbeck)
A tribute to collaboration, crystallography and Mike

18.30 Close

19.30 Dinner

Friday, 7th April

9.00 Simon Coles (Southampton)
Past, present and future perspectives in the Silver Anniversary Year of the National Crystallography Service

9.30 Bill Clegg (Newcastle)
The use of local, national and international facilities in the structural study of alkali metal complexes

10.00 Coffee

10.30 Philip Gale (Southampton)
Molecular recognition and structural chemistry of some new anion receptors

11.00 Paul Raithby (Bath).
Chemical crystallography: faster, bigger, brighter

All are most welcome.

Central Facility User Meeting

Organiser: **Mina Golshan** (SRS Daresbury Laboratory)

A combined meeting for the SRS XRD User Community and the Diamond SIG will take place on Monday, 3rd April.

Bursary Report 2005 - from the Treasurer

THE year of the International Congress is always a busy one for the Arnold Beevers Bursary Fund, and this year was no exception. The BSG donated £768.13, the interest from its reserves, to the fund and the Gift Aid refund of £801.50 on the membership subscriptions was also placed in the fund. Other membership donations amounted to £40.00.

There were 31 bursaries worth £4805 awarded to students attending the Spring meeting in Loughborough. Seven of these Bursaries had commercial sponsors, and we are very grateful to ICDD (1), PANalytical (4) and Rigaku (2) for this valuable support.

During the rest of the year, there were 19 Arnold Beevers Bursaries awarded, totalling £3790. 11 of these enabled students to attend the XX IUCr Congress in Florence, and the remaining 8 bursaries were used to attend some of the wide variety of conferences in which Crystallography has much to contribute. Many of the bursars' reports of these meetings have been incorporated into the articles which have been printed in Crystallography News.

The outlay on these bursaries has depleted the Bursary Fund, but it was very pleasing that so many students were assisted to attend such worthwhile and memorable conferences. All donations to build up the fund and enable future students to have similar opportunities are very welcome.

There were no requests for 'good works' funding in 2005.

IUCr Congress Bursary Fund

THE BCA Council is delighted that the 2005 IUCr Congress in Florence is able to return our loan, made in May 2004, towards congress bursaries. Once this money is repaid, we will be in a position to offer it to the organising committee of the XXI Congress in Osaka, Japan in 2008.

Name	University	Conference
Isabel Moraes	Reading University	School of Crystallography, Erice, Italy
Francesca Fabbiani	University of Edinburgh	XX IUCr Congress, Florence, Italy
Claire Jakeways	Cambridge University	Internal Friction and Mechanical Spectroscopy, Kyoto, Japan
Sophie Dale	University of Newcastle	XX IUCr Congress, Florence, Italy
Zhanhui Yuan	University of Newcastle	XX IUCr Congress, Florence, Italy
Kathy Guille	University of Newcastle	XX IUCr Congress, Florence, Italy
Gary Nichol	University of Newcastle	XX IUCr Congress, Florence, Italy
Ross Harrington	University of Newcastle	XX IUCr Congress, Florence, Italy
Ivana Evans	University of Durham	XX IUCr Congress, Florence, Italy
Shu Yan Zhang	University of Oxford	XX IUCr Congress, Florence, Italy
Pauline Gavan	University of Bradford	XX IUCr Congress, Florence, Italy
Michael Orley	Leeds University	Crystal Growth and Nucleation, Il Ciocco, Barga, Italy
Craig Bull	University of Edinburgh	XX IUCr Congress, Florence, Italy
Malcolm Guthrie	University of Edinburgh	XX IUCr Congress, Florence, Italy
Spoorthi Dharmayat	University of Leeds	Crystal Growth and Nucleation, Il Ciocco, Barga, Italy
Susanna Teixeira	Institut Laue Langevin	International Conference on Neutron, Sydney, Australia
Sean Harrison	University of Leeds	Crystal Growth and Nucleation, Il Ciocco, Barga, Italy
Elizabeth Harvey	University of Cambridge	Scientific Basis for Nuclear Waste Management, Ghent, Belgium
Helen Jones	University of Manchester	Symposium on Industrial Crystallisation, Dresden, Germany

From the Secretary Announcement of Election to Council - President

THIS year we have a vacancy on BCA Council for the Office of President, as Chick Wilson will have come to the end of his three-year term. Please send your properly seconded nominations for this position to me as soon as possible. I will accept nominations until two weeks before the date of the AGM on 5 April 2006. If you nominate someone, it is your responsibility to make sure that the person you nominate is willing to stand for election.

Christine Cardin
Secretary to Council

2006 Annual General Meeting of the BCA

THE Annual General Meeting of the British Crystallographic Association will be held on Wednesday 5th April 2006 at 4.35 p.m. in the University of Lancaster.

At this meeting we will elect a new President.

Draft Agenda

1. Approval of Agenda
2. Apologies for absence
3. Minutes of the last AGM (published in Crystallography News)
4. President's report
5. Secretary's Report to Council (published in Crystallography News).
6. Northern Networking Events' Report.
7. Report of the Treasurer to include Presentation of the Accounts for 2005 and the Examining Accountant's Report.
8. Acceptance of the Accounts
9. Membership Fees
10. Elections to Council
11. Appointment of Examining Accountant for 2006
12. Any other business

Christine Cardin (Hon Secretary)

BCA Young Crystallographers

Young Crystallographers - YC06

FOLLOWING the great success of the Young Crystallographers Meeting that took place at the BCA Spring Meeting two years ago, the event is being repeated. YC06 operates as a satellite meeting to the Spring Meeting, and will run from around lunchtime on Monday 3rd April until 10.30 on Tuesday the 4th.

The emphasis of YC06 is as much on the social interaction as the work presented, and is intended to open up new opportunities for young structural scientists, as well as allowing them to present their work in front of an audience of their peers. Contributions for talks are most welcome!

Registration is *free*, including accommodation, and is taking place online at http://www.chem.gla.ac.uk/yc06. Details of the program and other information will be posted here as and when they are announced. There is also the opportunity to design this year's logo...

A New Crystallographic Association: ATC: Association Tunisienne de Cristallographie

THE Tunisian Crystallographic Association organized its first Workshop on Crystallography at Monastir in June from 3 - 5 June 2005, and over 50 young researchers attended. It is now a member of the IUCr and the ECA. The First Tunisian Crystallographic Meeting (TCM 1) will be held in Hammamet (Tunisia) on 19, 20 and 21 March 2006.

Address:
Association Tunisienne de Cristallographie
Ecole Nationale d'Ingenieurs de Monastir
5019 - Monastir - Tunisia.
Tel/Fax: + 216 73501786

Email: tunicrystal@yahoo.fr

British Crystallographic Association

MINUTES of Annual General Meeting held on Wednesday, 6th April 2005 at 16.30 in Loughborough.

The President (**Chick Wilson**) in the Chair.

92 voting members were present.

1. **Approval of agenda.**
   The agenda was approved

2. **Apologies for absence.**
   An apology had been received from Kate Crennell.

3. **Minutes of the previous AGM.**
   These had been published in the March 2005 issue of Crystallography News. They were approved as a correct record of the meeting.

4. **President's report**
   The president recorded the deaths of six members, Sam Small, Mary Truter, Sue Bayliss, Francis Crick, Maurice Wilkins and David Blow. He asked that members reflect on their passing and celebrate their achievements. Three new Honorary members has been elected, Paul Barnes, Mike Glazer and George Sheldrick. Richard Catlow had been elected FRS.

   The most important subject group meeting had been the memorial meeting for David Blow, which had attracted about 240 attendees.

   The president commented on the membership figures, particularly the low number of students. He asked for a flat rate fee of £20 over the three years of the Ph.D. to be approved. A recruitment pack would be produced for the start of the next academic year.

   The main change on Council had been the addition of Sheila Gover as BSG representative. The Education website had been relaunched.

   No questions were raised.

5. **Secretary's Report.**
   The secretary, Christine Cardin, presented her report, which had been published in the March 2005 issue of Crystallography News. She thanked Dave Taylor for his extremely hard work as Treasurer.

6. **Northern Networking report.**
   This report was presented orally. Gill Houston said that there were now 867 members on the database. This beaks down as 558 Ordinary, 38 retired, 140 student, 5 unemployed and 20 Life. By group, there are 297 BSG members, 259 CSG, 116 IG and 118 PSG, with 77 recorded as unspecified. There are 13 companies as Corporate members.

   Crystallography News has been able to increase the number of advertising pages. Gill thanked Chick Wilson, Dave Taylor and John Finney for their major inputs to the success of the meeting, and their exhibitors for their support, without which the meeting could not be held. 78 posters had been presented; 31 students had applied for bursaries and all had been accepted.

7. **Treasurer's report.**
   The Treasurer, David Taylor, presented a detailed report, subsequently published in Crystallography News. In summary, subscription income was down, whereas advertising revenue from Crystallography news was up. He suggested that we should all give away any spare copies of Crystallography News to our colleagues, to encourage them to join. Expenditure was very similar to the previous year.

   Chick Wilson thanked David for his tireless work on behalf of members, and Michael Glazer proposed that the accounts be accepted. This was seconded by Paul Raithby. The reappointment of the accountant was also approved. David Taylor recommended that the Young Company be reappointed, seconded by Chick Wilson.

8. **Elections to Council.**
   Sheila Gould was nominated for the position of Treasurer by Chick Wilson, seconded by Christine Cardin. There were no further nominations, so Sheila Gould was duly declared elected.

9. **AOB.**
   1. Presentation of prizes. The Chairman announced that he proposed to present the prizes at the Conference Dinner.
   2. Student membership fees. The meeting discussed the question of the student membership fee. It was proposed that there should be a 4-year term for student memberships, rather than the existing three terms. The meeting agreed unanimously that there should be a three year fixed charge of £20; this three year term can take place contiguously at any point in a Ph.D. programme.

There being no further business the meeting closed at 17.20.

Christine Cardin
Secretary to Council

BCA 2006 Spring Meeting -

	Monday, 3rd April	Tuesday, 4th April			
	SATELLITE MEETING				
9.00 h		Young Crystallographers	An Introduction to Protein Crystallisation	Powder Diffraction Workshop	
9.45 h					
10.00 h					Coff
10.30 h		Coffee and Registration			
11.00 h	Young Crystallographers	Registration	Synchrotron Chemical Crystallography for all	Powder Diffraction Workshop	Neutron & Synchrotro Opportunitie
12.00 h		Lunch & Exhibition		PCG AGM	IG AGM
13.00 h	Young Crystallographers & User Meeting Lunch	Welcome and Keynote 1 Larry De Lucas		Powder Diffraction Workshop	K
13.30 h	Young Crystallographers	High pressure, liquid & surfaces	Crystal Stories		Crystallisatio Polymorphis
15.00 h			Tea & Exhibition		
15.30 h	Tea & Coffee	Tea & Exhibition	Crystal Stories	Powder Diffraction Workshop	Crystallisatio Polymorphis
16.00 h	Young Crystallographers	CCG Prize Lecture			
16.30 h		PCG Prize Lecture			
17.00 h	SR Users & Diamond SIG Meeting	Exhibitors' Forum			
17.30 h					
18.00 h					
18.30 h	Dinner for Young Crystallographers and User Group Members 18.30 - 19.30	Posters & Exhibition 18.30 - 22.00 Buffet & Wine Reception 19.00			
20.00 h					

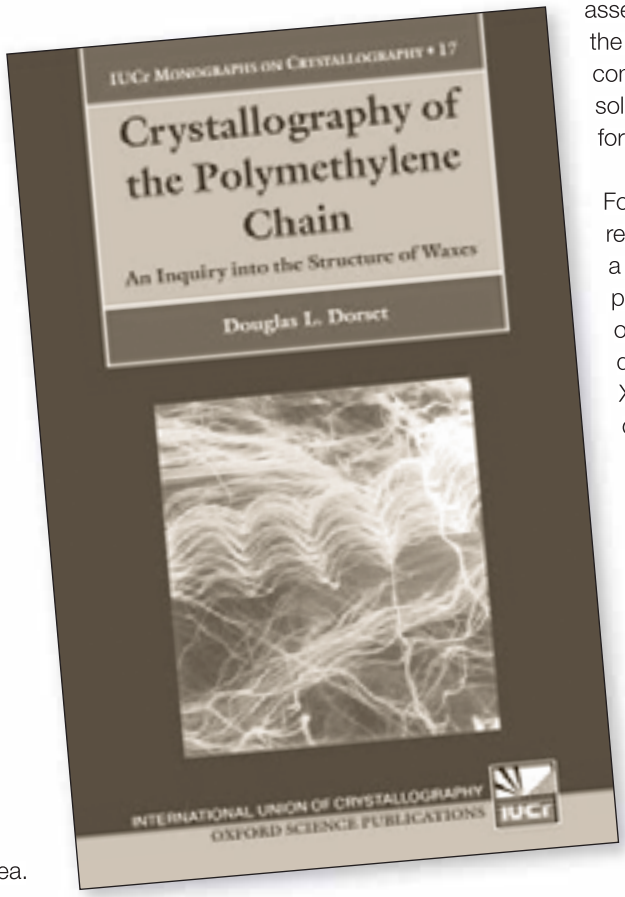
Timetable

Wednesday, 5th April			Thursday, 6th April			Friday, 7th April
						SATELLITE MEETING
Keynote 2 Mark Spackman			Keynote 4 - Teaching Plenary Garry Taylor			Hursthouse Event
ee & Exhibition		Topology	Coffee & Exhibition			
n es	Customised Crystallisation	Coffee	Charge Density	Crystal Structure and Growth at the Nano-scale	Getting the most out of your crystal	
		Topology				
	CCG AGM	BSG AGM				
hibition 12.00 - 13.00			Lunch & Exhibition 12.30 - 13.30			
Keynote 3 - Alun Bowen Lecture Ulrich Griesser						
n & sm	Customised Crystallisations	Topology	Powder Diffraction in Industry	Crystal engineering	TOPAS Academic Workshop	
Tea & Exhibition						
n & sm	Customised Crystallisation	Topology Workshop				
			Tea - Closing Ceremony 16.00 -16.15			
BCA AGM 16.35 - 17.20			Hursthouse Event			
Lonsdale Lecture 17.30 - 18.30 Mike Glazer						
Conference Dinner 19.30			Hursthouse Dinner 19.30			

Books

Crystallography of the Polymethylene Chain: An Enquiry Into the Structure of Waxes

Douglas L. Dorset, ExxonMobil Research, Annandale NJ USA
Oxford University Press, 2004 (IUCr Monographs on Crystallography 17)
Price £85.00 (hardback)
ISBN 0198529082, 232 Pages



THIS seventeenth title in the series of IUCr Monographs on Crystallography concerns the study of waxes, with particular emphasis on the structures of pure n-alkyl compounds and their binary mixtures as models for multicomponent systems containing linear polymethylene chains. The author's own research in this field spans nearly 35 years, and his significant contributions to the development of electron crystallography in particular have provided many new insights into earlier powder X-ray diffraction and spectroscopic studies of these systems. Electron diffraction images, mostly taken from the author's own archives, are prominent throughout the book, reflecting both the author's expertise and the importance of electron crystallography in this area.

The back-cover synopsis of the book specifies that it aims to elucidate three main features of waxes: "firstly, which modifications of molecular components are allowed for maintaining stable solid solutions; secondly, what happens when stability conditions are traversed and fractionation begins and thirdly, the structure of fractionated arrays". The opening chapter provides a more detailed statement of the book's scope, citing a multitude of everyday products and industries that rely on a thorough understanding of various waxes. One principal scientific objective is noted to be a critical evaluation of this understanding, specifically of the widely-accepted "Le Roux model" for wax structure. In short, this model suggests that a polydisperse wax - that is, a linear polymethylene chain assembly that contains a distribution of chain lengths, chain unsaturation, functionalisation and branching - can be considered to comprise four zones: the first, a mostly crystalline region in which polymethylene chains are arranged in a manner that resembles the pure materials; the second, a rigid amorphous zone that incorporates chain branches; the third, an amorphous region between the ends of the chains that may contain solvent molecules, and the fourth, a more fluid region that contains volatile lower molecular weight components. The book follows a course intended to assess this model by examining the structures of various pure wax components and their binary solid solutions in the most crystalline forms available.

Following the preliminary remarks, Chapter 1 comprises a concise and helpful primer concerning aspects of polymorphism, phase diagrams and solid solutions. X-ray diffraction, electron diffraction and differential scanning calorimetry are featured techniques. Chapter 2 treats the general packing features of linear polymethylene chains in the manner of Kitaigorodskii, including characteristic electron diffraction patterns that assist with the later discussion. Chapter 3 describes in some detail the known crystal structures of the n-alkanes (paraffins), establishing the structural basis for their extensive polymorphism. Inclusion in the discussion of recent experimental data is a useful expansion on earlier accounts. This chapter also touches upon branched and aromatically substituted paraffins, but highlights that experimental knowledge in this area remains somewhat sparse. Thermodynamic and structural aspects of disorder and phase transitions in the pure paraffins is expanded upon in Chapter 4, which again incorporates a good blend of crystallographic, spectroscopic and calorimetric data.

Chapters 5 and 6 provide a substantial discussion on

binary paraffin systems. In this section, Kitaigorodskii's well-cited rules for stabilisation of solid solutions are evaluated against newly available single-crystal electron diffraction data. While volumetric rules concerning size and shape matching of the molecular components are found to be largely robust, previous suggestions regarding the symmetries of the pure components do not stand. Some fractionated binary structures are discussed, in which phase separation is shown to involve both lateral and longitudinal chain segregation - i.e. the structures do not simply comprise layers of the pure components segregated at the methyl-group interfaces. The influence of unsaturation and heteroatom substitution on general chain packing and on the formation of binary phases is touched upon in Chapter 6, but experimental information is currently less abundant in this area.

The following four chapters are devoted to functionalised derivatives of the n-alkanes, considering respectively alcohols, carboxylic acids, fatty acid esters and cholesteryl esters. Each survey encompasses the structural features of the pure materials and also their binary solid solutions. These chapters are valuable summaries of a large and very diverse literature, and each is an excellent starting point for researchers wishing to consider the solid-state behaviour of these classes of compounds.

In Chapter 11 the author brings together all of the information from the preceding chapters, first providing an excellent summary, then discussing how the knowledge can be applied to polydisperse waxes incorporating much broader chain distributions. Specific examples are given in which structural knowledge provides insight into the physical properties of polydisperse waxes. Ultimately, Dorset arrives at the conclusion that growing experimental evidence requires re-evaluation of the Le Roux model, then goes on to suggest numerous areas for further progress.

As a whole, the book is impressive. The author brings together a huge amount of literature to provide a coherent and comprehensive account of the research area as it stands today. The pioneering research is faithfully documented, but it is critically re-evaluated where more recent results suggest this to be necessary. The range of analytical techniques discussed imparts an appreciation of their complementarity for examining these systems, while the focus on electron crystallography is justified and clearly written by an expert. The overall presentation, including plentiful diagrams and photographs, is excellent. The only possible negative comment regarding this book is that it seems likely to find a rather limited audience. Of the series of IUCr Monographs to date, the topic seems to be the most esoteric, and despite the fact that the author makes an admirable effort to stress its relevance in the opening remarks, it is perhaps unlikely that the book will find its way into the general reading of many crystallographers. Nonetheless, those who do venture into the book will be richly rewarded - it is a worthy addition to the series.

Andrew Bond

IUCr wins open-access funding for third successive year

THE International Union of Crystallography (IUCr) has won a third round of funding from the Joint Information Systems Committee (JISC) to support open-access delivery of its eight journals via its Crystallography Journals Online service. The award means the waiving of open-access publication charges for UK higher education staff who publish in these journals for a one-year period from 1 March 2006.

The investment received so far has helped the IUCr to provide UK authors with extra choice and improve access to published content, allowing the publication of over 570 open-access articles, 255 in 2004 and 322 in the first nine months of 2005.

The JISC programme continues to provide evidence about the impact of open-access models of publishing on the conduct and dissemination of research. The results of the full evaluation of the programme will be made available to the academic and research community in due course.

More information about the IUCr's open-access policy is available at **http://journals.iucr.org/services/openaccess.html**

Andrea Sharpe

A Useful PC Tool For Examining .pdf Files

Ever had the problem of printing out a publication from a .pdf file and finding out when you read it in the train or areoplane that you have printed a paper with colour illustrations on a black-and-white printer?

Kurt Tornare of the IT service of the University of Geneva recently drew my attention to the pc software **PDF - Analyzer 2.5** available as freeware from the site **http://www.pdf-analyzer.com/**

I use this software to determine whether the content of a pdf file is in black and white only or in colour BEFORE sending it to the printer.

Howard Flack

Groups

CCP4 at Leeds

THE annual Collaborative Computational Project in Macromolecular Crystallography (CCP4) Study Weekend returned to the University of Leeds for a stimulating meeting on January 6-7, 2006.

The meeting, "Crystallography of Complexes", presented a range of biochemical and computational methods with a key aim of obtaining crystal structures of proteins complexed with small molecules, nucleic acids or other proteins. The interesting and diverse scientific programme was organised by **Tadeusz Skarzymski** (GlaxoSmithKline, UK), **Airlie McCoy** (Cambridge University) and **Eugene Krissinel** (European Bioinformatics Institute, Cambridge). The meeting attracted delegates from all over the world and boasted the largest attendance of a CCP4 study weekend to date, numbering approximately 555 individuals from both academia and industry.

The chairman of CCP4 Working Group 1, **Jim Naismith** (St Andrews University) opened the workshop by encouraging the user community to continue its contribution to the effort and content of the package, nearing 30 years of age now. The relentless effort of one of the early pioneers, **Eleanor Dodson** (York University) was rewarded 2 years ago with election as a 'Fellow of the Royal Society.' The same accolade was accorded this year to another stalwart of the CCP4, **Phil Evans** (MRC Cambridge). Congratulations were offered by everyone present.

Joël Janin (Gif-sur-Yvette) started the first session, "Biology is Molecular Interactions" by posing the question 'What can one learn from looking at a PDB file?' There is a wealth of information that can be gleaned from PDB entries in relation to molecular aggregation. Proteins tend to work in tandem with other macromolecules, e.g. copies of the same molecule, proteins in cluster or cascade, or gene repression/restriction. Rules were drawn to distinguish biologically relevant interfaces from incidental interfaces arising from crystal packing. A strong, specific interface, such as antibody-antigen complexes, is usually a single-patch, rigid-body interaction. RMS deviation between atomic positions in the free protein and in the complex is below 1.0 Å. The solvent accessible area excluded by the complex formation is in the range of 1200-2000 $Å^2$. This is the sum of the areas on both molecules, as opposed to the interface area, which is half as large! Such an interaction is termed "standard", and has a characteristic distribution of non-polar contacts and H-bonds. Standard interfaces are encountered in biological homodimers. On the other hand, crystal packing interfaces tend to be smaller and more hydrated. But hetero-complexes often recognise each other in an induced fit interface spread over 2 or 3 patches. The total area is usually in the range 2000-3500 $Å^2$. Other metrics were introduced to quantify the specificity of interactions: Gap index, fraction of contacts that are hydrophobic and surface complementarity. Protein-DNA interfaces tend to be larger still, as they are more likely to be hydrophilic, and since DNA tends to bind to dimeric/oligomeric proteins.

Michael Rossmann (Purdue University) explored the path 'From structure of the complex to understanding of the biology', as encountered in his virus structure determination. Cell infection by a virus usually involves binding to a surface feature, initiating the formation of a coated pit. When internalised into the cell, the pH is lowered causing the capsid to unfold and the genetic material to be released into the cytosol. In the case of the canine parvovirus, which has a 5 kb ssDNA genome, capsid diameter 140 Å, electron microscopic (EM) reconstruction of an averaged particle did not show any electron density for the host transferring receptor that was known to be the viral infection promoter. Modelling a single TfR molecule on one of the 60 capsid faces, however, was able to retrieve phase information to trace the chain in the X-ray electron density, extending outwards from the centre at a distance of 140 to 210 Å. Comparing this model with the uncomplexed virus showed key conformational changes at the binding epitope right across the capsid, rendering the other faces unsuitable for binding. The TfR binding site was on a 3-fold axis of the icosahedral asymmetric unit, in a shallow recess, possibly promoting immune system evasion. The theme of a special vertex is also borne out in the T4 bacteriophage virus structure, where the tail part of the virus is connected to the icosahedral capsid. Here the viral genome is 1.2 Mb dsDNA, and a capsid diameter ~5000 Å. EM reconstruction experiments provided pictures of the various stages of the virus development. The head and the tail are assembled separately, and then fused by special cell machinery. The special vertex is on a 5-fold axis, where the baseplate protein has axial and peripheral domains, among many components. Mutations in the peripheral domain are associated with size variation of the capsid, also allowing interchangeable roles between GP23 and GP24, which have ~24% identity. The individual component protein structures were determined separately and EM reconstruction was used to dock them into the appropriate locations which were fortunately unambiguous. One of the baseplate components was a lysozyme-like protein, promoting the digestion of host cell wall components upon infection. A super helix of a beta-sheet domain forms a sheath around the neck, which is extended (1 turn) in the free virus, but gets shortened upon binding to the host (2 turns), as seen in EM reconstruction. Compiling all the structural information, a

mechanism of infection could be envisaged, where the initial host surface recognition is followed by tail shortening and lysozyme-like activity to allow the injection of a long rod of DNA into the hapless victim.

The second and third sessions, "Crystallography or Complexes between Macromolecules" focussed on preparation and characterisation of macromolecular complexes. **Kiyoshi Nagai** (MRC Cambridge) opened the session with hints and tips about preparation of large RNA-protein and protein complexes from his group's work on small nuclear ribonucleoprotein particles (snRNPs) involved in pre-mRNA splicing and the ~340 kDa signal recognition particle (SRP) involved in protein secretion or membrane insertion. His suggestions included the use of affinity purification under gentle conditions to purify complexes, and the use of two different approaches in tandem to ensure purity, 'Tandem Affinity Purification', TAP1. He described using proteomic analysis of protein bands to ensure that the purified complex is the one expected, i.e. in-gel tryptic digestion and MALDI-TOF analysis with a mass spectrophotometer. From the group's experiences with the spliceosome, he pointed to the Prediction of Natural Disorder website (http://www.PONDR.com) which predicts which parts are likely to be well ordered, and which parts of a protein should be first targets for deletion analysis. Using this information, one can then try to construct a more rigid crystallisable entity. He also discussed breaking multi-component complexes down into more manageable subsections, based on building up an understanding of which proteins interact with which in a complex. He warned the audience not to go too far by showing examples of proteins that had been insoluble on their own but folded into soluble complexes when co-expressed. Finally, he described achieving complexes of four proteins in *E. coli* by co-transfecting with two separate plasmids with different resistance markers that each coded for two proteins, to enable efficient overexpression of each protein. This four-protein complex could then be directly isolated from the *E. coli*.

Tim Dafforn (University of Birmingham) gave an overview of biophysical techniques that can form the basis of a study of macromolecular assemblies, and in particular the stoichiometry, affinity and configuration in solution. He described the principles of the use of Analytical Ultra Centrifugation in looking at changes in mass or size through complex formation. This talk started with a description of a machine the size of a room invented by Svedberg (who received the Chemistry Nobel prize in 1926 for his work on 'disperse systems'). To study conformation, Tim described various fluorescent techniques, taking advantage of either intrinsic fluorescence (Trp, Tyr, Phe, the cofactors NAD, FAD) or extrinsic fluorophores attached via cysteine or lysine residues. These included using changes in Fluorescence anisotropy to analyse ligand binding, and using FRET (Fluorescence Resonant Energy Transfer) to work out the relative positions of proteins in space in solution. And last but not least he reminded us of the use of running gel electrophoresis under native conditions rather than reducing conditions to examine the behaviour of a macromolecular complex. He suggested varying pH running conditions in these gels as a means to determine optimal conditions for complex formation.

John Ladbury (University College London) rounded off the session with a talk about the use of isothermal titration calorimetry in investigation the complex behaviour of macromolecules. He described the basis for isothermal calorimetry and demonstrated its use in investigating the formation of protein complexes in tyrosine kinase-mediated signal transduction. His results suggest that early signalling is accompanied by the formation of a multi protein complex - leading to the suggestion that we should be pursuing signalling complexes rather than signalling cascades. Systems biologists take note!

Overall the second session of the meeting was a pertinent and useful reminder of many techniques that protein crystallographers should be aware of and take advantage of, either in trying to obtain structures of macromolecular complexes or to better understand their function.

Airlie McCoy (University of Cambridge) opened the third session by reviewing the nature of crystallographic and non-crystallographic symmetry in biological complexes, showing that molecular replacement generally becomes more difficult when the number of protein molecules increases in the crystallographic asymmetric unit. After a brief description of the various steps involved in the molecular replacement program Phaser, she showed a couple of successful case studies ranging from an easy problem to a multiple copy (as many as 45!) and multiple domain search.

Kim Henrick (European Bioinformatics Institute, Cambridge) briefly described the comprehensive relation between the PDB and MSD. While PDB is the deposition of structures obtained by crystallography NMR or EM, MSD provides databases for derived attributes of these structures. Kim showed the problems and pitfalls encountered in processing the PDB to derive the biologically correct asymmetric units for biological assemblies and impact of the problems on fold recognition and active site matching.

Ruth Nussinov (SAIC-Frederick, U.S.A.) gave a brief introduction about the steps involved in her program ComboDock: Combinatorial Docking for Multimolecular Assembly and Protein Structure Prediction. She has demonstrated the success of the program as to how the 3D jigsaw puzzle was put together from individual macromolecular subunits. Examples included a transcription factor and RNA polymerase II.

Martin Noble (University of Oxford) closed out the day by showing that some computational tools have to be employed on a new structure to adequately describe its relevant features such as sequence conservation, functional epitopes, surface complementarity between interacting molecules, etc. He summarised the framework of concepts coming from empirical description of energetic terms and statistical analysis of known structures. He also showed how using the program GRID and the CXXSurface toolkit of the ccp4mmg program can enable one to analyse the surface properties of putative complexes.

The following day **Phil Evans** (MRC Cambridge) brightly opened Session 4, "Complexing Proteins with Small Molecules", with "Good morning boys and girls...Why do we need stereochemical restraints?" The answer, in the case of most protein structures is that the resolution of the X-ray data is not high enough to ensure that a chemically reasonable structure can be obtained without restraints. He then went on to methodically define and describe the different types of stereochemical restraints which are targets for minimisation in the refinement process (e.g., bond lengths, angles and chirality). He also showed how chemical structures, such as rings, may vary in their need for restraints as a consequence of their size. A clear message from this talk is that the crystallographer involved in refinement of a ligand in a protein structure must take full responsibility to ensure that the correct restraints and libraries are used. "Trust no one" …not even the PDB!

Chun-wa Chung (GlaxoSmithKline, UK) discussed how one uses biophysical methods to avoid producing crystals of 'apo-structures' (structures of proteins alone rather than in complexes). She explained how different techniques such as NMR, light scattering, calorimetry and circular dichroism can be used to determine the conditions favouring complex formation. It is evident from her talk that the investment of time and protein needed to define crystallisation conditions using biophysical methods can seem high depending upon the method used, but the rewards – obtaining a high resolution structure of an important protein-ligand - can be genuinely worth the effort.

Annie Hassell (GlaxoSmithKline, USA) complemented the previous talk by describing a range of strategies for obtaining protein-ligand complexes. She then described examples from four areas of interest: co-expression of a protein with a ligand present; the use of ligands during protein purification; co-crystallisation; and soaking methodologies. Interesting cases for 'encouraging' complex formation included the addition of a specific ligand during cell lysis or protein refolding. A specific ligand can also be introduced in the latter stages of purification as a means of displacing heterogeneous low affinity ligands bound to a protein target. Whilst it is clear that there is no single "magic bullet" to guarantee formation of any specific protein-ligand complex, there are a plethora of "tricks" available and the methodical variation of one small parameter (e.g., temperature, pH, chemical additives) can make all the difference in obtaining stable complexes suitable for crystallisation trials.

Session 5 "Molecular Interactions in Drug Discovery" involved complexes of proteins with inhibitor molecules for use in structure-based design of drugs. Three talks were presented from three pharmaceutical companies. All suggested that obtaining and interpreting inhibitor complexes could be a difficult exercise. **Sandra Cowan-Jacob** (Novartis) opened the session by describing the structure determination of wild type and mutant abl kinase, the target of Gleevec. Initial management pressure offered a window of 6 months to get structures if they were to be used in the design process. She described elegantly how the structure allowed new compounds to be made, and through looking at mutant structures the resistance of Gleevec could be addressed, leading to a compound that was effective against most of the resistance mutants.

Tomas Lundqvist (AstraZeneca), described how many validated targets have unappealing "druggability" and went on to discuss three cases where, despite challenges, use of structure enabled progress. In the Murl dimer, the active site is buried and binds charged molecules. NMR showed that Glu binding to a cryptic pocket remote from the active site is essential for compound binding. Whereas the active site was not druggable, specific compounds could be designed against the cryptic pocket. IL2 binds to a receptor through a protein/protein interaction "hotspot". Sunesis used "tethering" approaches (introducing covalent cysteine binding sites for potential compounds) and showed large conformational changes. In Caspase 7 an inhibitor was found (again by tethering) to bind at the dimer interface and to induce an allosteric conformation that stops substrate binding.

David Brown (Pfizer) discussed drug design efforts towards phosphodiesterase 5, PDE5. This protein is of therapeutic importance and is the target of the well known compound Viagra®. A clear aim of this work was to distinguish binding modes of inhibitors, a number of which were representative of different synthetic series of compounds. He described some beautiful work with many trials and tribulations on the way and confusion from results published elsewhere. The information obtained from this work helped to clarify subtle structure-activity relationships but was also of key importance in driving subsequent studies focussed upon the development of other potent and more specific inhibitors with wider applications in treating diseases demanding regulation of PDE's.

The conference rounded off with a "Case Studies" session on building small ligands into protein structures. The first speaker, Gerard Kleywegt (University of Uppsala, Sweden) discussed some tools for obtaining refinement dictionaries for your ligand and then described some bad examples in the PDB. All possible forms of error have been seen; ligands where refinement parameters should have been applied and were not, ligands where incorrect parameters had been applied, and correct restraints but incorrect refinement targets. He then outlined some bad examples such as the CoA structure with a 6.7 Å bond in it! His take home message was "Check your refinement parameters by

refining against just the parameters without any X-ray terms and do not trust anyone else's."

Tom Terwilliger (LAN, Los Alamos, USA) then presented the impressive PHENIX LigandFit wizard which will attempt to automatically identify the ligand in unknown density; an increasing issue in structural genomics projects where there is 'something lurking in the active site'. Using a list of 119 ligands which have a density correlation coefficient of less than 0.85, the right ligand is picked about half the time purely on correlation coefficient on a large test set. However using better statistics, such as normalising for how well this ligand fits all ligand densities in the test set, the accuracy can be improved to 90%. A fit to an asymmetric ligand with a similar correlation coefficient is more likely to be right than a spherical one.

Next **Victor Lamzin** (EMBL Hamburg) outlined automatic ligand building in ARP/wARP. He showed an interesting property of the connected volume of a real ligand, which declined more slowly with reduced contour level compared to noise. In most cases the ARP/wARP algorithm will identify ligand atoms close enough to the true position for refinement by refmac. Good B factors for the ligand not surprisingly correlate with success.

Finally **Paul Emsley** (University of York) described ligand fitting in Coot. He described the features of the algorithm, which includes the concept of crystal space where ligands are continuous even if they spread over an asymmetric unit boundary. He also described the use of FFT-based search for initial ligand (and protein fragment) fitting combined with real space refinement to optimise. Overall ligands should not be able to hide or distort with the impressive software now available to put them in their place.

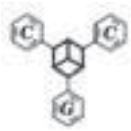
Finally, a meeting of this size and scope demands an excellent support team and in this regard we are truly indebted to the great work of the CCP4 organisation (Daresbury) which includes **Maeri Howard**, **Pat Broadhurst**, **Liz Kennedy** and **Sue Waller**. Special thanks are also due to **Stuart Eyres** who is responsible for the meeting photos (see http://www.ccp4.ac.uk/courses/stwk06/) and the web streaming of the meeting.

(Endnotes)

1 Puig, O., Caspary, F., Rigaut, G., Rutz, B., Bouveret, E., Bragado-Nilsson, E., Wilm, M. and Séraphin, B. The tandem affinity purification (TAP) method: a general procedure of protein complex purification. Methods. 24, 218-229 (2001).

Prepared by the Biological Structures Group Committee and edited by Kate Brown, Imperial College London

Computational Methods Applied to Crystallography



THE CCG Autumn meeting 2005 took place at Daresbury Laboratories on Wednesday November 16.

After much needed refreshments at the registrations, **Simon Parsons** opened the CCG autumn meeting with a warm welcome to the sponsors, Oxford Diffraction, Pfizer and Daresbury. This was followed by a brief but necessary outline of safety procedures, and especially of colour recognition of the stripes on the floor! (Apparently they are green and not orange…)

Angelo Gavezzotti initiated the day by introducing PIXEL, a semi-empirical method of calculating lattice energies, which may be used to investigate the relative contributions of different factors in crystal packing. Gavezzotti has studied intermolecular interactions for pairs of atoms using a frequency distribution function. Using this atom pairing method, it can be shown that there is no pattern for C…C, or indeed N…N or O…O interactions, but we start to see structure for C…S and H…Cl contacts. For classically hydrogen-bonded systems, such as acids, amides and alcohols, there is clearly structure. But then if H…Cl is a bond, is C…S also a bond? This would imply that everything is bonded to everything else but intermolecular bonds vary in strength so much that it questions the concept of a weak intermolecular bond - this being an oxymoron. *Ab initio* methods are generally limited by the size of the molecule and atom-atom methods are successful but totally empirical. The PIXEL method lies in between these two extremes. The method involves calculating the electron density of a molecule in a box split into a number of pixels. The contact is then defined as the overlapping of these two boxes (the overlap integral) and is calculated by numerical integration. The method may be used to investigate the packing forces involved in different polymorphs. He concluded that the shortest intermolecular interactions do not necessarily contribute to the crystal packing energy - such interactions have wide potential wells, and what is short is not necessarily also strong. PIXEL is useful, not for calculating lattice energies but to give insight into the relative importance of different interactions.

For the second talk, **Graeme Day** gave an overview of the current state of affairs in crystal structure prediction of organic molecules. The problem comes down to calculating the energy between molecules. However, the lattice energy surface may have many deep wells, all within a few kJ mol^{-1}. Finding the global minimum is a challenge, and even if we know it, is it the one that will be prepared? It is possible to search for patterns and get rough trial crystal structures using well-known methods such as Monte-Carlo, grid search or genetic algorithm methods. The energies of these structures are then minimised and clusters of structures emerge, often

many within 20-25 kJ mol^{-1} of the minimum. On examination, these clusters contain similar intermolecular interactions stacked in different ways. Success is assumed if the lowest energy (usually highest density) crystal structure matches the actual crystal structure. However, small changes in the molecular structure may have unpredictable effects on the crystal structure, and conformations, choice of Z', nucleation, kinetic effects and how energies are ranked also need to be considered - as well as computational cost. Although a small molecule can be extensively studied within about a day, a more complicated structure may take months. Pharmaceutical companies producing very flexible drugs are hence not yet interested! Graeme demonstrated the importance of the energy ranking by means of an example, oxazolidine-2,5,-dione, where fifty percent of the predicted possible structures lay within 5 kJ mol^{-1} of the global minimum. This was attributed to the fact that hydrogen-bonded structures appear to be much more difficult to predict than those with no hydrogen bonding. Thus better atom-atom approaches are needed, by improving electrostatics and atomic multipoles. This considered, predictions improved for hydrogen-bonded examples.

However problems still exist when thermodynamics are taken into account: when the entropy was considered, it was found that it affected the energy ranking significantly.

In conclusion, progress is being made in grasping the ideas of the changes in energy involved, but more work is needed to investigate kinetic and thermodynamic effects in the formation of individual crystal structures.

After tea had given us time to mull over the possibly disastrous consequences of failing to recognise the importance of kinetics in crystallisation, **Stewart Clark** gave his talk entitled "Applications of DFT in the Solid State". As Graeme previously highlighted, it would many people's dream to be able to predict physical and chemical properties of materials from knowledge of the atomic numbers, or to calculate properties beyond the capability of experiment to measure, or at least to enable interpretation of experimental results.

He explained the advantages of the plane wave pseudopotential approach, which included capturing the whole pressure-temperature range. Crystals can contain thousands of atoms per unit cell, which is significantly more than *ab initio* methods can deal with. Structural optimisation may be done from a given starting point, and temperature simulations may be performed in order to create a toolbox for calculating crystal properties, e.g. total energy, electronic structure, transition states, responses, polarisability, IR/Raman, all to a reasonable accuracy. However, these properties involve calculating the difference in total energy between two different states, and although the error on the initial states may be small, the error on the difference is relatively much larger.

In crystal structure determination, the plane wave approach may be used to calculate the structure where experiment has failed. The example of methanol was used, where each 'end' of the molecule has nine electrons (methyl and hydroxyl) and conventional x-ray diffraction could not distinguish the correct solution. The solution was known to be in P 1, and because a reasonable starting geometry was known, it was not difficult to isolate the minimum energy by considering all eight ways of arranging the methanol units together. He also highlighted the importance of the choice of exchange functional using amino acids as an example. In general, local density approximation (LDA) methods predict some sort of van der Waals (VDW) interaction, but generalised gradient approximation (GGA) methods give no interaction whatsoever. This leads to the former underestimating and the latter overestimating lattice (cell) parameters in glycine crystals due to the presence of VDW interactions, leading to the incorrect prediction of lattice energies and ultimately the wrong crystal structure. However in both cases the lattice parameters lay within 1% of the actual values and problems arise when these values are compared, again because of the large relative error - VDW forces suddenly becomes very important. In conclusion, DFT is not yet accurate enough for molecular crystal structure prediction.

Nic Harrison then changed the emphasis from molecular to inorganic structures, explaining how the stability of bulk phases could be predicted using titanates as an example and how this led to the discovery of a new ultra-hard material, comparable to diamond or boron nitride. Density functional theory may be applied easily and successfully to ionics, unlike molecular solids. There are eight known phases of TiO_2, of which rutile and anatase are the best known. Using DFT and experimental data, a phase diagram for the eight phases may be calculated and then projected under various experimental conditions such as increased pressure or temperature. Using this method, the cottunite phase was predicted to be the hardest at the highest pressure, which was confirmed experimentally. One application of TiO_2 phases is in lithium rechargeable batteries. The two phases, anatase and rutile, were compared for their ability to intercalate Li^+ ions, and found to have different properties. This was ascribed to the charge accommodation due to the split degeneracy of the t_{2g} orbitals in anatase. Orbital occupancy adopted with the donated charge is coupled to the structural deformation.

The last session before lunch by **Ashley Hulme** reintroduced molecular crystals and highlighted some of the problems of crystal structure prediction using 5-fluoracil as an example. The method used involved optimising the molecular structure *ab initio* and generating 2000 densely packed crystal structures using MOLPAK. In order for comparison, the energies of the actual crystal structures as well as those generated have to be minimised. The problem with fluoracil is that there are four molecules in the asymmetric unit, and although the correct structure was predicted, it lay nowhere near the lowest energy. Thus a polymorph screen was carried out and aside from various new solvates and hydrates arising, a new polymorph was discovered, which correlated with what was predicted to be the thermodynamically most stable form. (However the original polymorph was found experimentally to be the thermodynamically most stable form). In a second example related to fluoracil, 33 hypothetical structures were predicted within 10 kJ mol^{-1} of

the predicted minimum. A polymorph screen produced two new polymorphs amongst various other solvates. On close examination of the structures, it was found that there are only a few hydrogen-bonded motifs; this has resulted in a large number of polymorphs, and although the predicted minimum energy structure did not correlate with the actual structures, the correct hydrogen-bonded motifs were predicted.
After the delicious buffet lunch, which seemed to be enjoyed by all, especially those who snapped up the pudding before others had completed their main courses (no names mentioned!), **Anthony Stone** then went on to explain some of the difficulties in calculating intermolecular potentials *ab initio*. One possibility is the "supermolecule" model, where the intermolecular potential is calculated using the difference between the bonded and non-bonded molecules. Although a simple concept and easy to use, the method is subject to a number of problems, including basis-set superposition errors (BSSE), expense of calculations, and size consistency as well as giving a non-variational energy as a result. DFT can reduce the computational cost somewhat but does not solve the BSSE, and still produces only a single number. Perturbation theory (PT) gives the energy directly and gives a natural physical interpretation, with no BSSE, but for short-range distances, is complex and hard to extend to higher levels. The intermolecular perturbation theory (IMPT) gives the perturbation energy in terms of electrostatics, exchange-repulsion, inductive charge transfer and dispersion, and although the first two terms are calculated well, no correlation is taken into account. Symmetry adapted perturbation theory (SAPT) advanced on this, but there were perhaps too many energetic contributions, at very high computational demand. The Kohn-Sham extension to this (SAPT-KS) saw a simplification to the method, which was also faster, but gave disappointing results, partly because the functionals did not have the correct asymmetric behaviour. So the method was revised, and is still fast and relatively simple, and is accurate also. In conclusion, IMPT has been revised to provide an efficient and accurate source of intermolecular potential data. Electrostatics and exchange repulsions penetrations contributions are readily described, but other energy terms are more difficult to calculate.

Finally, **Gordon Barr** explained how we can get useful information from the CSD by data mining and pattern matching using cluster analysis. By defining all interatomic distances and angles in a given structure, or part of structure, it is easy to compare fragment similarity using D-SNAP, which is designed to be used in conjunction with the CSD. Up to 4000 hits may be analysed at any one time, making it possible to study almost any fragment of interest. New structures external to the CSD may also be included, allowing personal research to be included in the cluster analysis. It is easy to visualise the changes that differences in similarity cut-offs makes using a variety of clear graphical methods. Cluster analysis of this sort finds applications in powder pattern matching, quality control/analysis, polymorph and salt screening, as well as the more obvious database analysis looking for similarities in 3D structural geometry.

Mairi Haddow

CCG AGM

THE Annual General Meeting of the Chemical Crystallography Group will be held on Wednesday 5 April 2006 during the BCA Spring Meeting in Lancaster, starting at 12 noon.

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

Items for inclusion in the agenda should be sent to the secretary of the CCG, **Dr Georgina Rosair** and received no later than Wednesday 29 March 2006.

Call for nominations

Elections will be held for the post of one ordinary member of the committee. Dr Mary Mahon is not eligible for re-election to the same post (see rules 12 and 15 of the constitution). We thank her for her service to the committee.

The deadline for nominations is Wednesday 29 March 2006

Nominations may be sent in by email, they must be supported by no fewer than two members of the CCG and should be accompanied by the written consent of the nominee.

Current Officers

Chairman: **Dr Simon Parsons** (2005 - 2007)
Deputy Chairman: **Dr Richard Cooper** (2005 - 2007)
Secretary Treasurer: **Dr Georgina Rosair** (2004 - 2008)

Committee

Dr Andrew Bond (2004 - 2007)
Dr Charlie Broder (2005 - 2007)
Dr Mary Mahon (2003 - 2006)
Dr Andy Parkin (2004 - 2007)
Dr John Warren (2005 - 2007)
Ms Alex Griffin (co-opted student representative) (2005 - 2007)

Dr Georgina Rosair, Secretary - Treasurer
Email: G.M.Rosair@hw.ac.uk

The lecturing team, left to right: Ashley Hulme, Anthony Stone, Gordon Barr, Stewart Clark, Angelo Gavezzotti, Graeme Day and Nic Harrison

X - Ray Fluorescence Meeting - 10th May 2006

A Joint Meeting:

and

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For sponsorship and contact details see the web pages.

British Geological Survey (BGS), Keyworth, Nottingham.

We are pleased to announce that this one day meeting will be a joint meeting of the British Crystallographic Association - Industrial Group and the Royal Society of Chemistry Atomic Spectroscopy Group. By pooling our resources into this single one day meeting we hope to reach a wider audience and offer a wide ranging technical programme.

Programme Features: Note timings are provisional.

09:00	Optional tour of the BGS Facilities
10:00	Registration & Coffee
10:30	Introduction - Mark Ingham, British Geological Survey
11:00	Keynote lecture - "To be announced".
11:45	"Method Validation and Measurement of Uncertainties" - Ros Schwarz, LSM Ltd. Followed by discussion.
12:30	Lunch
13:30 - 17:00	Afternoon session - including:
	"Silver Determination in Photographic Emulsion by EDXRF" - David Beveridge, IlfordPHOTO
	"How Corus Group Share Best Practice" - an XRF user, Corus plc.

We will include short talks of 10 minutes duration so why not tell us how you use XRF in your laboratory or share the way you analysed a difficult sample.

Transport: The venue is conveniently located and should allow delegates from around the country to travel to BGS within the day. Nottingham East Midland Airport is nearby giving convenient travel links from Scotland, Ireland and mainland Europe.

Meeting Fees: £30 (£15 concessions) - open to non members at no extra charge.

Offers of Presentations at this meeting should be made through the local organiser: **Mark Ingham** (see the web pages for contact details)

More details and registration form will be posted on the meeting web page at:
http://bca.cryst.bbk.ac.uk/bca/ig/XRF/Meetings/meet06.htm

Industrial Group 23rd Annual General Meeting

WEDNESDAY, 5th April 2006 12:00 at The University of Lancaster

Chair **Jeremy Cockcroft**

1) APOLOGIES

2) MINUTES OF THE 22nd ANNUAL GENERAL MEETING

Held on Wednesday, 13th April 2005 at The University of Loughborough

3) MATTERS ARISING

4) CHAIRMAN'S REPORT

5) TREASURER'S REPORT

   a) Financial Report
   b) Charities Aid Foundation

6) THANKS TO SPONSORS OF THE IG

7) ELECTIONS TO COMMITTEE

   Vice Chair
   Secretary/Treasurer
   Three Committee Members

8) ANY OTHER BUSINESS ADMITTED BY THE CHAIR

Please send all nominations to

Judith Shackleton, Secretary Treasurer
Email: Judith.Shackleton@manchester.ac.uk

PCG AGM

THE 63rd Annual General Meeting of the Physical Crystallography Group of the British Crystallographic Association and Structural Condensed Matter Group of the Institute of Physics will be held at 12:15 Tuesday 4th April 2006, Lancaster.

Agenda:

1. Apologies for absence
2. Minutes from the 62nd AGM held at Loughborough, 13th April 2005
3. Matters arising from minutes
4. Chairman's report
5. IOP matters
6. BCA matters
7. Secretary/Treasurer's report
8. Elections to PCG/SCMP committee
9. Future Meetings
10. New Activities
11. Any other business

Elections to Committee

There are vacancies arising for Honorary Secretary/Treasurer and Ordinary Members. Nominations (with name of seconder and note of acceptance from the nominee) for any of these positions should be sent to the Honorary Secretary/Treasurer (john.evans@durham.ac.uk) by April 1st, or communicated to him in person at the 2006 BCA Spring Meeting.

Current Committee

Name	Grade	Since
Paolo Radaelli	Chairman	2005
Dave Allan	Vice Chairman	2005
John Evans	Honorary Secretary/Treasurer	2002
John Loveday	Ordinary Member	2003
Mina Golshan	Ordinary Member	2004
Andrew Wills	Ordinary Member	2004
Jonathan Wright	Ordinary Member	2004
Jacqui Cole	Ordinary Member	2005
Dave Laundy	Ordinary Member	2005

THE 62nd Annual General Meeting of the Physical Crystallography Group of the British Crystallographic Association and Structural Condensed Matter Group of the Institute of Physics

13:00 Wednesday 13th April 2005, Loughborough

There were 25 members present. Committee members present: **Pam Thomas, Paolo Radaelli, John Evans, John Loveday, Mina Golshan**.

1. Formal apologies for absence were received from **Andrew Wills, Jon Wright** and **Jeremy Cockcroft**.
2. Minutes of the 61st AGM held at UMIST were circulated and accepted as an accurate record of the meeting.
3. There were no matters arising from minutes
4. Pam Thomas reported on another active year for the PCG/SCMP. She also thanked everybody who had worked with her on the committee over 13 years. Specific activities mentioned were:
    a. A successful winter meeting on neutrons in biology (thanks to **Paolo Radaelli** as local organiser and **John Helliwell**).
    b. A white beam satellite workshop to the BCA spring meeting (thanks to **Mina Golshan**).
    c. A teaching (given by **Prof Mike Glazer**) and research session on phase transitions at the BCA spring meeting (this occurred after the agm but was again extremely well attended by a wide cross section of people).
    d. A two day Rietveld workshop (thanks to **Jeremy Cockcroft, Ivana Evans, Kevin Knight** and **John Evans**).
    e. The inaugural PCG/SCMP/Panalytical thesis prize awarded to **Dominic Fortes** (UCL); thanks to Panalytical for £500 sponsorship.
    f. A magnetic Rietveld workshop will be organised for September 2005.
    g. The PCG/SCMP prize will be awarded in 2006. Nominations were sought from all members.
5. There were no IOP matters raised.
6. There were no BCA matters raised.
7. The secretary presented the annual IOP activity report to the meeting and the financial summary appended. Several members raised the issue of ease of communication with the IOP regarding financial matters. JSOE will attend the annual representatives meeting and raise as appropriate.
8. Nominations for committee positions are detailed below. All were elected unopposed. The committee sought and received the approval of the meeting to co-opt John Evans as secretary/treasurer for a further 12 months to provide continuity amongst the officers.
    a. Chair: **Paolo Radaelli**. Proposed: **Pam Thomas**; Seconded: **John Evans**.
    b. Vice chair: **Dave Allan**. Proposed: **John Evans**; Seconded: **Jon Loveday**.
    c. Ordinary Member: **Jaqui Cole**. Proposed: **Andrew Wills**; Seconded: **Paolo Radaelli**.
    d. Ordinary Member: **Dave Laundy**. Proposed: **Pam Thomas**; Seconded: **Jon Loveday**.
9. Future meetings will include a magnetic Rietveld workshop in September. The topic for the autumn meeting is under discussion. A structural Rietveld workshop will be held in 2006. The group will consider making a significant contribution to cmmp meeting in 2006.
10. **Paolo Radaelli** outlined his plans for the PCG/SCMP over the next 3 years. An “education portfolio” will be produced to highlight the important educational work being undertaken by the committee.

The meeting closed with an expression of thanks to the retiring chair for her work at all levels on the committee over the past 13 years and the presentation of a long-service certificate and small gift.

Prize Lecture for Physical Crystallography - Call for Nominations

THE PCG/SCMP is proud to invite nominations for the Prize Lecture in Physical Crystallography. This award takes over from the Phillips/Panalytical award and will be presented biannually.

The £1000 award will be for the best recently published work (say 2-3 papers in the last few years) by a relatively young person (usually 35 years of age or younger) working in the general field of Physical Crystallography. His or her research must be judged to have a significant present or future impact in this field. The award is traditionally presented at the Annual BCA Spring Meeting, where the recipient is expected to give an oral presentation of his or her work. The committee of the Physical Crystallography Group (also known as the Structural Condensed Matter Group of the IoP) selects the best candidate from a list of nominees.

Nominations should be sent to the Chair of the Physical Crystallography Group, **Prof Paolo Radaelli**, by 28th February 2006.

Recent Winners have included:
Andrew Wills
Jon Loveday
Daniel Bowron

Magnetic Structure Determination From Neutron Powder Diffraction

FOLLOWING the success of a similar event held in December 2002, this workshop, sponsored by the Physical Crystallography Group and by CCLRC, was held at The Cosener's House, Abingdon, in November.

The workshop aimed at providing essential theoretical foundations and some working experience in solving and refining magnetic structures from neutron powder diffraction data. Compared to its first edition, the present workshop reached an unexpected international scope, with about 50% of the 34 attendees coming from outside the UK. A much awaited event, indeed! **Lingfei Zhang** from the Materials Science group of the University of Salford commented: *"I have been waiting for 2 years! […] this workshop gave me a unique chance to interact with the most specialised experts in the field; otherwise the mystery of magnetic powder diffraction refinement might never have been cleared up for me".* The teachers/tutors that had made the 2002 workshop a success (**Juan Rodriguez Carvajal** - LLB, **Paolo G. Radaelli** - ISIS and **Andrew Wills** - UCL) gathered once again at Cosener's House, this time effectively "complemented" (guess who did all the hard work!) by **Laurent Chapon** (ISIS) and me.

The objectives of the workshop were quite ambitious: the task of teaching how to solve and refine magnetic structures from neutron powder diffraction data, in the words of **Michael Banks** from the Max Planck Institute, Stuttgart is *"difficult to get right in a few days; I think the organisers did the best possible job"*. The first half day was devoted to lectures on experimental techniques. During the second day, special emphasis was placed on the essential theoretical foundations, with a series of lectures dedicated to the use of symmetry, as well as to the methods of solving and refining magnetic structures. The last morning was a practical session, allowing us to get hands on the most popular computer programs that are used in the field. This session was a deliberate compromise, dictated by the diversity of the background of the attendees, who ranged from PhD students to confirmed researchers, and from crystal chemists and solid state scientists working in conventional laboratory environments, to experienced neutron scatterers from the ISIS facility and other European neutron sources.

Overall, the feedback received from the participants is excellent: *"Great course, many thanks for all the effort put in. For next time, perhaps recommend some reading for participants to do before they arrive"* (**Nicola Wilson**, PhD student from Warwick University). *"I learned and now understand a lot, and, well, surely not everything! But in any case I have the great handbook you provided us for further reading. I enjoyed everything very much, not just the topic, but also the surroundings and the accommodation. Also, you were very patient in explaining everything during the practice lessons and answering our questions."* (**Michael Tovar**, Post Doc at the HMI neutron source, Berlin). A general lesson for the future is that the workshop in general, and the hands-on session in particular, was just too short. People ask for more, and extending the workshop by 1-2 days sounds to us a promising improvement for next time!

Aziz Daoud-Aladine, ISIS Facility, CCLRC

More pictures at http://www.isis.rl.ac.uk/conferences/MagnetismCoseners05/

PANalytical Thesis Prize for Physical Crystallography

Call for Nominations

THE Physical Crystallography Group is pleased to invite entries for the PANalytical Thesis Prize in Physical Crystallography.

The prize will be awarded for the best use of techniques or methods of Physical Crystallography in a successfully-examined thesis submitted in the period from September 1st 2004 to December 31st 2005. The amount of the prize, which will be sponsored by PANalytical Ltd, will be £500. To be eligible for the prize, candidates must be a member of the Structural Condensed Matter Group of the IOP and/or the British Crystallographic Association (BCA). Non-members may enter the competition but will be required to join the BCA at the student rate (currently £20.00 for three years) to progress their nomination further.

To enter the competition, candidates must submit:

(a) a copy of the Thesis on CD-ROM.

(b) a personal statement of not more than 500 words explaining why the Thesis should be considered for the prize and including a clear description of the role of Physical Crystallography (as interpreted below or otherwise) in the research.

(c) The names and contact details of two academic referees, one of whom may be the Thesis supervisor, who will be able to comment on the Thesis research of the candidate.

In order for a thesis to be eligible for the award, the Physical Crystallography element must be central to the work of the thesis, which must also demonstrate a context over and above structural work for its own sake.

Nominations for the prize must be submitted to the Chair of the Physical Crystallography Group, **Prof Paolo Radaelli**, by February 28th 2006 and the prize will be awarded at the 2006 BCA Spring Meeting in Lancaster, April 2006.

Remit of Physical Crystallography in connection with Prizes: Methods and techniques of Physical Crystallography will be interpreted in a broad fashion, for example, to include x-ray and neutron diffraction or scattering, Rietveld analysis and structure refinement, total scattering, structure-property relationships, development of structure-solution techniques, crystallography under non-ambient conditions, use of complementary techniques to diffraction (e.g. optical studies, NMR), computational crystallography and modelling, electron diffraction, diffuse scattering, applications of physical crystallography in biology.

Prof Paolo Radaelli, Chair of the Physical Crystallography Group, ISIS Facility, R3, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX, UK.
P.G.Radaelli@rl.ac.uk

The Honours List: Honour a Crystallographer?

A campaign aimed at getting more women active in technology and science who go that extra mile nominated for the Queen's honours awards has been launched by the Cabinet Office. In the 2006 New Year's Honours list just under 37% of the Honours awarded were given to women, despite the fact that they make up 51% of the population.

The "Do the Honours" campaign (**www.honours.gov.uk/**) is aimed at getting more nominations from women who make a real difference, whether it is in their field of work, through their interests or pursuits or on a local level. It is also raising awareness of the fact that any member of the public can send in a nomination.

The full story is at **http://www.publictechnology.net/modules.php?op=modload&name**

Kate Crennell

Meetings of interest

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

2-3 March 2006
Diffraction de poudres: - Laboratoire Léon Brillouin, France
http://www-llb.cea.fr/SOLEIL-LLB/DiffractionPoudres/diffractionpoudres.html

6-8 March 2006
Joint Meeting of German and Polish Associations for Crystal Growth, Berlin-Adlershof, Germany
http://jm2006.dgkk.de/

6-8 March 2006
Basic and Advanced X-Ray Powder Diffraction: Pharmaceutical Applications,Part I Stamford, CT, USA
http://www.assainternational.com

9-10 March 2006
Basic and Advanced X-Ray Powder Diffraction: Pharmaceutical Applications, Part II, Stamford, CT, USA
http://www.assainternational.com

15-19 March 2006
3rd International Conference on Structural Analysis of Supramolecular Assemblies by Hybrid Methods. Lake Tahoe, CF, USA.
http://www.burnham.org/hybridmethods2006

19-21 March 2006
TCM 1 : First Tunisian Crystallographic Meeting, Hammamet, TN
Information from **tunicrystal@yahoo.fr**

20-21 March 2006
Modulated and Classical Procedures in Thermal Analysis, Pharmazentrum, Basel, CH
http://www.eurostar-science.org

21-22 March 2006
Polymorphism & Crystallisation 2006, Thistle Marble Arch Hotel, London
http://www.iqpc-pharma.com/cgi-bin/templates/genevent.html?topic=237&event=9197

3-6 April 2006
Jahrestagung der Deutsche Gesellschaft für Kristallographie (DGK), Freiburg, Germany
http://www.dgk-2006.de

4-6 April 2006
BCA/BACG Spring Meeting, University of Lancaster
http://www.crystallography.org.uk

6-7 April 2006
Polarized Inelastic Neutron Scattering (PINS) followed by HYSPEC IDT Meeting, Brookhaven National Laboratory, Upton NY USA
https://www.bnl.gov/pins/

23-28 April 2006
Rapid Data Collection and Structure Solving at the NSLS: A Practical Course in Macromolecular X-Ray Diffraction Measurement, Bloomington IN USA
http://www.px.nsls.bnl.gov/RapiData2006/

24-28 April 2006
Practical X-Ray Fluorescence: ICDD, Pennsylvania, USA
http://www.icdd.com/education

25-27 April 2006
Process Crystallization in the Pharmaceutical & Chemical Industries, Philadelphia, PA USA
http://www.acsprospectives.org

27-29 April 2006
ILL Millennium Symposium and European User Meeting, Grenoble, France
http://vitraill.ill.fr/symposium/firstCircular.jsp

2-5 May 2006
Polymorph Screening: Techniques and Applications, Mallorca, Spain.
http://www.assainternational.com

8-9 May 2006
International Workshop on the Pharmaceutical Physical Characterization of the Amorphous State, Stamford, CT, USA
http://www.assainternational.com

8-10 May 2006
Sixth Canadian Powder Diffraction Workshop, Waterloo ON, Canada
http://www.cins.ca/cpdw/

10 May 2006
X-Ray Fluorescence meeting of general interest, British Geological Survey, Keyworth, Nottingham
www.crystallography.org.uk/ig

12 May 2006
Journée Scientifique "E.F. BERTAUT", CNRS-Polygone, Grenoble, France
Contact: **jean-louis.hodeau@grenoble.cnrs.fr**

14-19 May 2006
First European Workshop in Drug Synthesis, Certosa di Pontignano, Siena, Italy
http://www.unisi.it/eventi/ewds

22-25 May 2006
Polymorph Screening: Techniques and Applications, Stamford, CT, USA
http://www.assainternational.com

28 May - 3 June 2006
Ninth International Conference on Synchrotron Radiation Instrumentation. Daegu, Exco, Korea
http://sri2006.postech.ac.kr/

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

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

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

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

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

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

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

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

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

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

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

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

1-4 August 2006
X-El 2006 - School on structure determination by the combination of X-ray powder diffraction and Electron Crystallography: Antwerp, Belgium
http://www.emat.ua.ac.be/XEl2006/XElhome.htm

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

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

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

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

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

31 August – 9 September 2006
Neutron Techniques In Molecular Magnetism, Jaca, Spain
http://magmanet.unizar.es/

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

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

3-8 September 2006
13th BCA Summer School in Protein Crystallography, Biochemstry Department, Oxford University (website not yet available)

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

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

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

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

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

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

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

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

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

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

23-26 October 2006.
Polymorph Screening: Techniques and Applications</A> Mallorca, Spain
http://www.assainternational.com

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

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

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

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

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

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