Crystallography News

British Crystallographic Association

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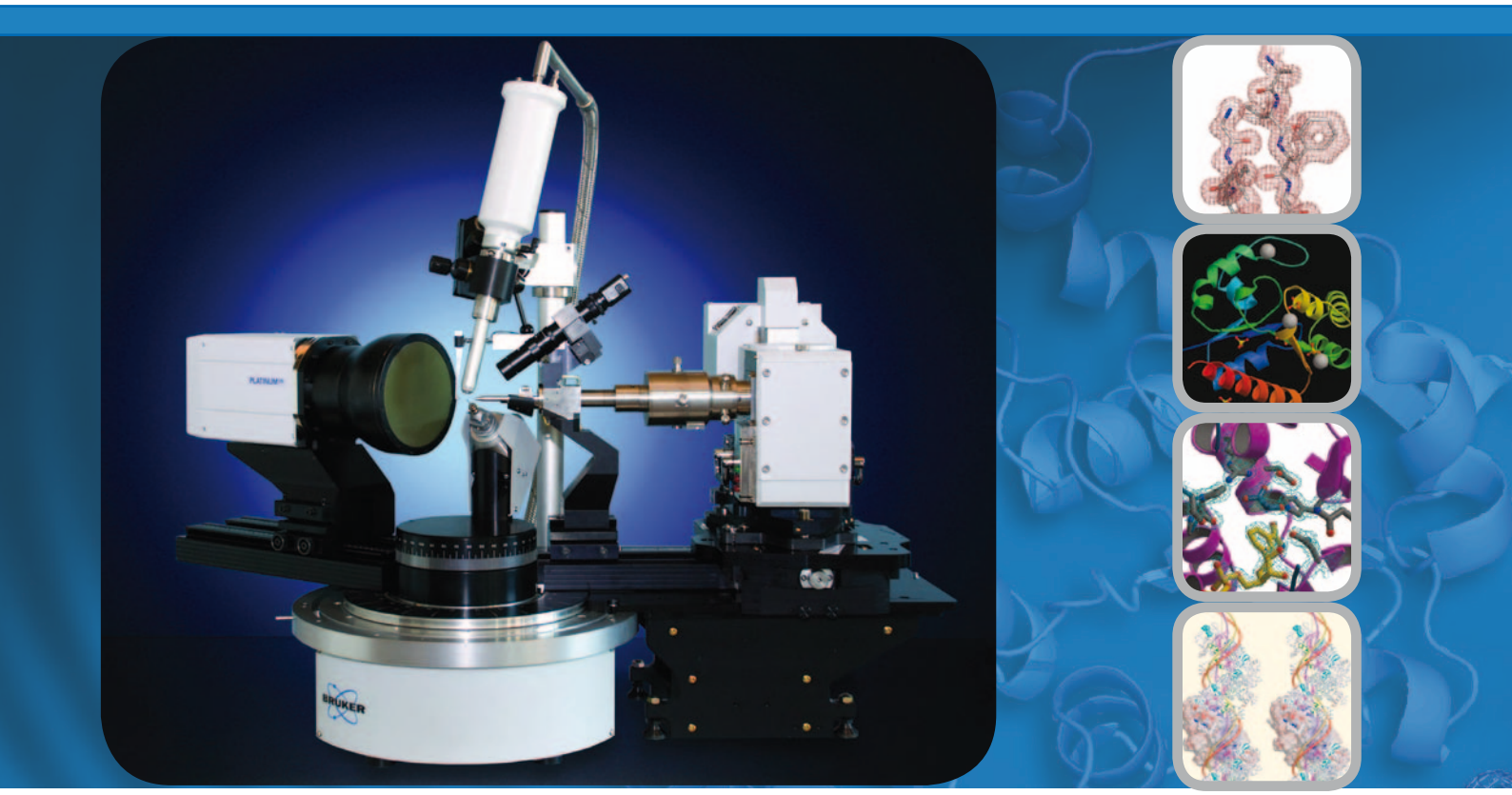
2011 C CHEMISTRY

International Year of CHEMISTRY 2011

SEE INSIDE



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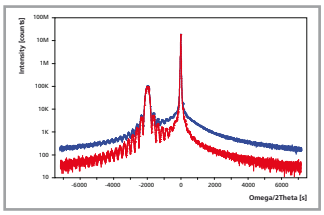

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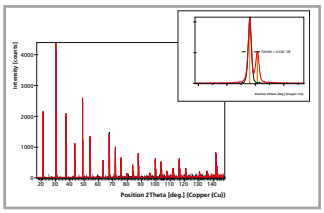

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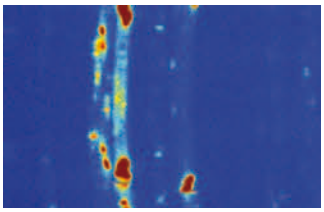
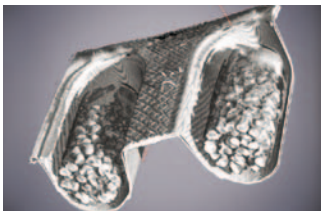


3D



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Crystallography News March 2011

Contents

This month's cover:

CCDC art,
BCA AGM,
Spring meeting &
Autumn meetings.

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by William Anderson and Sons Ltd, Glasgow. 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 March 2011 issue are sent to the Editor to arrive before 25 January 2011.

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As required by the DATA PROTECTION ACT, the BCA is notifying members that we store your contact information on a computer database to simplify our administration. These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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From the Editor

AS I write this column, the typical January weather we are experiencing feels like springtime after our unusually cold December. My thoughts are directed to daffodils, Easter bunnies and, above all, the BCA Spring Meeting. The latest iteration published in this issue should convince everyone that the programme is both interesting and well integrated. The venue, Keele University, is easily accessible and reasonably priced. Once again we shall be joined by our friends from the XRF community, providing an additional opportunity to forge collaborative links.

Other meetings also deserve our attention. At the end of March there will be another CPOSS meeting. After a period of frustratingly slow progress crystal structure prediction has recently made rapid strides. Its application to pharmaceutical compounds may change failure in drug delivery to success. April 15 is an important date: it is the deadline for submission of abstracts to the 22nd Congress of the International Union of Crystallography. Taking place in Madrid, this meeting offers the ideal combination of easy access and a fascinating culture. Further details of both meetings appear in this issue.

Meeting reports here should convince every reader that once again we enjoyed a series of lively Autumn Meetings organised by our Groups. We also present the announcement by the International Centre for Diffraction Data of the Ludo Frevel awards, listed by recipient, nationality and research area. Sadly, there are no UK award winners, but I am assured by the ICDD that UK applications are welcome. I hope that this information, particularly about research areas, may be helpful to applicants in future rounds.

Anyone with an interest in crystallographic teaching is encouraged to look at the open access special issue of the *Journal of Applied Crystallography*, "Crystallography education and training for the 21st century", which is volume 43, part 5, number 2 (October 2010). This issue begins with a thought-provoking editorial that conveys both excitement and anxiety: crystallography has broadened out from a specialist research area with highly trained practitioners to a technique with a much wider user community, leading to new application areas but also new chances to make mistakes. A series of articles outlines methods for teaching fundamentals, the use of databases and software tools, ways to incorporate crystallographic science into secondary and early university education, science-based critical validation of data, workshops and on-line resources, and enriching learning everywhere by remote use of real facilities and realistic virtual environments.

Our cover displays the interplay of art and crystallography as exemplified by an art installation entitled "Repeat, Evolve" recently made by **Jessica Hymas** for the Cambridge Crystallographic Data Centre. Our appreciation of the beauty of crystals goes back thousands of years, when people first admired the regular faces of gemstones. More recently **M. C. Escher** applied the crystallographic concepts of symmetry and space-filling in the creation of his highly imaginative drawings. It is appropriate that the CCDC collaborates with an artist. One of the delights I have become able to enjoy in retirement is that, while searching the Cambridge database for a specific purpose, I can pause and appreciate the intricate beauty of the packing arrangements. Jessica's blog explains the significance of the title in relation to her artwork as follows: "'Repeat' describes the symmetries and regularity to be seen in all crystal structures and is reflected in the wrapping, stitching, folding and repeated printed motifs. 'Evolve' captures the artistic temperament, with Hymas's creative autonomy displayed in vibrant colour and sharp geometric elements. It also speaks of the physical aspects of disorder and defects in crystal growth." The work can be viewed by appointment by contacting **admin@ccdc.cam.ac.uk .**

With 2013 being the International Year of Crystallography I am grateful to the American Crystallographic Association for permission to reprint an article from *ACA Reflexions* which points to numerous websites that can help us to prepare imaginative illustrations that are instructive for non-crystallographers. In the aftermath of the Oscar ceremonies we should even consider adapting Hollywood techniques! We have also been invited by the International Union of Crystallography to apply our well-honed skills to the design of a logo for IYCr2013. The logo for this year's International Year of Chemistry is displayed, partly as a model and partly as a reminder of the intimate association between crystallography and chemistry. Most of us either are chemical crystallographers or use chemistry to prepare the samples for biological or physical crystallography or industrial applications.

In late January a major news story has revealed the actions of *News of the World* employees in hacking into celebrities' electronic mail. This left me wondering what I would find if *Crystallography News* hacked into leading crystallographers' mail. There would be lots of "shop talk", for sure. I'm certain that I would find a great deal of altruism, too: supervisors helping postgrads and postdocs to find jobs, and research leaders assisting less well-resourced crystallographers. Above all I would expect immense enthusiasm for our subject. No doubt *NotW* readers would find most of the material stupefyingly boring, but I hope they would also derive some inspiration.

Carl Schwalbe

BCA Council 2010

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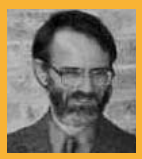

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(The dates in parentheses indicate the end of the term of office).

Full committee details on the BCA website **www.crystallography.org.uk**

Spring Meeting Registration and Subscriptions:

www.crystallography-meetings.org.uk

From the President

DEAR MEMBER

The heavier than usual (for the UK) snows appear to be behind us and thankfully it feels as though Spring is already in the air: I spotted some seasonally challenged primroses already flowering in my garden today.

Thank you to those of you who sent me nominations for new Honorary Members of the BCA: we again have a number of very strong candidates to consider.

The annual one-day BCA Group Meetings were all held very successfully in November and December. Unfortunately this year my undergraduate teaching commitments meant that I was only able to attend the Biological Structures Group gathering hosted and arranged by **Kim Watson** at the University of Reading on ''Metal-protein interactions in transport and disease' By all accounts the other Meetings, at which **Dave Allan**, our Vice President, represented me, were also lively. The Industrial Meeting took place at the Diamond Light Source and was organised by **Elizabeth Shotton** and **Matthew Johnson**, and the Physical Crystallography Group Meeting, arranged by **David Keen**, was held in Coseners House, Abingdon in conjunction with the ISIS Crystallography Users Group on 'Current Research in Physical Crystallography'. The Chemical Crystallographers were in Edinburgh hearing talks 'On Understanding the Solid Sate', organised by **Stephen Moggach**. The BCA is very grateful to the researchers who devote time to masterminding such meetings which due to their focus and attendee numbers, usually below 100, encourage free discussion and comments from the floor. In my experience this makes the scientific dialogue much more stimulating.

The BCA Spring Meeting in Keele, for which **Arwen Pearson** is the Scientific Organiser, is fast approaching, and details of the exciting and wide ranging programme are now available (see later in this issue). At the BCA AGM in Keele, we will be seeking a new Treasurer of the Association, since **Harry Powell** will come to the end of his three year term of office. The Association is particularly indebted to him for his determination to move to less administratively onerous methods of Membership payment, and his successful efforts to transfer all our bank accounts to within the Charities Aid Foundation umbrella. The key job of Treasurer tends to be unsung, but efficient management of our finances is pivotal to the growth of the Association, and we will miss Harry's eagle eye and wisdom, as well as his every ready advice on all areas of our activities. I am personally indebted to him for being so prepared to spend several hours on the phone with me recently trawling through and discussing appropriate action on 30 or so issues which had arisen through e-mail over the last 8 months, and to which I had been unable to attend due to other demands on my energies.

The agenda for the BCA AGM can be found later in this issue, and includes a proposal by Council to raise the subscriptions in Jan 2012 to a more realistic level in order to ensure the sustainability of the Association.

We are very pleased that the Lonsdale Lecture and Teaching Plenary this year will be delivered by Professor **John Helliwell** on "The evolution of synchrotron radiation and the growth of its importance in crystallography" and John will no doubt draw on his long association with synchrotrons during his career in crystallography, which has seen many developments in the field. The Lonsdale lecture is named in memory of **Kathleen Lonsdale**, 1903-1971, crystallographer and pacifist, who determined the structure of benzene, and among other 'firsts' was the first woman President of the IUCr: for some information on this fascinating scientist see for instance http://understandingscience.ucc.ie/pages/sci_kathleenlonsdale.htm.

The IUCr have designated 2013 to be the International Year of Crystallography (IYCr2013), and are holding a logo competition to help advertise this. The logo should symbolize and represent the fundamental importance of crystallography to society, and will be used for announcements, letterheads, brochures, publications, web sites and other purposes as may be decided by the IUCr. Designs should be sent by email to the IUCr Executive Secretary (execsec@iucr.org) by 1 July 2011. For more details of the competition and how to enter, go to http://www.iucr.org/iycr/logocompetition/. I strongly encourage anyone with graphic and/or artistic skills to submit their entries for consideration.

Talking of the IUCr, the XXII IUCr Congress and General Assembly in Madrid (22nd-29th August 2011) is now in an advanced state of planning, and the second circular has just been released with a more detailed programme (see http://www.iucr2011madrid.es/). The BCA's financial contribution to the IUCr entitles us to have 5 delegates at the Congress meetings; if there are Members who would be interested in being one of these, please let me know.

If anyone is in any doubt as to the vitality of crystallography, they will be reassured by the very exciting report in the 3rd February issue of Nature by **Henry Chapman** *et al*. (pp 73-77) on 'Femtosecond X-ray protein nanocrystallography'. I strongly recommend reading of this paper, which opens up a bold 'new frontier' in our field.

Lastly, you might remember that in last April's CN letter, I mentioned Professor **Grzegorz Jezierski**, of Opole University of Technology in Poland, who wrote to me to enquire about the possibility of obtaining donations of used (damaged) X-ray tubes, and there was a photo of him in *Crystallography News* with some of his collection. He now has a wonderful WWW site which is well worth a visit: It is in English as well as Polish and has close-up pictures of many X-ray tubes: www.xraylamp.webd.pl

I look forward to seeing many of you in Keele in April!

Elspeth

Puzzle Corner

A camel has 300 bananas, and he has to eat 1 per mile as he goes along to fuel his locomotion. However, he can only carry 100 at a time. What is the maximum distance from his starting point in the desert that he can reach? (Contributed by Elspeth Garman)

Answer to December Puzzle

The accepted chemical names and symbols follow the non-standard names. The column of first letters of the chemical symbols spells out the message "Happy Hols. Santa". We hope that this has come true for you.

Hydrargyrum	Mercury	Hg
Anglohelvetium	Astatine	At
Florentium	Promethium	Pm
Illinium	Promethium	Pm
Aldebaranium	Ytterbium	Yb
Norium	Hafnium	Hf
Nebulium	Oxygen	O
Cassiopium	Lutetium	Lu
Stibium	Antimony	Sb
Unnilhexium	Seaborgium	Sg
Alabamine	Astatine	At
Columbium	Niobium	Nb
Masurium	Technetium	Tc
Emanium	Actinium	Ac

The prize is awarded to **Jim Trotter.**

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 starting from 1 January to 31 March 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.
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BCA Annual Spring Meeting 2011

University of Keele 12th-14th April 2011

THE 2011 BCA spring meeting will be held at the University of Keele 12th-14th April. As is traditional the Young Crystallographers Meeting will occur before the main meeting on the 11th and 12th April. This year we are also joined by the XRF community who will hold a workshop on the 12th April followed by scientific sessions during the main meeting.

For registration and the latest programme information please visit the meeting website at:
http://crystallography.org.uk/spring-meeting-2011

The Annual General Meeting of the British Crystallographic Association will be held on Wednesday 13th April 2011 at 6pm at the University of Keele.

SCIENTIFIC PROGRAMME

Plenary Lectures

Lonsdale Lecture (BSG)
John Helliwell (University of Manchester)
The evolution of synchrotron radiation and the growth of its importance in crystallography
CCG Plenary
Judith Howard (University of Durham)
Intermolecular interactions: their influence on structure and properties
PCG Plenary
Gilberto Artioli (University of Padova)
Crystallography in the cultural heritage: personal experiences
IG Plenary
Nora De Leeuw (University College London)
Computational studies of biomaterials
XRF Keynote
Margaret West (West X-ray Solutions Ltd)
It began with a helping hand

Sessions and Confirmed Speakers

Protein Crystallization: dealing with low solubility proteins and protein:ligand complexes (BSG)
Chair: **Ray Owens**
Zygmunt Derewenda
Macromolecular crystal engineering - from serendipity to rational design
Magnus Alphey
Contrasting projects of a complex nature
Elena Seiradake
Crystallization of secreted mammalian glycoproteins: Eph-ephrin complexes

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Membrane Proteins (BSG)
Chair: **Chris Tate**
David Drew
Benchmarking membrane protein detergent stability of improving throughput of high resolution X-ray structures
Jenny Miller
Structural studies of a β-adrenergic receptor: stabilising a membrane protein by mutagenesis for improved crystal quality and higher resolution X-ray diffraction
Stephen Muench
The mechanical and regulatory complexity of the vacuolar ATPase revealed

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Radiation Damage (BSG, PCG & CCG))
Chair: **Colin Nave**
Elspeth Garman
Scavenger effects on specific versus global radiation damage
Robin Owen
Running away from radiation damage: microfocus MX at room temperature
Frank von Delft
Dealing with radiation damage in practice

Bacterial Cell Walls - synthesis, virulence and inhibitors (BSG)
Chair: **Klaus Futterer**
Helge Dorfmueller
The GT-2 enzyme NodC as a model for studying chitin synthase

David Albesa-Jové
Structural insights into the molecular organisation of the surface layer from Clostridium difficile
Andrew Lovering
Structure and function of TagF, polymerase for the secondary wall polymer teichoic acid

---

Young Crystallographer Showcase (BSG)
Chair: **Dean Rea & Vilmos Fulop**
James Lillington
A Bacterial Alkaline Phosphodiesterase with the Structure of a Purple Acid Phosphatase
Geoffrey Masuyer
Botulinum Toxin in pieces: crystal structure of a functional fragment of Botulinum Neurotoxin B
Simon Tanley
Structural studies of Anti-cancer platinum complexes with hen egg white lysozyme as a model protein
Paul Acklam
X-ray Crystallographic Studies of Rationally Designed Dihydroorotate Dehydrogenase Inhibitors
Thembaninkosi Gaule
Copper amine oxidases: From homodimer to heterodimer

Hot structures (BSG)
Chair **Ravi Acharya**
Yvonne Jones
Cellular Satnav: structural studies on the semaphorin-plexin cell guidance system
Susan Lea
Structural insights into the control of type three secretion
Aiwu Zhou
A redox switch in angiotensinogen modulates angiotensin release

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Twinning and Pseudosymmetry (BSG)
Chair: **Eleanor Dodson**
George Sheldrick
Handling small molecule and macromolecular non-merohedral twins
Roberto Steiner
Andre Lebedev

New Developments at Diamond (CCG & PCG)
Chair **Helen Maynard-Casely & David Keen**
Ian Robinson
Coherent Diffraction Imaging of Nanocrystals: Effects of Partial Coherence
Steve Baker
Tailoring Magnetism in Nanoparticles through Control of Crystal Structure
Jawwad Dear
Combinatorial Direct Solid State Syntheses of Doped Lanthanum Nickelates from Nanoceramic Precursors; Is This The End of Shake and Bake?

From Molecular to Supramolecular (CCG)
Chair **Peter Byrne**
Neil Champness
Andy Cooper
John Warren
Suck it and see

Macro and small molecule crystallography - a combined future (CCG & BSG)
Chair **Paul Raithby**
Christine Cardin
From molecular tweezers to DNA light switching in the home lab
Arwen Pearson
Using Terahertz time domain spectroscopy to probe long range dynamics in molecular and macromolecular crystals
Isabel Moraes
Challenges and Opportunities in Structure Determination of Membrane Proteins

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Time resolved structural science (PCG, CCG & BSG)
Chair **Dave Allan**
Tom Penfold
SwissFEL to applications: Ultrafast time-resolved X-ray scattering in the condensed phase
Simon Kimber
Decoupling of charge, orbital and lattice relaxation in frustrated $Ba_3NaRu_2O_9$
Jacqui Cole
Time-resolved photo-crystallographic studies of ruthenium sulphur dioxide complexes

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Structure/Property Correlations in Luminescent Materials (CCG)
Chair **Andrew Bond**
Prof Lee Cronin
Dr Jamie Gould
CCDC/CCG Young Scientist Prize Lecture

Dynamic Data, dealing with limited data (CCG & PCG)
Chair **Peter Wood**
Iain Oswald
Andrew Stewart
Trials and tribulations of solving organic structures from 3D electron diffraction data
Paul Smart
Multi-step synthesis and reactions of metal-organic frameworks

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Getting more from diffraction data (CCG)
Chair **Hazel Sparkes**
Michael Probert
Moving beyond the standard experiment, without moving house
Chris Gilmore
New methods in electron crystallography
David Watkin
What's all this MoOing about?

Local Structure (PCG)
Chair **Andrew Goodwin & Matt Tucker**
Serena Corr
Local Structure studies of the metal-insulator transition in rutile VO_2
Joe Hriljac

High Pressure and Energetic Materials (PCG)
Chair **Christoph Salzmann & Matt Tucker**
Colin Pulham
Modification of the structures of energetic materials using high pressures and co-crystallization
Peter Portius
Ben Slate
Simulation of materials at high pressure

Stress-strain Microstructure (IG & PCG)
Chair **Judith Shackleton**
Steve Norval (IG Award Lecture)
Raising The Standard
Moatez Attallah
In-Situ Strain Measurement during Tensile Loading of Ti-Alloys

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Materials Science: white beam methods (PCG & IG)
Chair **Bob Cernik**
Xu Song
Characterisation of polycrystal deformation at different scales by white beam X-ray diffraction
Simon Jaques

Cultural Heritage (PCG & XRF)
Chair **Winfried Kockelmann & David Taylor**
Julia Farley
A comparison of WDXRF and neutron diffraction analysis techniques for the study of ancient silver coins from the Hallaton Treasure
Panagiota Manti
The Cu_6Sn_5 phase 'problem' of tinned archaeological bronzes

Andy Smith
A host of golden angels - Coin making in Tudor times explored by XRF and neutron diffraction

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Crystallization I (CCG, IG & BACG)
Chair **Louise Male & Sven Schroeder**

Crystallization II (IG & BACG)
Chair **Anne Kavanagh & Robert Hammond**
Patrick Stewart
Random microseeding: a theoretical and practical exploration of the Microseed Matrix Screening (MMS) method, with new recommendations for achieving crystallization success
F Gorrec
Macromolecular Crystallization: Robotics, Procedures and Innovations
Young Crystallographer Prize Lecture

Materials Science - Powder methods (IG)

Novel Techniques (XRF)
Chair **David Taylor**
Joanna Collingwood
XRF analysis of neurodegenerative brain tissue using synchrotron radiation
Rainer Schramm
ISO 17025 accreditation for fused bead methods
Adrian Wright
Challenges in the characterisation of amorphous metal phosphates and fluorophosphates

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New Developments (XRF)
Chair **Mark Ingham**
David Lane
Using low cost CMOS sensors for X-ray imaging and spectroscopy
Stefan Kneip
Bright spatially coherent synchrotron X-rays from a table-top source
Mike Dobby
Enhancing the light element performance of EDXRF by using a new Silicon Drift Detector with high transmission window

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Applications (XRF)
Chair **David Beveridge**
Didier Bonvin
Applications of High Power XRF in Geochemical and Environmental Laboratories
Phil Russell
New Test Methods for WDXF: Trace elements in Burner Fuels
Dirk Wissmann
The Balancing Act Between Versatility and Analytical Performance when Using ED XRF Instrumentation
Paul Vanden Branden
X-ray fluorescence analysis of rocks by fusion method using a benchtop WD-XRF
David Bellis
Novel applications of XRF for mapping metals in industry, health and the environment

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Applications in XRD/XRF (XRF)
Chair: **Guest Chair**
David Beveridge
Characterisation of the phosphate surfactant in a latex using XRF and other techniques
Leah Cliff
Environmental Applications for a new Benchtop XRD/XRF Instrument

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XRF WORKSHOP 12th April 2011

11:00 - 12:30 **Sample preparation**

Organiser and Chair **Margaret West**

This Masterclass is designed to offer practical advice on the ever expanding range of techniques available to prepare samples for analysis in the laboratory and in the field.

The session will be devoted to fusion techniques including

- calibration beads from CRMs and pure chemicals
- routine samples
- samples requiring special care
- fluxes and additives
- care of platinum ware
- practical lab demonstrations

Delegates are invited to submit requests to margaretwest@blueyonder.co.uk for hints and tips to get the best from their samples and this Masterclass.

13:30 - 15:00 **Sample preparation (cont).**

This session will concentrate on grinding and pressing powders, handling liquids and gels and dealing with those "unknowns" that sometimes demand attention.

15:30 - 17:00 **Calibration**

Organiser and Chair **Ros Schwarz**

This Masterclass will focus on common problems in the selection of line and background positions. Some of the topics to be considered include:

- when and why is it difficult to calibrate XRF?
- matrix mass absorption
- lack of standards
- line overlaps
- background overlaps
- range (Majors, Minors, Trace)
- line and background selection
- resolution
- why do you need a background?
- background correction

Contact the session chair (r.schwarz@sheffield.ac.uk) with details of your calibration if you would like it discussed during the Masterclass.

YOUNG CRYSTALLOGRAPHERS MEETING
11-12th April 2011
Plenary Lectures

Matthew Johnson (GlaxoSmithKline)

Industrial Action: Striking at the heart of Materials Science

Arwen Pearson (University of Leeds)

Getting more than just diffraction from a crystal: How complementary methods can add to your experiment

Parkin Lecture

Helen Maynard-Casely (The Royal Institution of Great Britain)

Session YC1

Chair: **Duncan Sneddon**

Henry Wong (University of Nottingham)

Structural analysis of metal coordination complexes under pressure

Sarah Jane Ewing (Heriot Watt University) *Solvothermal synthesis of Indium Selenides*

Oliver Zeldin (University of Oxford)

High-throughput metallo-protein analysis by microPIXE

Lauren Hatcher (University of Bath)

Thermal and photocrystallographic studies on a nickel-nitro complex

Laura Thompson (University of Birmingham) *Structure solution of two nicotinamide: succinic acid cocrystals*

Ines Collings (University of Oxford)

Flexibility in cadmium and mercury imidazolate

Session YC2

Chair: **William Lewis**

Andrew Jones (University of Glasgow/ Institut Laue-Langevin)

Proton migration in molecular complexes of urea and its derivatives

Claire Murray (University of Reading)

Synthesis and structural characterisation of multi-nuclear cages with ortho-palladated ligands

Miriam Walden (University of Leeds)

Control of asymmetric cell division in developing Drosophila neuroblasts

Nick Funnell (University of Edinburgh)

Using pressure to direct polymorph formation: overcoming isotope effects in the 4-methylpyridine pentachlorophenol co-crystal

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Session YC3

Chairs: **Claire Murray & Peter Byrne**

Flash Presentations for Poster Contributors: Sell your poster in no more than 3 sentences!

Session YC4

Chair: **Susanne Coles** (née Huth)

Helen Mason (University of Durham)

Structural studies of selected photochromic compounds

Matthew Mold (University of Keele)

Complementary structural studies of serum amyloid P component from Limulus polyphemus

Daniel Bailey (University of Nottingham)

High Pressure Studies of d-block Thioether Co-ordination Complexes

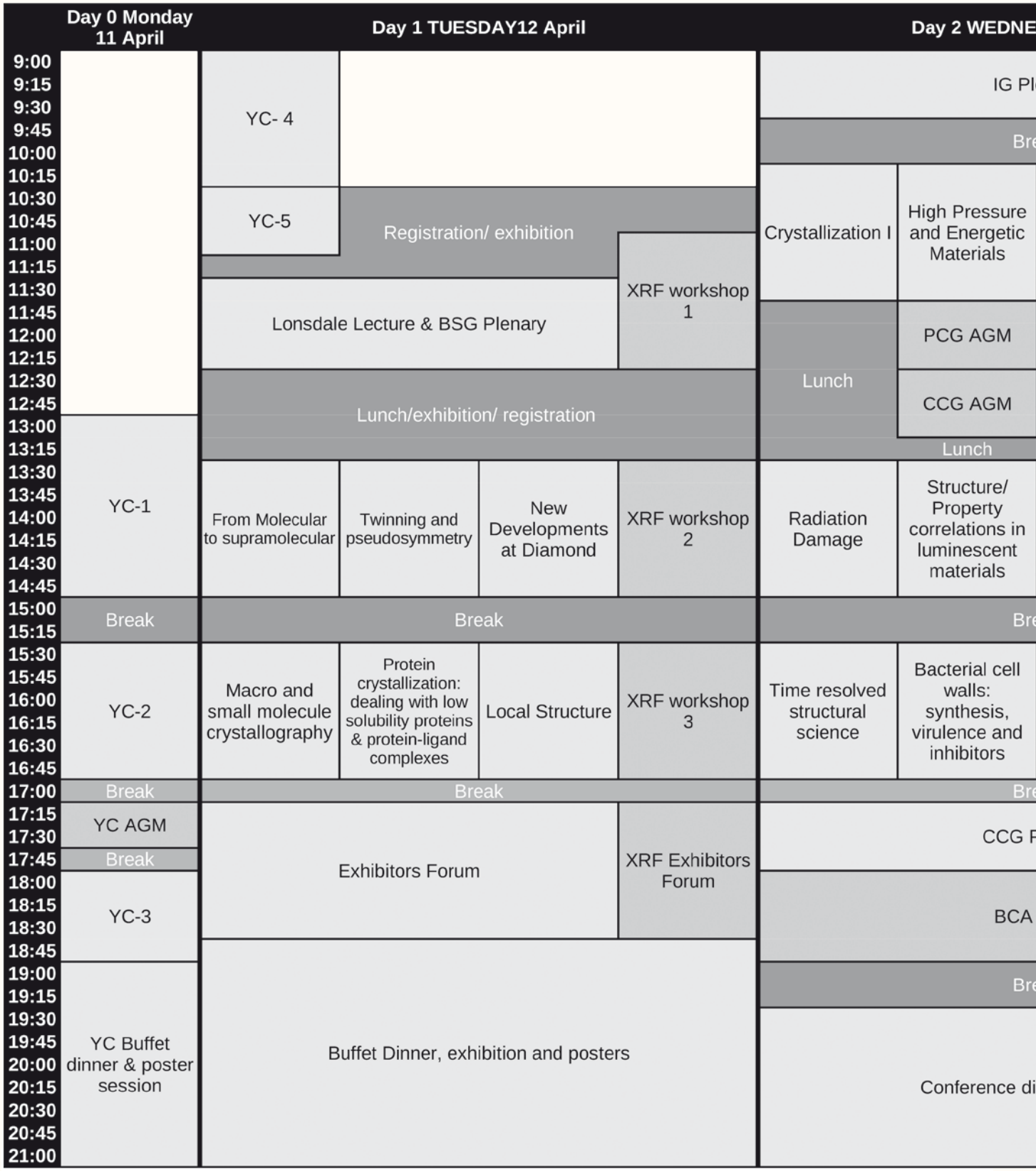
Kirsten Christensen (Diamond Light Source) *Trimesic Acid – a simple molecule with an unsolved packing problem*

Session YC5 Professional Development

Paul Raithby (University of Bath)

The Rocky Road to becoming an Academic

A Career in Industry (speaker tba)



SOCIAL PROGRAMME & POSTER SESSIONS

The Spring Meeting Conference Dinner will be held on Wednesday the 13th April 2011, in the spectacular venue of Keele Hall, a 19th Century Grade 2 listed mansion house. Surrounded by beautiful gardens, Keele Hall has the added advantage of being within walking distance of all of the Halls of Residence.

Make sure to bring your dancing shoes to the meeting as following the conference dinner, to help work off the calories, there will be the BCA Spring Meeting 2011 Ceilidh. Music and directions will be provided by "The Moody Food Ceili Band". http://www.moodyfood.co.uk

EXHIBITOR FORUMS

We are glad to welcome back our many exhibitors to the 2011 meeting and the Exhibition will run throughout the meeting after a formal launch on Tuesday evening at 5:15pm with the main Exhibitor's Forum (chaired by Arwen Pearson) and a parallel XRF Exhibitor's Forum (chaired by Dave Taylor).

SDAY 13 April		Day 3 THURSDAY 14 April			
enary		PCG plenary			XRF Keynote
eak		Break			
Membrane proteins	New Developments in XRF	Dynamic data, dealing with limited data	Materials Science: white beam methods	BSG YC Showcase	Novel Techniques in XRF
BSG AGM	XRF/XRD Applications	Break			
Lunch	IG AGM	Cultural Heritage	Materials Science: powder methods	Hot Structures	Getting more from diffraction data
Lunch		Close 13.30			
Crystallization II	XRF Applications				
eak					
Stress-strain microstructure	XRF Applications				
eak					
Plenary					
AGM					
eak					
nner & Ceilidh					

Registration*	After 7th March 2011
Full registration	**£240**
Student/Unemployed/Retired	**£105**
One-day-registration	**£140**
Young Crystallographers Meeting (Full)	**£67†**
Young Crystallographers (S/U/R)	**£40†**

* A supplement will be charged for non-members. † The full registration fee and S/U/R concessionary fee for the main meeting include registration for the Young Crystallographers Meeting

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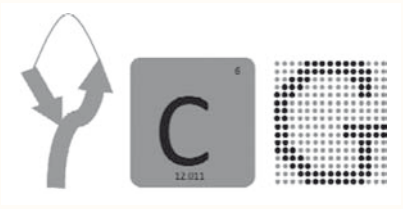
ACCOMMODATION & MEALS

Accommodation for the meeting will be in the Halls of Residence at Keele University and can be booked when you register for the meeting. Both single ensuite and single rooms with shared bathrooms are available. Breakfast is included with the accommodation.

Packed lunches will be provided during the meeting, however, these must be pre-booked when you register. Buffet dinners are provided free-of-charge on Monday 11th April (YC members only) and on Tuesday 12th April as part of the exhibitors forum for all delegates.

PARKIN LECTURE



It is with great pleasure that I can announce the YCG Parkin Lecture 2011 has been awarded to Dr Helen Maynard-Casely from the Royal Institution of Great Britain. This prize lecture acknowledges Helen's outstanding engagement with the public and scientific community in order to promote science. Whether it is the BBC, newspaper and magazine articles, course demonstrating, student supervision, public lectures, school outreach activities, blogging, you name it - Helen enthusiastically conveys her passion for science and I am looking forward to Helen delivering the Parkin Lecture at the YC Satellite in Keele!

Susanne Coles (née Huth)
YCG Chair

AGM BCA 2010

MINUTES of The Annual General Meeting of the British Crystallographic Association held on Wednesday 14th April 2010 at 6.00 p.m. at the University of Warwick.

68 people were present.

1. Approval of Agenda. A revised agenda was approved such that the elections took place at the end of the meeting.

2. Apologies for absence were received from Paul Raithby, Mike Probert and Andrés Goeta.

3. Minutes of the 2009 AGM were published in the March 2010 issue of Crystallography News and no corrections were requested.

4. President's Report
The President, Elspeth Garman, said the spring meeting was successful and enjoyable though with slightly fewer numbers than 2009 which was joint with the XRF group. She thanked Simon Coles and the Programme committee for putting together such a good meeting. There were 70-80 delegates present at the Young Crystallographers meeting for which EPSRC gave £2000 sponsorship and she thanked them for this. The Hodgkin lecture was given by Dame Louise Johnson and the Bragg Lecture was delivered by Sir John Meurig Thomas. Prof Simon Parsons gave the inaugural Parkin lecture.

The cost of this meeting is the same as last year. Spring meeting costs are being addressed by Council. In 2011 the meeting will be in Keele though the venue for 2012 has not been finalized. Council decided there would be no spring meeting in 2013 since the European Crystallography Meeting will be held here in Warwick in 2013.

There are up-coming elections for IUCr commissions. The President encouraged UK representation on these commissions so interested members should contact the President. Each position is held for a maximum of 6 years.

At this AGM the terms of office for the Secretary and Vice President finish. The current Secretary, Georgina Rosair, is willing to stand for a further 3 years. Sandy Blake will stand down as Vice-President and we will elect a new Vice President at this AGM. The elections for Ordinary member of Council will be staggered so one current Ordinary member will step down for one year and be co-opted immediately.

An electronic option is being considered for Crystallography News and Council is working with advertisers and NNE on this. As requested, Jena Bioscience have changed their magazine name to "Crystallization News" from "Crystallography News" to avoid confusion with the BCA publication. She thanked Carl Schwalbe for his Editorial work on Crystallography News.

The President then reported the passing of John Rutherford and Gordon Squires and there was a minute's silence.

The President has the pleasure of reporting three new Honorary members Prof. Bill Clegg, Prof. Venki Ramakrishnan and Mr Dave Taylor.

Council is concerned about the drop in Membership numbers to 512. She asked members to encourage colleagues to join the BCA. 80 incorrect email addresses had been corrected by Council members. The proposal to increase membership in 2012 to £30 from £20 will be put to vote at the next AGM in 2011.

In response to any proposed political activity, the BCA officers and Council will send out information regarding petitions but not actively support one view in the name of the BCA as we do not want to split the membership.

Richard Cooper was thanked for his excellent work on the BCA website. The President visited all the group meetings last year. Funds from the European Synchrotron Radiation Society will be used to enable students to attend IUCr and ECM meetings. She thanked NNE and Council for their assistance in the first 12 months of her Presidency.

5. Secretary's Annual Report
The Secretary, Georgina Rosair, reported that the BCA website has been updated to allow Council members and group representatives to add their own content which has been made possible by Richard Cooper's excellent work on the website. She encouraged all members to put a link to the new BCA website on their own web pages. At the 2009 European Crystallography meeting in Istanbul the UK won the bid to host the ECM in 2013 here in Warwick. She thanked Sandy Blake who led the bid, Gill Moore of Northern Networking Events, the Young Crystallographers Group and the President who presented the bid in Istanbul. She was delighted to report that Prof Bill Clegg has been elected to serve as an Individual Member Representative on the European Crystallographic Association Council and thanked fellow Officers and members on Council.

The President said she is working with the Secretary in homogenizing the BCA archives and thanked Moreton Moore for donating his BCA records.

6. Northern Networking Events Report
David Massey presented his report stating that the BCA has 518 members; according to interest group: 180 (BSG), 202 (CCG), 75 (PCG), 38 (IG) and 23 (Unspecified); according to category: 302 (Ordinary), 107 (Student/retired/unemployed), 60 (Corporate), 25 (Term/overseas) and 25 (Honorary).

Corporate members have dropped to 10; economic circumstances were cited. He thanked Crystallography News advertisers who enable Crystallography News to be produced at no net cost to the BCA. At this Spring meeting 267 attendees have registered with 20 exhibitors. The BCA are indebted to our exhibitors for their essential financial support for the meeting. David Massey thanked the exhibitors listing them individually.

The President added that each company which takes out Corporate membership is eligible for up to ten individual BCA memberships but not all companies take out the full ten. Membership is at an all-time minimum because of the bank account/payment changeover. More than half the membership paying by standing order were paying less than the correct membership fee.

Moreton Moore asked how many Young crystallographers we had. David Massey replied that they were included in the student numbers.

Colin Groom asked how many attendees are BCA members and suggested including membership fee in the meeting registration fee, The Treasurer replied that this was a good idea and already happened at BSG and CCG group meetings.

Peter Collins asked what impact the increase to £30 in the membership fee would have on the Corporate rate. The President replied that there were no plans yet and would welcome feedback on Corporate membership rates.

7. Report of the Treasurer to include Presentation of the Accounts for 2009 and the Examining Accountant's Report
The Treasurer, Harry Powell, presented the accounts. Whereas income is stable, membership subscriptions and income from interest are both down but investment income is up slightly. At the start of economic crisis cash was considered a better place for funds but since investments have performed better than cash, more money will be put in investments. The value of BCA sweatshirts and ties will be written off. The total BCA funds are just over £200,000. Approximately £100,000 exists as restricted funds (controlled by Groups or Funds) and the remainder just covers the cost of one spring meeting (£100K); therefore these reserves are needed to cover a Spring meeting going wrong. The President pointed out that the increase in administration costs for NNE include Gill's visit to Istanbul in 2009 for the ECM2013 bid which will be reclaimed from the ECM meeting in 2013.

Awards and bursaries (Cruickshank prize award) should read £250 not £2,250.

David Beveridge pointed out that the total for awards and bursaries was incorrect. The Treasurer will check and correct this before publication of the accounts. Colin Groom asked if the meeting was designed to break even. The Treasurer replied that it was, although a surplus was welcome. John Helliwell queried this in that a small surplus is needed rather than break even. The President stated that in planning, the registration fee was fixed at a rate at which the meeting would break even but this was with estimated attendee numbers.

8. Acceptance of the Accounts
After the above correction was made, the accounts were accepted. Nominated by David Beveridge and seconded by Pierre Rizkallah.

9. Appointment of Examining Accountants for 2010
The Treasurer said that the Accountants had not raised their fee and continued to work well with the BCA. The Accountants Young and Company were reappointed for 2010, nominated by Arwen Pearson and seconded by Simon Philips.

The President thanked Harry Powell for all his hard work as Treasurer and reminded members that a new Treasurer will be elected next year and encouraged interested members to stand for election.

10. Amendments to the Statutes and By-laws of the BCA
Sandy Blake presented the proposed changes to the Statutes and By-laws. These were previously published in Crystallography News (December 2009) and published on the BCA website. All were accepted.

Proposal 1. Amend Statute B (Membership)
The purpose of this group of amendments is:

(a) to formally recognise the category of "Student Member" "Student Members are entitled to a concessionary annual or a single discounted concessionary four-year membership fee, the latter

to commence no later than during their first year of postgraduate study. In all other contexts the expression Ordinary Members shall include Student Members." (Passed).

(b) to acknowledge the change in the name of the Physical Crystallography Group within the Institute of Physics; from "Physical Crystallography Group of the Institute of Physics" to"Structural Condensed Matter Physics Group of the Institute of Physics. (Passed).

(c) to replace the upper limit on the number of Honorary Members (20) with a limit on the number of people who may be accorded this status in any one calendar year.. "Honorary Membership shall normally be accorded to a maximum of two persons in any one calendar year." (Passed with one abstention).

Edward Bilbe asked why would there be more honorary members. To which the President replied that we had many worthy nominations but the upper limit needs to be removed otherwise we would be waiting for existing Honorary members to pass away before appointing new ones. Sandy Blake stated that there were three Honorary members appointed this year since there were extraordinary circumstances one being that a UK Crystallographer won a Nobel Prize. Jeremy Cockcroft asked if Honorary members paid fees. Sandy Blake replied that whilst many did not, several made substantial donations to the BCA (Passed with one abstention).

Proposal 2. Amend Statute G.2 (Finance)
This proposal is intended to clarify the liabilities of the BCA Trustees, by stating that if they follow the advice of the Charity Commission they will generally be protected. The proposed amendment to Statute G.2 is to add as the second sentence:**"The Trustees of the BCA shall be guided in the exercise of their responsibilities by the advice published by the Charity Commission."**
Jeremy Cockcroft asked about liability insurance. Harry Powell replied that this had been investigated and was found to be expensive. Sandy Blake added that when Trustees had been found liable it had been when criminal acts have been committed, and going against the advice of the Charity Commission would render any insurance invalid. (Passed).

CHANGES TO BY-LAWS

Proposal 3. Amend By-Law E.2 (Nominations and Elections) This proposal is to ensure that the Secretary is in a position to receive nominations and where necessary prepare ballot papers. It will require nominations to be received four days before the relevant AGM rather than two. The President added that vacancies were advertised in Crystallography News. (Passed).

Change to By-Law D.4, to reflect current accounting practices.
"The **audited** accounts shall be despatched to Members at least **two weeks** before the date of the Annual General Meeting, preferably with the agenda paper" will be changed to "The **independently examined** accounts shall be made available to Members at least **two days** before the date of the Annual General Meeting, preferably with the agenda paper". (Passed).

Proposal 4. By-Law G (Groups and Joint Group) was updated as follows:

1.Change the name of "The Physical Crystallography Group of the Institute of Physics" to "The Structural Condensed Matter Physics Group of the Institute of Physics " (Passed).

2.Ordinary Members of the Association have the right to become members of **another** Group of the Association without payment of a further subscription. **Members of the Association entitled to membership of the Young Crystallographers Group have the right to become members of another Group of the Association without payment of a further subscription;** such Ordinary or Student Members shall not be counted in determining any subvention to be paid by the Group to the Association. (Passed).

3.The Council shall determine what additional subscription, if any, shall be paid by **someone who is a Joint Member by virtue of paying a subscription via another organisation** who wishes to be a member of more than one Group [as set up under Statute D.4(f)]. **The introduction of any such additional subscription, and any subsequent modification to it, shall require the approval of the next Annual General Meeting.** (Passed with one abstention).

Proposal 5: Changes to By-Laws G (Groups and Joint Group) and I (Financial Arrangements with Joint Groups under Statute B.4):
The deletion of By-Law I.3 which reads:

"The Association shall not be required to meet any expenses of Group representatives attending Council and General Meetings. (Passed).

By-Laws I.4 and I.5 were moved to By-Law G as G.4 and G.5, thereby referring to all Groups and not just joint groups.

I4. The production and distribution of notices of conferences and similar meetings shall be provided for in the budget for the meeting. The Groups have no financial liability for any loss and no financial benefit from any surplus that may arise in connection with conferences and similar meetings arranged by the Association.
I5. Each Group shall submit an annual financial

statement to the Treasurer of the Association, giving details of its income and expenditure during the year. (Passed).

Proposal 6: Minor change to the wording of By-Law H (Reduced Subscriptions to allow Members who have never been in full-time employment, as well as those who have left it, to qualify for a reduced subscription.

> "Ordinary Members who are enrolled students for a degree or diploma, or who are **not** in full-time employment, shall pay such subscriptions, not exceeding one-half the regular subscription for Ordinary Members, as the Council shall determine, but shall have the same rights and privileges as Ordinary Members." (Passed).

Proposal 7: All text from "Version 5, 26 April 2000" onwards listing amendments shall be removed. (Passed).

11. Elections to Council: A new Vice-president and one new Ordinary member of Council were elected. There were two vacancies and two nominations so they were elected unopposed.
Vice president
Dr. Dave Allan (Diamond Light Source)
Nominated by Prof. Paul Raithby
Seconded by Prof. Chick Wilson

Ordinary member of Council
Dr. Arwen Pearson (Leeds University)
Nominated by Dr. Katherine Brown
Seconded by Prof. Simon Philips
The President thanked retiring members of Council Bill Clegg, Paul Raithby and Sandy Blake.

12. Any other business
There was no other business so the meeting was closed at 7.15pm.

2011 Annual General Meeting of the BCA

The Annual General Meeting of the British Crystallographic Association will be held on Wednesday 13 th April 2011 at 6.00 p.m. at the University of Keele.

At this meeting we will elect a new Treasurer and one new Ordinary member of Council.

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 Annual Report
6. Northern Networking Events Report
7. Report of the Treasurer to include Presentation of the Accounts for 2010 and the Examining Accountant's Report
8. Acceptance of the Accounts
9. Appointment of Examining Accountant for 2010
10. Raising of membership fee for 2012 from £20 to £30
11. Elections to Council
12. Any other business

Georgina Rosair
(Secretary to Council)

From the Secretary

Announcement of elections to Council

At the 2011Annual Meeting in Keele we will elect a new **Treasurer** and **one Ordinary member** of Council. Nominations for these posts are invited. Any two Members may make nominations for any vacancy. Such nominations shall be accompanied by the written consent of the candidate to serve if elected and must be received by the Secretary not less than four days before the Annual General Meeting which will be held on 13th April 2011 at 6pm. These may be sent by email to secretary@crystallography.org.uk

Georgina Rosair
Secretary to Council

Central Facility News

IN the previous issue of Crystallography News we made a brief visit to the macromolecular Xray diffraction beamlines. We will now complete our clockwise orbit of the synchrotron building (in the direction of travel of the electrons) by visiting two beamlines that also support crystallographic studies but offer a complementary range of diffraction techniques to those we have already seen. As we continue our walk around the experimental hall floor away from the MX village we eventually reach beamline I07, also called XENA (X-ray scattering Experiments for Nanostructure Analysis). The beamline is designed for the investigation of the structure of surfaces and interfaces at high resolution and under a variety of different conditions, including harsh and real-world environments.

Surface X-ray diffraction (SXRD) became a widely used technique following the 1986 publication by **Ian Robinson** (Phys. Rev. B, 33, 3830) who realised that the x-ray scattering between Bragg spots had an intensity distribution that depended on interferences both within the bulk and at the surface. This led to the understanding that these intensities could be used to solve well-ordered surface structures with high accuracy. Several groups worked at synchrotron facilities on traditional 4-circle or 6-circle diffractometers to implement the measurements and analysis strategies. This led to the development of beamlines specifically designed for surface diffraction experiments that were able to incorporate large ultrahigh vacuum chambers whilst still enabling the sample motion required for the diffraction.

In the UK, **Colin Norris** (Leicester) had also recognised the importance of the technique and applied (together with **Mike Hart**) to SERC in 1984 to build a surface diffraction beamline on station 9.4 at the SRS in Daresbury. A consortium of groups was established including the Leicester group together with **Emyr Macdonald** (Cardiff) and **Friso van der Veen** (FOM Institute). Two UHV systems were produced, one built in Leicester and the other at the FOM Institute in the Netherlands. One of the early students in this developing area was **Elias Vlieg**, who went on to write the widely used analysis software ROD. The 5-circle diffractometer was specifically designed for surface diffraction and enabled a number of operational modes including an option to work with a fixed incidence angle, thus preserving the surface sensitivity and penetration depth. In addition to solving surface structures (e.g. gold on germanium (111)), methods were developed to understand real-time growth dynamics (e.g. germanium on germanium (111)) through modelling growth oscillations at specific regions in reciprocal space. The interpretation was simple compared with other techniques due to the ability to use single scattering kinematical diffraction theory. Another chamber (INGRID) was developed by **Ronan McGrath** (Liverpool) and **Geoff Thornton** (Manchester) to extend the possible experiments on beamline 9.4.

The beamlines on second generation sources were superceded by purpose built beamlines on new third-generation facilities (notably by **Salvador Ferrer** on ID3 at ESRF), where the high flux and small spot from the insertion device had an immediate impact in terms of data collection speed and signal-to-noise. Not only did the studies of surfaces in ultrahigh vacuum continue but surface structures could now be studied in other environmental conditions including in atmospheric gases, in liquids or electrochemical environments. SXRD remains one of the only techniques that allows the study of surface structures in a non-vacuum environment.

In 2002, **Chris Nicklin** (Leicester) put together a working group to propose a surface x-ray diffraction beamline for Diamond Light Source. The concept included two end-stations, one to house small purpose-built chambers while the rear hutch would contain a fully equipped ultrahigh vacuum end-station. This was approved by the Diamond Scientific Advisory Committee as one of the Phase 2 beamlines. Chris Nicklin left Leicester to become Principal Beamline Scientist for the project in 2005, where it further developed to include the complementary Grazing Incidence Small Angle Scattering technique. The beamline team, which includes **Tom Arnold** and **Jonathan Rawle**, were able to commission the beamline on time and took first users in October 2009.

The beamline has two experiments hutches with the upstream and larger hutch, EH1, housing an impressively large 6-circle Huber diffractometer – though, to be frank, the term 6-circle rather underestimates the number of motorised axes the instrument has. The diffractometer is remarkably flexible and sections can be detached to accommodate the large variety of experiments, with their accompanying complex sample environment cells, that the beamline needs to support. A key element of the diffractometer set-up is the hexapod sample stage which not only allows the sample to be translated linearly in x, y, and z but also allows limited rotations around three orthogonal axes. This can be accommodated on various locations on the diffractometer and this is often implemented by removing one of the more conventional axes from the goniometer. The detector arm, which can be independently rotated around the horizontal 2Θ

axis and an orthogonal vertical axis, holds a number of detectors which can be selected on a rotary stage. There is also room on the arm for a large detector stage, which can support a Pilatus 2M photon-counting area detector. Immediately upstream of the diffractometer is the large vacuum vessel for the beam deflecting optics. This allows the beam to be directed downwards onto the sample position so that the surfaces of liquids or liquid-substrate surfaces can be examined over a range of grazing incidence angles. As the sample must remain horizontal during the experiment (to avoid a pool of liquid on the hutch floor) both the beam and the detector need to be scanned through the required angles. At the time of writing the deflecting optics are in the process of being commissioned and they will be made available to users later in 2011. The second, and relatively small, experiments hutch on I07 is currently under construction but it will eventually house the vessels and instrumentation for ultrahigh vacuum experiments. This will be made available in early 2012.

As we continue our walk around the experiments hall we pass beamline I11, which we've already seen in the September 2010 issue, and cross over the beam pipes for the long beamlines I12 (JEEP) and I13 – though the latter involves going upstairs onto the office level of the synchrotron building while the construction area remains closed off. We eventually come to beamline I16, the Materials and Magnetism beamline, which is tucked in between beamlines I15 (Extreme Conditions) and B16 (Test).

I16 was one of the first Diamond Phase-I beamlines to become operational for users, in January 2007. Since then it has provided a single crystal diffraction facility that had not previously been available in the UK. While it has much in common with I19 (the small-molecule single-crystal diffraction beamline), the focus for I16 is high-resolution diffraction, typically involving very weak resonant and magnetic scattering. In the late '80's and early '90's there was a great deal of excitement about the possibility of using intense x-ray beams to study magnetic structures – an activity previously monopolized by neutron scattering. Some heroic experiments were carried out at Daresbury by **Bill Stirling**, **Malcolm Cooper** and their colleagues and collaborators, but the technique did not become commonplace until the arrival of dedicated beamlines at third-generation synchrotron sources and the first of these was ID20 at the ESRF. In order to satisfy the demands of a growing UK community, and give them somewhere to call home, Cooper, Stirling et al won funding for the XMaS UK CRG at the ESRF, which has been supporting UK and international users since the late '90's. Meanwhile, at Daresbury, Station 16.3 provided a facility that could challenge XMaS on resolution, but certainly not on flux. For that, the UK had to wait for its own third-generation source and the dedicated beamline I16.

The fact that I16 was chosen as one of the four Phase-I beamlines for the physical sciences is testament to the enthusiasm of the UK user community. Since the early years of magnetic scattering, it has become apparent that high-flux high-resolution resonant scattering facilities can probe a wide variety of fascinating phenomena in Xray physics, including resonant and non-resonant magnetic scattering, anisotropic resonant scattering - often going beyond the dipole approximation - and studies of minute atomic displacements in strain waves. Most of these phenomena exhibit complex behaviour with respect to beam energy, azimuthal rotation and photon polarization, and so I16 was designed with such studies in mind. The beamline combines very high flux with no compromise in resolution with a focal spot size down to 20 x 185 microns. The Principal Beamline Scientist, **Steve Collins**, developed station 16.3 at SRS Daresbury and he used the experience gained on this facility for the subsequent design and construction of I16. The beamline scientific staff also includes **Alessandro Bombardi**, the Beamline Scientist and **Gareth Nisbet**, the Beamline Support Scientist.

Beamline I16 has a single but capacious experiments hutch which houses a large Newport 6-circle diffractometer and a motorised table which supports a range of secondary optics. Although the instrumentation is broadly reminiscent of that available on beamline I19, which we also saw in the September 2010 issue, there are key differences which are crucial to the determination of magnetic structure. Perhaps the most significant of these differences is the provision of a wave-plate (composed of a single-crystal of diamond) in the optics hutch, which allows the polarization of the beam to be varied. This is a crucial element as the intensity of those reflections that are most sensitive to the underlying magnetic structure are strongly affected by both the polarization of the X-ray photons and the azimuthal scattering angle. (By magnetic structure we mean the spatial correlations between the magnetic vectors of the atoms in the sample.) The two additional diffractometer circles enable the detector arm and the crystal goniometer to be rotated independently around vertical axes and these extra degrees of freedom allow azimuthal scans of the magnetic reflections to be carried out more readily. The detector arm supports a variety of detectors and these are arranged, rather like the fingers of a hand, on a rotary stage so that a specific

Central Facility News (Cont.)

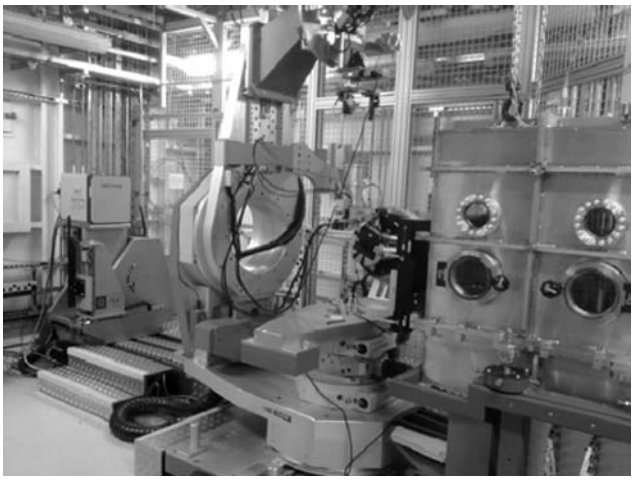
detector can be selected for a particular measurement. Additionally, the detector stage can also be rotated along an axis parallel to the detector arm, rather like a wrist (to continue with our hand analogy), so that the analyser crystal can additionally probe the polarization of the beam diffracted by the sample. For a more rapid surveying of reciprocal space, the detector arm also holds a Pilatus 100K area detector, which is now used for the majority of experiments that the beamline supports. Beamline I16 is also equipped with Pilatus 2M detector which is mounted to the diffractometer on a separate, detachable, platform. When this detector is in operation the detector arm is oriented and fixed in the vertical position.

As many magnetic structures are stable at only cryogenic temperatures, the diffractometer can support a closed-cycle cryostat which provides sample cooling to 4 K. The cryostat is designed specifically for the Newport geometry diffractometer and it mounts neatly onto the axis stage with an unrestricted opening to the sample position for both the primary and diffracted beams. Apart from the cryostat, the sample stage can accommodate standard (though extremely large) IUCr goniometer heads and a variety of alternative sample environments (although these custom items are more usually brought by users for specific experiments).

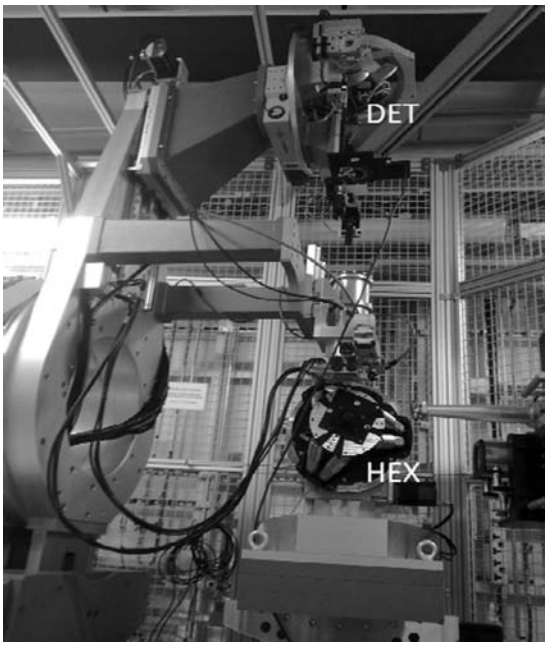
As the arrangement of the detectors is designed for the measurement of individual reflections, one at a time, with high spatial resolution, the beamline is also regularly used for the study of incommensurate and modulated systems where the careful characterisation of the positions of the weak satellite reflections is a crucial factor in the determination of an accurate structure. Although extremely detailed studies can be conducted on materials that have had some previous investigation, and thus where some prior knowledge of the expected structural behaviour exists, it is time-consuming to map a sufficiently large volume of reciprocal space to fully characterise some new or unexpected behaviour. Consequently, the current trend for this type of study is for closer links to be formed between small-molecule diffraction facilities, such as I19, and the physics-oriented beamlines. At Diamond, both beamlines are situated on high-flux undulator sources and both are making increasing use of very sensitive photon-counting pixel detectors. We believe that this trend will continue, with many future users seeking access to both types of facility: I19 to get a rapid overview of the crystal structure and large-scale reciprocal space maps, then I16 to focus in on specific diffraction features such as magnetic and pure-resonant diffraction peaks and their polarization dependence.

Further information on beamline I07 is available at http://www.diamond.ac.uk/Home/Beamlines/I07.html or contact **Chris Nicklin** (chris.nicklin@diamond.ac.uk) and further information on I16 is available at http://www.diamond.ac.uk/Home/Beamlines/I16.html or contact **Steve Collins** (steve.collins@diamond.ac.uk). I'd like to express my gratitude to both Chris and Steve for their very significant contribution to this article.

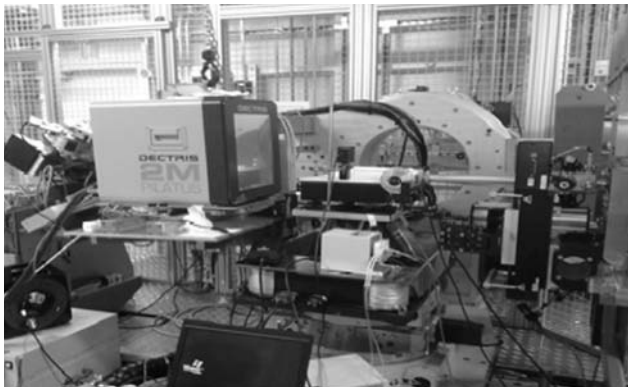
Next time we will be crossing the site to catch up on the updates at ISIS where a great deal of work has been carried out on many of the crystallography instruments in the last few months.



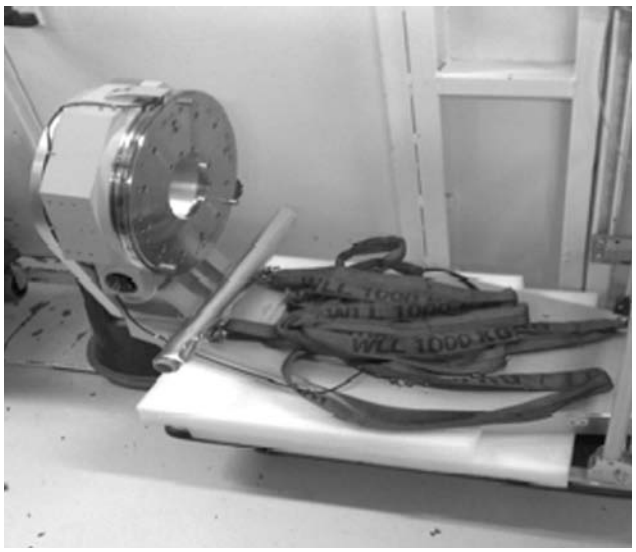
The layout of experiments hutch (EH1) on beamline I07. The diffractometer is shown in the centre of the image with the detector arm oriented in the vertical with the rotation axis of 2Θ rotated so that it is parallel with the incident beam direction. The Pilatus 2M detector is shown on the left of the image mounted to its independent motorised stage. The vacuum vessel for the beam deflecting optics is on the right of the image.



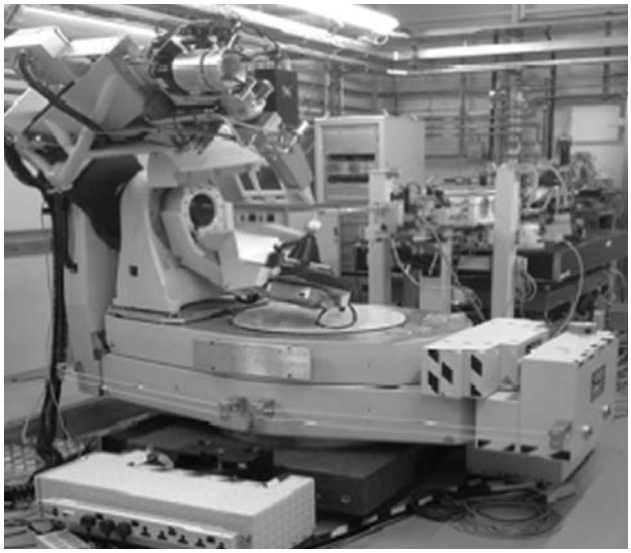
A detailed view of the I07 diffractometer. The hexapod (HEX) is shown on the detachable sample axis and the rotary detector stage (DET) is also indicated.



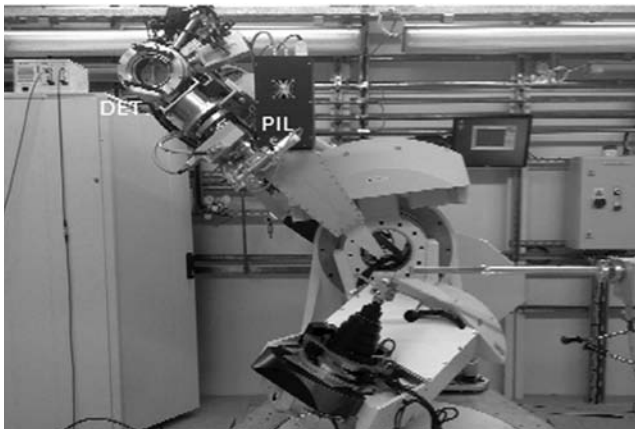
The I07 diffractometer in an alternative mode of operation. The detachable sample stage has been removed and the hexapod has been mounted in such a way that it supports a horizontally oriented sample cell for liquid interface experiments. The Pilatus 2M has also been mounted, via a detachable platform, to the diffractometer's detector arm.



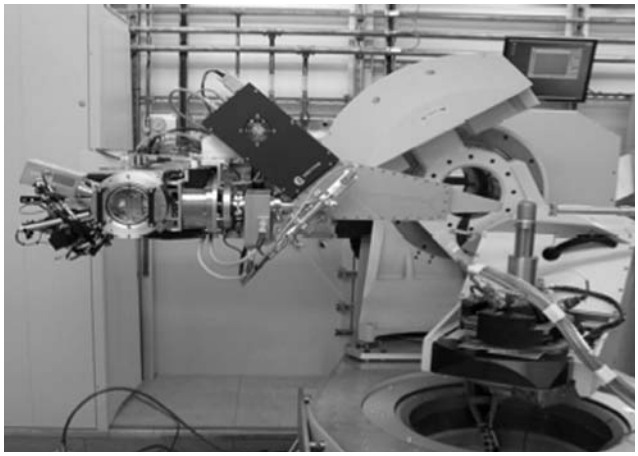
One of the detachable elements of the I07 diffractometer.



The layout of the experiments hutch of beamline I16. The 6-circle geometry diffractometer is shown in the foreground while the optics table is shown in the background.



A detailed view of the I16 diffractometer. The rotary detector stage (DET) is indicated, with the analyser crystal clearly visible, and the Pilatus 100k detector (PIL) is also shown. Note that in order to save space, the Pilatus detector is mounted at an angle to the main axis of the detector arm – a geometrical correction is applied to the recorded diffraction images to take account of the angle of incidence of the diffracted beam.



The diffractometer on beamline I16 with the closed-cycle cryostat mounted. The cables and hoses are close to the base and can be held away from the sample position. The -axis contains an integral motorised x,y,z translation stage which can be used to centre the crystal while it is contained within the cryostat. The finger-like arrangement of the detectors around the rotary stage at the end of the detector arm is readily apparent.

Science as Art / Art as Science

IMAGINE the surprise when the earliest molecular models were presented to the public by Hoffmann in his 1866 Faraday Lecture, or the anticipation when Fischer used bread clumps and toothpicks to model the stereochemical properties of carbohydrates in the 1890s. A few of us were around in 1968 when a color monitor was first used to display 3-D images of molecules. The challenges then were daunting – it was not until 1975 that it became possible to fit a protein structure to density with molecular graphics. Early programs like ORTEP, DISPLAY, BILDER, FRODO evolved and matured, but were seldom used outside the lab. Later, visualization software, such as GRAMPS, and 16mm movies taken from the graphics terminal in the 1970s made it into the lecture room and laid the groundwork for videos now easily made from programs like KiNG or VMD (cf. http://molvis.sdsc.edu/visres/sculpture/subjects.jsp). David Goodsell (http://mgl.scripps.edu/people/goodsell) took molecular visualization into the art gallery and Edgar Meyer started carving wooden sculptures of molecules (http://molecular-sculpture.com/); Byron Rubin (http://www.umass.edu/microbio/rasmol/history.htm#bender) and Julian Voss-Andrae (http://www.julianvossandreae.com/) made secondary skeleton sculptures in metal.

Rapid prototyping (Scripps, 3dmoleculardesigns.com) made it possible to create precisely scaled models. To commemorate the sesquicentennial of the polio vaccine in 2005, the Smithsonian commissioned scaled bronze sculptures of the polio virus capsid structure and the capsid+receptor complex (Hogle's lab, HMS). Mixing fantasy with art and science, images of molecules have been juxtaposed with flowers or in sculpture gardens (http://molecular-sculpture.com/Campus-sculptures/Imagine.html). Can we place life-sized bronze sculptures of biomolecules in public spaces, like a model of penicillin in a hospital terrace or a blockbuster drug in the offices of a pharmaceutical company? These sculptures of monumental molecules will have lasting value, telling future generations about the 'golden age' of crystallography and the heroic efforts to elucidate the individual molecules of life.

The recent increased use of physical, hand-held static models has been well complemented by the growing use of dynamic visualization tools. In the past decade, an increasing number of scientists have turned to 3-D animation software to create Pixar-quality movies of dynamic molecular events. These molecular animators, including recent MacArthur Foundation awardee Drew Berry (http://www.macfound.org/site/c.lkLXJ8MQKrH/b.6241243/k.30C1/Drew_Berry.htm), Janet Iwasa (http://iwasa.hms.harvard.edu), and Graham Johnson (http://fivth.com) use animation software from Hollywood, such as Autodesk Maya, Maxon Cinema 4D and Blender, to bring static molecular structures to life within their natural biological context. Efforts are currently underway to give these animation programs some of the capabilities of molecular viewer software (http://www.molecularmovies.com/toolkit/, http://mgltools.scripps.edu/epmv) and to provide tutorials specifically targeting researchers (http://www.molecularmovies.com/learning/).

Imagine going to a movie theater near you to see the latest 3-D blockbuster, a film rippling with dramatic tensions between molecules competing for scarce resources, or with heroic (also photogenic) scientists using cutting-edge technology to combat dreadful diseases – yes, fellow crystallographers, that too is part of our heritage, so why not go public with it, in 3-D!

With the centennial of the discovery of X-ray diffraction and the International Year of Crystallography just around the corner, here is our chance to make a visual and lasting impact on public consciousness and sensitivity.

Janet Iwasa & Edgar Meyer

Useful links:

http://biovisions.mcb.harvard.edu/

http://www.proteopedia.org/wiki/index.php/Main_Page

Delightful eyesfull:

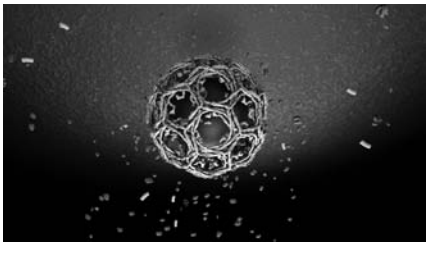
http://www.youtube.com/watch?v=mbcWGU8fpxA&feature=related%20?

http://www.nytimes.com/imagepages/2010/11/16/science/16anim5.html

http://www.nytimes.com/imagepages/2010/11/16/science/16anim6.html

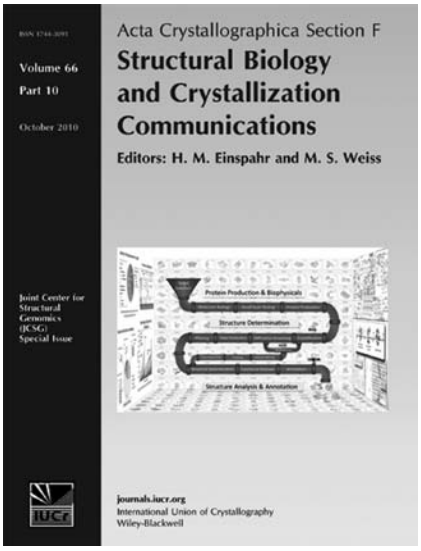
http://www.nytimes.com/2010/11/16/science/16animate.html?scp=1&sq=science%20animation&st=cse

http://www.nytimes.com/2010/11/16/science/16animate.html?hpw



Acta Crystallographica Section F showcases structural genomics publications

THE application of high-throughput methods to structural biology has generated an abundance of new macromolecular structures. In order to help ease the resultant publication backlog, Acta Crystallographica Section F now offers a special publication strategy to showcase these structures and the experiments upon which they are based. The first example was published in December 2009 and contained eight papers from the RIKEN-UK structural genomics consortium in a **special section** of the journal.



More recently (October 2010), the journal published a **special issue** that focuses exclusively on 35 structures, grouped into context, from the Protein Structure Initiative Joint Center for Structural Genomics. The issue, which is open access, is available from http://journals.iucr.org/f/issues/2010/10/00/issconts.html. This milestone publication has been enthusiastically welcomed by the community, and new requests and proposals for further special issues and special sections are under consideration.

For more information, please contact the Editors, **Howard Einspahr** (hmeinspahr@yahoo.com) or **Manfred Weiss** (msweiss@helmholtz-berlin.de).

The ICDD Announces the Recipients of the 2011 Ludo Frevel Crystallography Scholarship (January 19, 2011)

THE ICDD Ludo Frevel Crystallography Scholarship Committee has selected thirteen recipients for the 2011 Scholarship Program. These recipients were selected, on a competitive basis, from sixty-five commendable applications received by the ICDD Scholarship Committee. The recipients are:

Gokhan Barin, Northwestern University, Evanston, Illinois, USA

Metal-Organic Frameworks Incorporating Copper-Complexed Rotaxane Struts

Jeffrey Bertke, University of Notre Dame, Notre Dame, Indiana, USA

Synthesis and Characterization of Azolate Functionalized Metal-Organic Frameworks for the Sequestration of CO_2

Sharon Bone, University of California, Berkeley, California, USA

X-ray Absorption and Scattering Analysis of Hg Sorption by Nanocrystalline FeS

Honghan Fei, University of California, Santa Cruz, California, USA

Solvothermal synthesis of cationic framework materials, including zeotypes, inorganic extended materials and cationic metal-organic frameworks

Hua He, University of Delaware, Newark, Delaware, USA

Single-crystal and high resolution powder x-ray diffraction studies on new antimonides with layered and framework structures

Zachary Hudson, Queen's University, Kingston, Ontario, Canada

Triarylboron Compounds for Optoelectronic Materials: Applications in Solid-state lighting and chemical sensing

Shmuel Samuha, Ben-Gurion University of the Negev, Beer Sheva, Israel

Characterization of the Structure of a New Ternary Phase in Al-Ru-Rh system

Pradeep Sharma, All India Institute of Medical Sciences, Delhi, India

An approach towards prevention of septic shock syndrome: Structural and functional studies of PGRP and its complexes with various PAMPS

Chutchamon Sirisopanaporn, Universite de Picardie Jules Verne, Picardie, France

Crystal Chemistry and Electrochemical properties of Lithium Transition Metal Silicates; Li_2MSiO_4 where M are Fe and Mn

Vedran Vukotic, University of Windsor, Ontario, Canada

Development of new materials which have application in non-linear optics, ferroelectronics, piezoelectrics, and other technologically important physical properties

Andrew Warren, University of Central Florida, Orlando, Florida, USA

X-ray scattering of nanometric films and interfaces

Julie Wilkerson, The University of Texas at Austin, Austin, Texas, USA

Synthesis, characterization, and study of new luminescent materials based on conducting metallopolymers

Jeongho Yeon, University of Houston, Houston, Texas, USA

Investigation of New Polar Oxides: Crystal Structure and Physical Property Relationship

The ICDD will present each of these students with a check in the amount of $2,500 to assist in the continuation of studies in their selected fields of crystallographic research.

These scholarships are made possible through corporate and private donations. If you would like information on how you can make a tax-deductible donation, please contact the ICDD at +610-325-9814.

News (Cont.)

Logo design competition for the International Year of Crystallography – 2013 (PRIZE: Apple iPad)

IN 1912 Max von Laue showed that X-rays were diffracted by crystals, and in 1913 W. H. and W. L. Bragg demonstrated that the diffraction of X-rays can be used to determine the positions of atoms within a crystal. These groundbreaking experiments mark the birth of modern crystallography. The International Union of Crystallography (IUCr) is marking the centennial of these events by declaring 2013 the International Year of Crystallography (IYCr2013).

Logo design competition

Entries are invited for the design of a logo for the International Year of Crystallography.

The logo should symbolize and represent the fundamental importance of crystallography to society.

The logo will be used for announcements, letterheads, brochures, publications, web sites and other purposes as may be decided by the IUCr.

Designs should be sent by email to the IUCr Executive Secretary (execsec@iucr.org) by 1 July 2011.

For more details of the competition and how to enter, go to http://www.iucr.org/iycr/logocompetition/.

Successful logos in widely different styles for three recent International Years: Biodiversity (2010), Astronomy (2009) and Natural Fibres (2009), are reproduced here. They can be viewed in more detail on the relevant websites, http://www.cbd.int/2010 , http://www.astronomy2009.org and http://www.naturalfibres2009.org/images/iynf-logo-en.jpg .

Control and Prediction of the Organic Solid State - 30 March 2011

THE 2011 meeting of the CPOSS project will be held in the Old Refectory at University College London on Wednesday 30th March 2011. The theme of the meeting will be "Towards Understanding the Pharmaceutical Solid State", and will include speakers from the Solid State Pharmaceutical Cluster in Ireland and the Cambridge Crystallographic Data Centre. To complement the recurring theme of polymorphism causing catastrophic problems in pharmaceutical production drugs, the successes of the recent International Blind Test of Crystal Structure Prediction will be highlighted.

cposs

The meeting is free of charge to all academic groups, thanks to the sponsorship of the CPOSS Industrial Alliance. Lunch and coffee is included, and all participants are welcome to bring posters for the extended networking sessions. Full details of the programme are available at http://www.cposs.org.uk/ To register, please complete the online form, email Louise Price (l.s.price@ucl.ac.uk) or write to Dr **Louise Price**, Department of Chemistry, University College London, 20 Gordon Street London WC1H 0AJ.

Autumn Meeting Reports

CCG Autumn meeting 2010

"Understanding the Solid State"

Royal Society of Edinburgh conference centre.

LOCAL organiser **Stephen Moggach** arranged an historic and conveniently located venue via his connection to the Royal Society at the Royal Society of Edinburgh conference centre. The CCG programme was arranged by **Hazel Sparkes**.

The meeting started with opening welcome and introduction by CCG chairman **Andrew Bond** and additional remarks by BCA vice-president **Dave Allan**. Thanks were expressed to Bruker for providing funding for the meeting.

The first session was chaired by Andrew, with the first speaker being **Terry Threlfall** from Southampton. He spoke about first and second order transformations in crystals, which is important in understanding how crystals grow. Using examples, he showed how crystal defects would influence the transition, and he demonstrated the use of differential scanning calorimetry to study these phase transformations. He ended his talk by leaving us with a conundrum: two crystals which undergo a phase transition to the same structure but have different melting points 46 degrees apart, the only difference being their treatment in acids or bases. The second presentation was by **Jonathan Foster** who talked about "changing the old habits in new mediums: influencing crystal growth using supramolecular gels". Championing the use of gels as a crystal growth technique, he showed how by extending the library of available "gelators" one could encourage the growth of different polymorphs by mechanisms of kinetic trapping or thermodynamics.

Stephen chaired the second session held after lunch. We started with a talk entitled "Bananas, pear and other fruitful discussions" by **Carole Morrison**. She gave a very engaging talk with audience participation about these "fruits": code for the shapes of thermal ellipsoids. She discussed how molecular dynamic simulations could be used to improve our interpretations of the ellipsoid models and how they can give significant improvement over current polynomial expressions and their effect on bond lengths. This was followed by a talk by **Craig Robertson** from Durham on "solid-state properties of organic neutral radicals". He talked about his work on imidazolyl type radicals and the formation of novel dimer like compounds using the cryo-temperature equipment available at Durham to give interesting magnetic and conductive properties.

The third and final session chaired by Hazel began with the penultimate talk by **David Millar** on the high pressure crystallography on energetic materials at extreme conditions. He discussed work briefly done during PhD studies on RDX explosive materials and their latest work into azide compounds. Controlled high temperature and pressure conditions reveal new polymorphs and the possibility of recovering these forms back to ambient conditions. The final talk of the meeting was given by **Russell Morris** of St Andrews on metal organic framework materials but with the unusual tack of their medical applications. He demonstrated the use of MOFs in taking up biologically important gases and how they could be used in controlled drug delivery. Also he discussed some variable temperature work and how Pair Distribution Functions can be used to follow the changes within poorly diffracting crystals as they undergo a phase change.

Henry Wong

University of Nottingham

BCA Industrial Group Autumn Meeting at Diamond

THIS year's BCA Industrial Group (IG) Autumn meeting was held on the 3rd and 4th of November at Diamond Light Source. With over 40 delegates at the meeting discussions were lively. The meeting report below was written by the winners of the student bursaries for the meeting.

The IG Autumn meeting at Diamond certainly had an eye on the trend for practical applications of synchrotron science. Welcomes from the meeting organisers, Dr **Elizabeth Shotton** and Dr **Matthew Johnson**, as well as the BCA vice-president Dr **Dave Allan** were followed by an introduction to Diamond from Prof. **Trevor Rayment**, the Physical Sciences Director at Diamond. After providing some of the background to the applications of synchrotron science, Trevor encouraged everyone to review the proposals for the Phase III beamlines and to contribute to the shortlisted proposals, which focus on imaging, high throughput solutions, and the electronic structure of materials.

Dr **Emily Longhi**, an insertion device physicist at Diamond, guided us through the inner workings of a synchrotron, highlighting the importance of precision and angles as the final destination of the X-rays produced from the LINAC is to form a 100 micron beam targeted at a 100 micron sample! It was very interesting to learn that the majority of the 5MW electricity is spent on powering and cooling for the 240 quadrupole magnets, 168 sextupole magnets and 48 dipoles. 3MW of electricity is used when the magnets are not powered, i.e. just for cooling the water. There are also two RF cavities (eventually there will be three).

The merits of high resolution powder X-ray diffraction were extolled by Dr **Julia Parker**, senior support scientist on the PXRD I11 beamline at Diamond. High intensity, and high

Autumn Meeting Reports (Cont.)

resolution powder diffraction are powered by an undulator, operating at 15 kEV, and data are detected by the multi-analysing crystals detector, with 9 crystals on five 2θ arms. Time resolved powder diffraction can be obtained through the use of the position sensitive detector, which has 90° coverage. The development of a High-Throughput Continuous Hydrothermal (HiTCH) flow synthesis reactor by Cockcroft et al. was aided by the rapid characterisation of a series of 66 unique nanoceramic samples with composition varying around $Ce_xZr_yY_zO_{2-\delta}$ generated via this technique. High resolution PXRD diffraction were acquired for the entire heat-treated library in <1 day, enabling the characterisation of a complete ceria–zirconia–yttria ternary phase diagram.

"Big opportunities for small molecules" were presented by Dr **Harriott Nowell,** beamline scientist on the single crystal X-ray diffraction beamline I19 at Diamond. A broad range of experiments were presented, including a series of high-capacity hydrogen storage materials by Blake et al. The ever-present issue (for this crystallographer at least!) of very small and weakly diffracting crystals benefited greatly from the high flux on I19, and sensible and solvable data were obtained. The growing choice of sample environments will soon include a tuneable laser and chopper for performing pump-probe experiments, as well the installation of a Pilatus detector in EH2.

Dr **Michael Engel**, the industrial liaison scientist for macromolecular crystallography (MX), enlightened us on the structure of proteins, and emphasized the many degrees of freedom which hindered facile structure solution for macromolecular crystals. The somewhat small complication of contending with secondary, tertiary and even quaternary structures is brought about via hydrogen bonding in the 'local' ordered structure. This layered issue was highlighted in the structure solution of the Baculovirus polyhedra on I24 (Microfocus MX beamline), where the virus was packed so tightly around the protein that is almost impossible to break apart. Other work on protein-ligand interaction and binding on I04-1 (fixed λ MX side station) is attempting to target structure based drug design.

An adventure into the strange world of microstructure and small angle X-ray scattering (SAXS) was led by Dr **Claire Pizzey** (industrial liaison scientist for scattering). SAXS data gives an average of the entire bulk of the sample, and is particularly good for in-situ measurement and for non-volatile or opaque samples. Data are complementary to microscopy, which gives an image of a single local area. Studies carried out so far have included proteins, biomaterials, colloids, surfactants and catalysts.

Dr **Michael Drakopoulos** (Principal Beamline Scientist on I12) provided an excellent introduction to the very recently launched beamline I12, which is for joint engineering and environmental processing science (JEEP). High energy X-rays (50-150 KeV) and a large beam size allow access to a wide range of diffraction and imaging techniques. The ability of these energies to penetrate up to 20 mm of steel is very impressive, and recent studies of turbine blades by Rolls-Royce in EH2 highlighted the potential for improved characterisation and understanding of materials on an industrial scale. A recent publication by Korunsky et al. highlighted the quantification of strain partitioning between phases and grain orientations within polycrystalline two-phase titanium alloy Ti–6Al–4V from white beam energy-dispersive diffraction patterns on I12, and the resulting data achieved a strain measurement accuracy better than 50×10^{-6}.

Dr **Anna Kroner-Niziolek** (industrial liaison scientist-spectroscopy) introduced the wide range of spectroscopic techniques available at Diamond, and focused on the power of the photoelectric effect to describe the local structure of a wide range of materials. Information about the elemental distribution, chemical speciation in the local environment and long range order can be acquired for complex inhomogenous materials and systems under realistic conditions. A recent paper by Hart et al used data from beamline I18 (Microfocus XAS) to study the role of the chemical form of metal species in the unexplained failure of metal-on-metal hip arthroplasties. The speciation of the metal was observed to be unrelated to the hip type, blood level of metal ions nor the method of tissue preparation, and so future research can potentially be focused on the human synovial tissue response to $Cr(III)PO_4$.

The second day of the meeting started with a tour of the facilities at Diamond. Delegates were able to visit the beamlines which had been presented on day one of the meeting as well as getting to visit the inner workings of the synchrotron including the storage ring. The tours stimulated a lot of discussion about applications of Diamond to various crystallographic problems.

Prof. **Bill David** (ISIS/University of Oxford) presented a talk entitled 'From pharmaceutical research to the low carbon economy: the potential of powder diffraction' discussing the advantages and multi use of powder diffraction. The talk focused on 2 different drug molecules: paracetamol and zoplicone hydrates illustrating how the phase transitions involved with these compounds can be seen and analysed through the use of powder diffraction and the structures indexed and solved. The talk ended with a discussion of how powder diffraction data can aid the research into hydrogen storage in which an ammonia storage system is promising due to it being safe and efficient at room temperature, with powder diffraction investigating the variation of stoichiometry and polymorphism.

Prof. **Chris Frampton** (Pharmorphix) followed with a talk entitled 'Structural Characterisation of Pharmaceutical Materials: Application of Synchrotron Methods' in which the multi use of single crystal along with its advantages and disadvantages were outlined and how the use of synchrotron methods can overcome some of these problems. The talk focused on a discussion about sodium diclofenac (an anti-inflammatory) in which only one structure was previously known, however a further two hydrate forms have been discovered. In this case the bright X-rays created at the synchrotron allowed enough data to be collected from a small weakly diffracting crystal to determine one of the diclofenac

crystal structures. This in turn led to greater understanding of the stability of the sodium diclofenac drug phase.

'Conformational Change of Mammalian Serine Racemase upon Inhibitor Binding' was the title of the talk presented by Dr **Myron Smith** (Evotec) investigating the possibility of forming a mammalian serine racemase (protein in the brain). After screening 3000 possible conditions, the optimised crystallisation conditions were discovered and the structure was solved using synchrotron X-ray crystallography, showing a closed conformation with both a large and small domain. An alternative form was discovered under different conditions which had an open conformation, again solved using synchrotron X-ray crystallography.

The afternoon session commenced with Dr **Emyr Macdonald** (Cardiff University) presenting a lecture entitled the 'Grazing incidence diffraction studies of in-situ thermal processing of organic photovoltaic film'. Photovoltaic films have the benefits of being inexpensive, flexible and with the ability of covering large surface areas they are ideal substitutes to silicon in the capture of solar energy. By using GI-WAXS, the annealing process was tracked in real time at 140°C revealing a number of interesting trends regarding, crystallinity, domain size, disorder and expansion, all important factors when developing future energy sources.

Prof. **Dave Rugg** of Rolls-Royce gave an interesting and timely lecture, entitled 'Crystallography and safety critical structures' in which we are reminded of the role material science plays in the area of aerospace. Designing and manufacturing gas turbines with the capacity to move 1.2 tonnes of air/sec and a reliability of 1:100 million flights place heavy demands upon both engineers and scientists. It is clear that the understanding of macrostructure, in particular the residual stress, elasticity and grain orientation is critical for this to be achieved. Through the use of such techniques as high resolution topography, it is possible to track the growth of cracks and with EBSB providing information on grain orientation, it is clear that high powered analytic technique have a central role to play within this area.

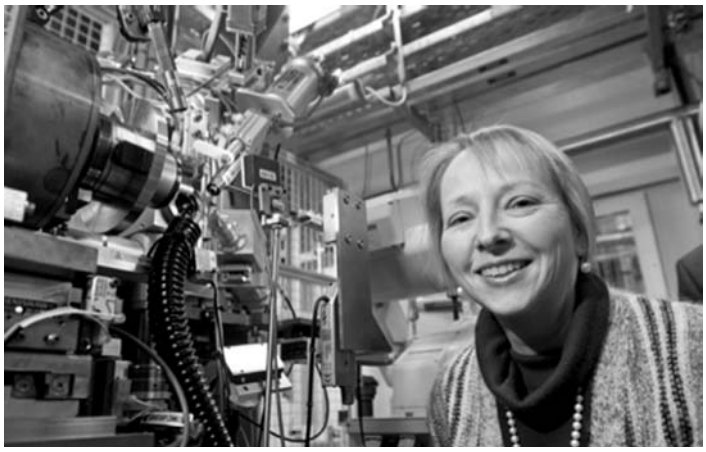
Dr **Gemma Newby** (University of Warwick/ESRF) lectured on 'Pluronic Properties and Applications'. The structural properties of these block polymers, which are widely used in biomedical and personal care products due to their biocompatibility and unique gel properties were discussed; SAXS and SANS, in addition to a unique rheo-SAS system, were employed for the investigation of shear alignment. The effect of varying temperature and concentration were investigated using SAXS, with phase diagrams constructed based upon the combination of these results.

The final lecture of the day was given by Prof. **Gopinathan Sankar** (UCL) on the 'Application of Synchrotron Radiation Techniques for the Determination of Structure of Industrial Catalytic Material'. The lecture focused on aluminophosphate frameworks and the incorporation of transition metals in a high oxidation state, eg Co, Mn, Fe within the structure. The crystallisation of CoAlPO-5 provided an eloquent example of how analytical techniques including EDXRD, SAXS and WAXS can be used in tandem to reveal to structural changes occurring within the system.

Claire Murray (University of Reading), **Laura Johnson** (University of Birmingham), **Catherine Greenan** (Queen's University of Belfast)

Julia Parker (Diamond) and Rebecca Sheridan (Pilkington Group Limited) on beamline I11.

Delegates at the BCA Autumn Group meeting held at Diamond

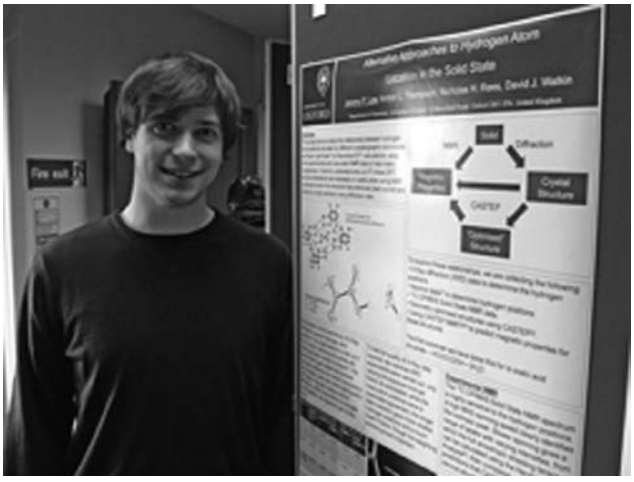


Dr Alison Burke (Huntsman) on beamline I03

Autumn Meeting Reports (Cont.)

The PCG-SCMP Winter Meeting

The PCG-SCMP Winter Meeting took place on Monday 15th and Tuesday 16th November at Cosener's House, Abingdon in conjunction with the ISIS Crystallography Group User Meeting. This is a format that has worked particularly well in previous years and this year was no exception. Just over sixty people attended the two-day meeting to hear about developments within Crystallography at ISIS as well as a series of talks under the heading "Current Research in Physical Crystallography". The meeting also included a poster session with punch and an excellent dinner on the Monday evening. After dinner a prize was awarded to **Jeremy Law** (pictured) for his poster on "Alternative Approaches to Hydrogen Atom Location in the Solid State". Jeremy is a 4th year undergraduate student working with **Nicholas Rees** and **David Watkin** in Oxford and the prize was awarded for his enthusiastic presentation and the potential outcomes of the work.



We had an eclectic mix of talks within the broad physical crystallography theme with **Mike Hayward** (Oxford), **Pam Thomas** (Warwick), **Andrew Wills** (UCL), **Joe Hriljac** (Birmingham), **Eddie Cussen** (Strathclyde), **Richard Walton** (Warwick) and **Steve Bramwell** (UCL) discussing Multiferroics, NBT, Frustrating Metals, High Pressure PDF, Li-ion Mobility, Flexible MOFs and Spin Ice, respectively. All talks were very well received and each elicited a good deal of discussion. We also had a session for 'younger' researchers to present their work with contributions from **Emma McCabe** (Durham), **Alex Gibbs** (St Andrews) and **Chris Knee** (Gothenburg) and we heard about the work on high-pressure methane phases contained in the thesis that was awarded the 2010 PANalytical-sponsored PCG Thesis prize from the recipient, **Helen Maynard-Casely** (RI).

The meeting benefitted considerably from the convivial atmosphere of Cosener's House made possible through the financial support from ISIS Crystallography and the Structural Condensed Matter Physics Group of the Institute of Physics. We are already looking forward to the next meeting!

Dave Keen
Rutherford Appleton Laboratory

XXII Congress and General Assembly

The Spanish Crystallographic Community warmly invites you to participate in the XXII Congress and General Assembly of the International Union of Crystallography (IUCr) to be held in Madrid, Spain, in August 2011. The Local Organizing Committee together with the International Program Committee, are working hard to offer a scientific program of the highest quality, aimed at showing the latest developments and topics in the field of one of the most interdisciplinary sciences that links together frontier areas of research.

With an attractive and weighty Scientific Program and taking into account all the different research interests, the timetable has been organized trying to avoid any overlap in topics, making sure that every attendant can make the most of their participation.

Crystallography plays a key role for the development of many important scientific fields, from Mineralogy up to Chemistry, Physics, Material Sciences, Nanotechnology, Biochemistry, Biology and Biomedicine. No scientist is a stranger to the crystallographic forum.

Learning about new trends in all these scientific areas surrounded by Madrid´s friendly and cosmopolitan atmosphere, a European city privileged with its cultural and historical heritage, will be an unforgettable experience.

We look forward to welcoming you in Madrid!

Enrique Gutiérrez-Puebla
Chairperson
XXII IUCr Madrid 2011 Congress

Important Dates

January 15, 2011 - Opening of abstracts submission
March 15, 2011 - Deadline for bursary applications
April 15, 2011 - Deadline for abstracts submission
May 15, 2011 - Deadline for "Early bird" registration
August 22, 2011 - Opening Ceremony
August 29, 2011 - Closing Ceremony

Congress Scope

Contributions, either poster or oral, should be assigned to one MS when submitted. In the following list the MS are ordered by different IUCr commissions; one MS could be under more than one commission.

Meeting Reports

CCP4 at Warwick

THE annual Collaborative Computational Project in Macromolecular Crystallography (CCP4) Study Weekend was held at the University of Warwick on January 5-7, 2011 in modern and comfortable facilities at that venue. The meeting entitled "Model Building & Refinement & Validation", covered the latest developments in these latter-stage steps of determining a protein crystal structure. The scientific programme was organised by **Roberto A. Steiner** (King's College London, UK) and **Bernhard Rupp** (k.-k. Hofkristallamt, Livermore, CA, USA). Registered participants numbered 379 and drew scientists from a range of academic and industrial institutions in the UK and from 12 other European countries as well as the United States, China, India, Malaysia and Singapore.

The first session, "Introduction to Meeting Themes" opened with **Roberto Steiner** welcoming the participants and wishing them a useful outcome from the meeting.

Bernhard Rupp then set the scene for the meeting with his talk, provocatively titled "Why is crystallography (still) difficult?". Macromolecular biological crystallography has become streamlined to the extent that users tend to think of it as "magic box" requiring little interaction with the user. Thankfully, this was a spur for some researchers to increase the complexity and size of the systems they study, creating many more challenges on the way: Sample procurement, crystallisation and data collection. Low resolution, high mosaicity, twinning, modulation, absence of native phases and other problems often lead to poor models. Non-linearity of protein and data behaviour, coupled with low determinacy of the problem, yield incomplete models, requiring cross-validation and stereo-chemical restraints. The treatment of the solvent masks is probably the biggest source of discrepancy between observed and expected amplitudes. Problems with twinning, correlated partial occupancies and anisotropic diffraction have exercised the minds of crystallographers over the years, and they are constantly being reassessed as crystallography develops. Model bias in Molecular Replacement, and real-space v reciprocal-space refinement are two more topics that keep arising. Ultimately, one hopes to obtain the best model from the data available and the subsequent speakers each addressed aspects of the topics introduced in this lecture with a view to achieving this goal.

George Sheldrick (Georg-August-Universität Göttingen, Germany) discussed "Using Prior Structural Information in Model Building and Refinement". Typical small molecule structure refinement yields R-factors of 3-4%, while macromolecule R-factors are around 5 times as large. Many underlying reasons were assessed, e.g. multiple conformations, heterogeneity of sample and poor modelling of the solvent mask. For example TLS (Translation/Libration/Screw) restraints have been reasonably successful, particularly when combined with residual B parameter refinement. The solvent mask remains the most significant component, and has classically been left flat. Attempts were made recently to allow solvent mask variations, but further work is needed. Special position constraints are automatically generated, and prior knowledge of both model geometry and electron density distribution is still necessary to generate appropriate restraints. The Engh & Huber dictionary is being updated, and new libraries of ideal geometry are being introduced. Model reliability seems to correlate well with R-free, but is unreliable when twinning is present. Full matrix refinement of all parameters, as encoded in SHELXE, gives estimated standard deviations for model assessment, and also allows chain extension and auto-tracing.

The after lunch session, "Building a Model: Automated, Manual, Sometimes Easy, Sometimes Not", was notable for its juggling of order. First up was **Paul Emsley** (University of Oxford, UK) with "New Tools for Model Improvements in Coot Using Concerted Torsions Description". He demonstrated some of the new features of his leading structure-rebuilding programme Coot. He showed how the Ramachandran plot can be used in real space refinement and how the use of the main chain can improve side chain rotamer fitting.

Next, **Kevin Cowtan** (University of York, UK) presented "Recent Developments in BUCCANEER for Model Building and Refinement." He discussed new features in his model building programme and in its sister ship Sloop for building poorly defined loops, and bravely compared refinement protocols not only within programmes but between programmes. Although on individual structures some protocols were worse, over a set of 55 there were no significant differences between REFMAC and *phenix.refine*.

Alwyn Jones (Uppsala University, Sweden) then presented his talk "Low Resolution Model Building" in O with a provenance back to the idea of skeletonisation by Greer in 1974, predating much of the audience. He reminded everyone that "We all make mistakes" and that out of register errors were most common in protein structures, which is incorrect numbering of the amino acids, and so the wrong side chains, for a section of the structure, which is obviously easier to miss at low resolution.

Technical problems with an HTML presentation finally being largely overcome, **Isabel Usón** (ICREA at Instituto de Biologia Molecular de Barcelona, Spain) presented her talk "New Structures Solved and Built with ARCIMBOLDO…and a Glimpse of SUBIX". ARCIMBOLDO (also a 16th century Italian artist who drew faces made from fruit- google arcimboldo to see some!), is a package that solves protein structures by placing individual helices or other small fragments by conventional molecular replacement and then using density modification. It requires good resolution (better than 2 Å) and often many attempts before a solution emerges.

Finally, **Willy Wriggers** (D.E. Shaw Research, New York, NY, USA) presented "Course-Grained Models for Molecular Structure Refinement and Dynamics". He described the SITUS suite and SCULPTOR an interactive front end, which is more commonly used by the protein EM community, but can also be used for fitting domain structures into low-resolution crystallographic, tomographic or SAXS density. A detailed

Meeting Reports (Cont.)

description of the capabilities of the package including online tutorials is available at http://situs.biomachina.org.

The final session of the first day, "Refining a Model: General Strategies and Novel Developments" focused on developments in *phenix.refine* and BUSTER. **Pavel Afonine** (Lawrence Berkeley National Laboratory, Berkeley, CA, USA) started the session with "Crystallographic Structure Refinement and Validation Using PHENIX" and broke the refinement process into three constituent parts: model parameters, the target function and the optimisation method, each of which should be carefully defined for optimal refinement. The aim of *phenix.refine* is to choose these such that the refinement process is automated from low to atomic resolution. New tools such as dual space refinement and automatic determination of TLS groups realising this were introduced as was a tool comparing your refinement statistics with those of comparable deposited PDB entries so you can see how well (or badly) your refinement is progressing.

Oliver Smart (Global Phasing Ltd., Cambridge, UK) introduced the audience to "Recent Developments in BUSTER: autoNCS, Targetting, and Improved Ligand Restraints". Exploitation of non-crystallographic symmetry (NCS) is a powerful tool and NCS with local structural similarity restraints can be enforced between two or more chains within a structure or alternatively the model under refinement can be coupled to another known structure. Both methods can result in more readily interpretable electron density. Reliable restraints are highly important in ligand refinement and BUSTER can now use mogul to survey the Cambridge Structural Database to determine restraint information and use prior knowledge of ligand chemistry in refinement. If information is not found, quantum chemical information can be used as part of geometry refinement.

Jeff Headd (Lawrence Berkeley National Laboratory, Berkeley, CA, USA) returned us to *phenix.refine* with "Knowledge-Based Restraints in phenix.refine for Improved Macromolecular Refinement at Low Resolution", but the focus this time was on improving refinement at low resolution (3 Å or worse). In order to achieve this, three new restraint models have been added to *phenix.refine.* These were reference model restraints for use when a higher resolution model exists: from the reference model restraints on dihedrals can be determined. Secondary structure restraints for restraining hydrogen bond length in helices or base-pair distances in RNA are particularly useful during the early stages of refinement. And finally Ramachandran restraints steer outliers towards favoured regions of the Ramachandran plot. All three models were shown to improve molprobity statistics and reduce Rfree; work is ongoing to tie all three models together in *phenix.refine.*

The first session on Friday morning was "Refining a Model: Low Resolution, Twinning and Complex Cases" and began with a talk by **Axel Brunger** (Stanford University, Stanford, CA, USA) entitled "Computational Approaches to Improve the Quality of Structures Obtained from Low-Resolution Diffraction Data". He introduced a new method, termed DEN (Deformable Elastic Network) that adds specific information from known homologous structures but allows global and local deformations of these homology models. For test cases at 3.5-5 Å resolution with known structures at high resolution, this method gave significant improvements over conventional refinement techniques.

Garib Murshudov (University of York, UK) the presented his talk "Low Resolution Macromolecular Crystal Structure Refinement: Problems with and Approaches to". He described novel developments implemented in the refinement program REFMAC. These included refinement against twinned data, and tools for low-resolution applications, such as "jelly restraints" (a form of local NCS), external restraints, B-value restraints and map sharpening applications.

Pietro Roversi (University of Oxford, UK) spoke about "The Structure Solution and Refinement of Human Complement Factor I, or: Tetartohedral Twinning Can Happen to You Too". He described how a special twinning problem was observed during the crystal structure determination and refinement of human Complement Factor I. A special case of ntwins=4 *aka* tetartohedral twinning was found, which was invariably associated with 222 rotational non-crystallographic symmetry - a challenging problem to say the least.

The next session "Ligands and Nucleic Acids: How to Properly Treat Non-Amino Acids" began with a talk from **Judit Debreczeni** (AstraZeneca, UK) "Modern Methods of Ligand Refinement and Analysis Using Coot". Judit demonstrated several new developments in Coot and its interface with tools for the modelling and validation of small molecule ligands (JLigand, LIBCHECK, CPRODRUG and Mogul). Accessed through the extensions menu of Coot, these allow you to rapidly draw a small molecule and generate sensible geometric parameters. The use of Mogul, in particular, for the validation of automatically generated restraints is based on a knowledge base of geometric parameters. Mogul is also able to flag up poor real space correlations between the ligand and experimental data.

Andre Lebedev (University of York, UK) next presented "JLigand: a Graphical Editor to Create Ligand Descriptions". JLigand now allows you to create a CIF library that describes covalent modifications to existing monomers (for example a pyruvoyl-lysine) in the CCP4 library. This can then be included as a LINK card in the PDB file rather than requiring the construction of a new monomer library specifically for the modified amino acid or ligand. There have also been advances in the ability of LIBCHECK and JLigand to deal with bound metals, although it is necessary for the user to define the coordination geometry correctly.

Bill Scott (University of California at Santa Cruz, CA, USA) gave the next talk "Challenges and Surprises that Arise with Nucleic Acids". He described his experience solving novel RNA structures. The approach he presented is to first use the "nucleotide builder' functionality of Coot to create fragments of A-form RNA based on secondary structure predictions from sequence data. These fragments are then used as molecular replacement models by PHASER to generate an initial "dodgy" model. The resulting molecular replacement solutions were then used to generate "MIR" phases that could be passed to CNS for solvent flattening. This final step produced an

amazingly readily interpretable map from which the structure could be built!

The final talk in this session was by **Victor Lamzin** (EMBL-Hamburg, Germany) who described the use of ARP/wARP for building protein, nucleic acid and ligands. NCS matching will be implemented in the next release that will look for matching short fragments of density related by NCS and then attempt to combine these into a single molecule. This does seem to improve initial model completeness. The nucleic acid building begins with locating phosphate groups and then searches for adjacent planar density that could correspond to bases. This works well and could be used to automatically build much of the 30S ribosome from data at 3.05 Å in ~ 6 hours. Finally he described the use of ARP/wARP to locate ligands in the electron density map. Using a user defined initial model of the ligand ARP/wARP attempts to dock the ligand into the density. Conformational fitting, such as permitting rotation around rotatable bonds is used. A cocktail approach is also possible, where a variety of ligands can be tested in order to identify the species that best fit the experimental data - something that is likely to be very useful when trying to figure out what your mystery density might be.

In summary, this was a useful session that included a wealth of practical tips to enable crystallographers to better deal with those pesky non-protein bits of macromolecular structures!

The final session of the meeting "Validation: Keep Checking You're on the Right Track" was opened by **Frank von Delft** (Structural Genomics Consortium and University of Oxford, UK) who presented a talk entitled "2 Copies Good, 4 Copies Better: Validated by Non-Crystallographic and Cross-Crystal Symmetry". He began by reminding the audience how under-defined the crystallographic problem is, but that in many cases we can get "multiplicity for free" using NCS or cross-crystal symmetry (CCS). He discussed key issues associated with weighting and model building (both of multiple copies of protein chains and solvent) and highlighted, with reference to Gerard Kleywegt's 1996 Acta Cryst. D paper [vol. 52, no. 4(7), 842] how NCS and CCS influence validation in refinement processes. The overall message was that multiple views of a structure can improve the quality of the final model but that it is important to use multiplicity properly.

The next talk, "Statistical Quality Indicators for Electron Density Maps", was given by **Ian Tickle** (Astex Therapeutics, Cambridge, UK). He explained how the use of the real-space R-factor and the real-space correlation coefficient in validation is sub-optimal, owing to the inability of these quantities to distinguish between the accuracy of the model and its precision. He described correlation effects involving B-factors and emphasised the importance of using difference maps in the model building process. Finally, he illustrated, using an example from his work at Astex, his maximum likelihood-based method for assessing local model accuracy using a real-space difference density Z-score as an effective means for model validation.

Ethan Merritt (University of Washington, Seattle, WA, USA) presented the rather imaginatively titled talk "To B or not to B? What's Appropriate in Models from 1 Å to 4 Å (And Thus the Native Hue of Resolution is Sicklied o'er With the Pale Cast of Thought – W. Shakespeare)". He began by explaining why it is important to obtain a final model that does not contain inappropriate levels of complexity – an inherent problem arising from the drive to add parameters to compensate for the often low number of observables in protein crystallographic datasets. His talk included a critical discussion about how one chooses the appropriate treatment of parameters such as B-factor in crystallographic refinements, introducing the use of the Hamilton R-factor test as a statistical test for aiding in this choice. He also described several programs that could be use to guide refinement strategies and validation processes involving a range of parameters such as using anisotropic B-Factors for modelling at either the atomic level or as a bulk quantity (e.g., TLS; see for example the programs PARVATI or SKITTLS).

Sameer Velankar's (EMBL-EBI, Wellcome Trust Genome Campus, Hinxton, UK) presentation "The Future of Validation in the PDB" began by recounting the history of the PDB (established in 1971 for archival purposes) and the current goals of the PDBe (Europe site) that involve transforming this database into a valuable resource for both experts and non-experts with interests in biomedicine and related areas of research. He described a recent outcome of a Validation Task Force (chaired by Professor Randy Read from the University of Cambridge, UK) that resulted in the production of a set of recommendations (to be published this year) for enabling the generation and reporting of validation metrics in an easy-interpretable format. A clear goal is that this information can help guide and inform researchers about the strengths and limitations of individual PDB entries. Key areas of future development within the PDBe include improving the presentation of quality checks, errors and outcomes of validation analyses for all users, regardless of their level of expertise.

The final talk of the meeting was by **Robbie Joosten** (Netherlands Cancer Institute, Amsterdam, The Netherlands) who presented an ambitious project entitled "PDB_REDO: Constructive Validation, More Than Just Looking for Errors". He described the development of the PDB_REDO pipeline aimed at optimising existing models in the PDB using validation and rebuilding tools in a constructive manner. A key driver for this effort is that a great number of PDB entries have not benefitted from recent developments in model-building and refinement strategies and thus the models available to PDB users could be improved. The new structure models are available at http://www.cmbi.ru.nl/pdb_redo. This subject sparked a lively discussion at the conclusion of the meeting about how these new models could be associated with the existing PDB entries and whether the original depositor would have any approval role.

The meeting concluded with the current chair of CCP4 Working Group 1, **Martin Noble** (University of Oxford, UK) thanking the organisers for their work in producing an excellent programme of talks. Finally, the smooth and successful running of this year's CCP4 workshop was ensured by the dedicated and professional support provided by the STFC team of **Shirley Miller, Damian Jones, Laura Johnston**, and **Stuart Eyres** (photography).

Prepared by members of the Biological Structures Group Committee and the BCA Council, and edited by **Kate Brown** (BSG Vice-chairman).

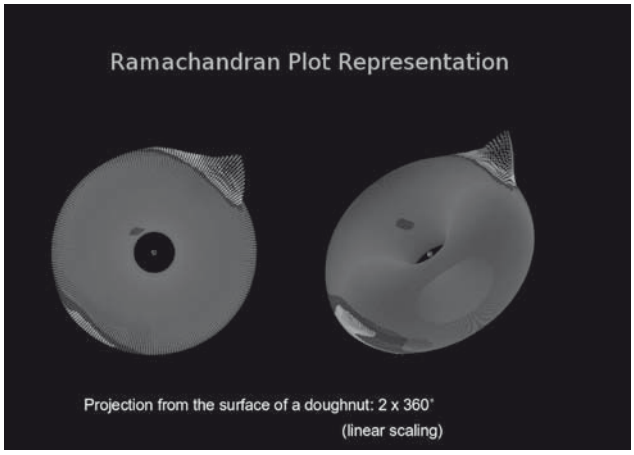


Figure 1: "Dough-nut" representations of Ramachandran Plots. Ramachandran plots are usually represented using a 2d plot with logarithmic scaling. Here we represent the same data using the surface of a dough-nut. The height of the point from the surface of the dough-nut represents the probability density of a given phi,psi pair. This representation uses linear scaling - the lowest non-zero level being at the 5% level (that is, less than 5% of residues in the PDB have phi, psi values that are less likely than this) and shows the data as continuous in 2 dimensions and the regions of low probability density are rather more extensive than one might imagine using a conventional representation. (Figure prepared by P. Emsley)

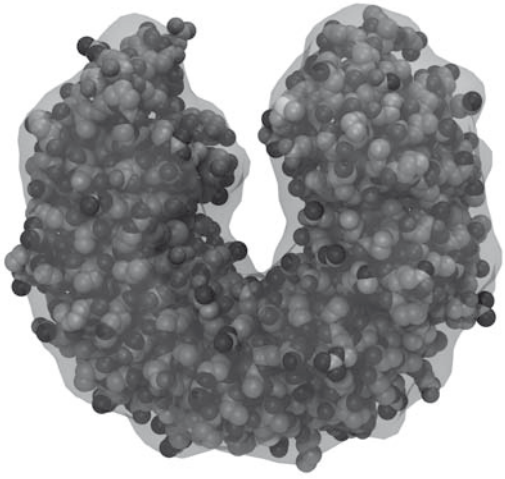


Figure 2: Real-space fitting and visualization of SAXS bead models with Situs[1,2]. Atomic structure of ribonuclease inhibitor (PDB entry 1BNH) fitted in to a coarse-grained bead model (393 beads, 3Å radius, hexagonal close-packed; generated from with the *Situs* tool *pdb2sax*) using the *Situs* tool collage. To show the embedded structure the bead model is rendered as a transparent envelope. The envelope is the half-max isosurface of a density map created from the beads with the *Situs* tool *pdb2vol*, using Gaussian kernel convolution with (half-max) kernel radius 3Å. This image rendered with Tachyon ray tracing using VMD [3]. For an updated review of the complete SAXS workflow see [2] and the SAXS tutorial at http://situs.biomachina.org. (Figure prepared by W. Wriggers)

[1] *Wriggers W, Chacón P (2001)* Using Situs for the Registration of Protein Structures with Low-Resolution Bead Models from X-ray Solution Scattering. *J. Appl. Cryst.,* 34:773-776

[2] *Wriggers W (2010)* Using Situs for the Integration of Multi-Resolution Structures. *Biophysical Reviews*, 2:21-27

[3] *Humphrey WF, Dalke A, Schulten K (1996)* VMD - Visual Molecular Dynamics. *J. Mol. Graph.,* 14:33–38

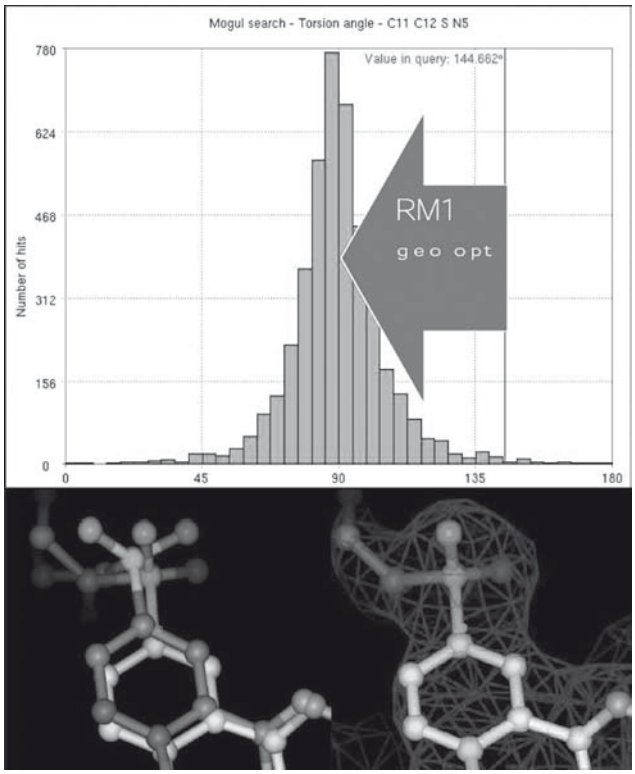


Figure 3: BUSTER refinement of 1udt using quantum mechanical (QM) restraints for Viagra. This figure shows how ligand strain motion can be assessed by QM and compared with the Cambridge Structural Database (CSD) data using the programme MOGUL. (Figure prepared by O. Smart)

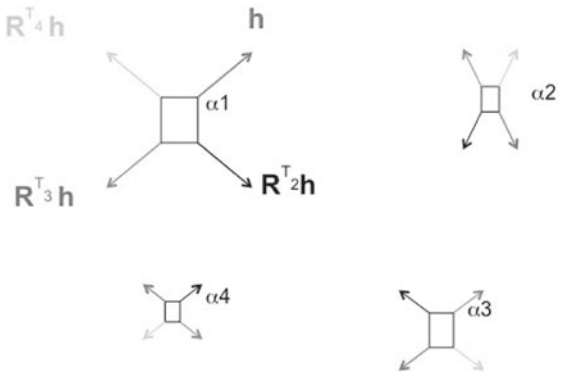


Figure 4: A tetartohedrally twinned crystal consists of four crystal domains (here represented by the four black boxes, separated in space for clarity). The ratio of the volume of each domain is a1:a2:a3:a4 (twin fractions). Each reflexion **h** will have twin-related reflexions $\mathbf{R}^{T}_{2}\mathbf{h}$, $\mathbf{R}^{T}_{3}\mathbf{h}$, $\mathbf{R}^{T}_{4}\mathbf{h}$, where $\mathbf{R}^{T}_{i}$ is the i^{th} twin operator, a 3x3 rotation matrix; the spot containing the scattering at **h** from the first crystal domain will contain scattering from the other domains at the twin-related vectors. (Figure prepared by P. Roversi)

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to list please send them to the Editor, c.h.schwalbe@aston.ac.uk. Assistance from the IUCr website is gratefully acknowledged.

14-18 March 2011
ICDD 2011 Spring Meetings, Newtown Square, PA, USA.
http://www.icdd.com/profile/march11.htm

21-25 March 2011
American Physical Society March Meeting 2011, Dallas, TX, USA.
http://www.aps.org/meetings/march/

26 March - 3 April 2011
13th Intensive Teaching School in X-ray Structure Analysis Durham.
http://www.dur.ac.uk/durham.x-ray-school/

27-31 March 2011
ACS National Meeting & Exposition. Spring 2011, Anaheim, CA, USA.
http://portal.acs.org/portal/PublicWebSite/meetings/spring2011/index.htm

30 March 2011
Control and Prediction of the Organic Solid State - Towards Understanding the Pharmaceutical Solid State
http://www.cposs.org.uk/

3-8 April 2011
European Geosciences Union General Assembly 2011, Vienna, Austria.
http://meetings.copernicus.org/egu2011/

4-5 April 2011
ACTOP11 - 4th Workshop on Active X-ray & XUV Optics, Didcot.
http://www.diamond.ac.uk/Home/Events/actop11.html

4-7 April 2011
Microscopy of Semiconducting Materials XVII, Cambridge.
http://msmxvii.iopconfs.org/

6-15 April 2011
Synchrotron Radiation & Free Electron Lasers. Joint US-Cern-Japan-Russia School, Erice, Italy.
http://www.cern.ch/schools/CAS

11-14 April 2011
BCA Spring Meeting, Keele University.
http://crystallography.org.uk/spring-meeting-2011

2-4 May 2011
HSC Industry: Neutrons and Synchrotron X-rays for Industrial Applications, ESRF Grenoble, France.
http://www.esrf.eu/events/conferences/HSC/HSC13/hsc-industry-neutrons-and-synchrotron-x-rays-for-industrial-applications

2-6 May 2011
Practical X-ray Fluorescence Spectrometry International Centre for Diffraction Data , Newtown Square, PA, USA
http://www.icdd.com/education/xrf.htm

5-6 May 2011
Dynamic X-ray Diffraction/Spectroscopy Experiments at Extreme Conditions: Implementing time resolved experiments for 3rd and 4th generation synchrotrons, DESY, Hamburg, Germany.
http://indico.desy.de/conferenceDisplay.py?confId=3942

6-9 May 2011
3rd APPA Conference in conjunction with the 3rd Symposium of the CPS, Shanghai, China.
http://cms.shu.edu.cn/Default.aspx?tabid=15853

9-11 May 2011
Wilhelm and Else Heraeus Seminar: Energy Materials Research by Neutrons and Synchrotron Radiation, Bad Honnef, Germany.
http://www.helmholtz-berlin.de/events/we-heraeus-seminar/index_de.html

9-13 May 2011
E-MRS Spring Meeting and IUMRS ICAM 2011, Nice, France.
http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=359&Itemid=134

10-14 May 2011
ICSG 2011 International Conference on Structural Genomics, Toronto ON, Canada.
http://www.sgc.utoronto.ca/ICSG2011/

10-18 May 2011
International School of Biophysics: Channels and Transporters, Erice, Italy.
http://www.physiology.vcu.edu/erice/index.html

15-22 May 2011
ESI 2011. EIROforum School on Instrumentation Grenoble France
http://www.epn-campus.eu/esi-2011

16-19 May 2011
PPXRD-10. 10th Pharmaceutical Powder X-ray Diffraction Symposium, Lyon, France.
http://www.icdd.com/ppxrd/

22-26 May 2011
IXth European Symposium of The Protein Society, Stockholm, Sweden.
http://www-conference.slu.se/proteinsociety2011/welcome.html

22-27 May 2011
3rd Intl School on Biological Crystallization, Granada, Spain.
http://www.isbcgranada.org/

23-27 May 2011
SMARTER 2 Workshop. Structure Elucidation by Combining Magnetic Resonance, Computation, Modelling and Diffraction, Aveiro, Portugal.
http://smarter.web.ua.pt/

23-27 May 2011
2nd Course on Neutron Scattering Applications in Structural Biology, Oak Ridge, TN, USA.
http://neutrons.ornl.gov/conf/gcnb2011/

25-27 May 2011
Joint Annual Meeting of GAC-MAC-SEG-SGA, Ottawa, ON, Canada.
http://www.gacmacottawa2011.ca/http://www.gacmacottawa2011.ca/

28 May - 2 June 2011
American Crystallographic Association Meeting, New Orleans, LA, USA.
http://www.amercrystalassn.org/content/pages/2011-homepage

1-4 June 2011
2011 North American Solid State Chemistry Conference, Hamilton, ON, Canada.
http://www.brockhouse.mcmaster.ca/news-events/details/23-2011-north

2-12 June 2011
The Power of Powder Diffraction, Erice, Italy.
http://www.crystalerice.org/Erice2011/2011pd.htm

2-12 June 2011
Electron Crystallography: New Methods to Explore Structure and Properties of the Nano World, Erice, Italy.
http://www.crystalerice.org/Erice2011/2011ec.htm

6-7 June 2011
XDL 2011 Workshop 1: Diffraction Microscopy, Holography and Ptychography using Coherent Beams, Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

6-10 June 2011
TXRF2011. 14th International Conference on Total Reflection X-ray Fluorescence and Related Methods,, Dortmund Germany.
http://www.txrf2011.org/http://www.txrf2011.org/http://www.txrf2011.org/

6-10 June 2011
Fundamentals of X-ray Powder Diffraction, International Centre for Diffraction Data , Newtown Square, PA, USA.

13-14 June 2011
XDL 2011 Workshop 2: Biomolecular Structure from Nanocrystals and Diffuse Scattering, Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

13-16 June 2011
Nanotech Conference & Expo 2011, Boston MA, USA.
http://www.techconnectworld.com/Nanotech2011/

13-17 June 2011
Advanced Methods in X-ray Powder Diffraction, International Centre for Diffraction Data , Newtown Square, PA, USA.
http://www.icdd.com/education/xrd.htm

13-17 June 2011
Resonant Elastic X-Ray Scattering, Aussois, France.
http://rexs2011.grenoble.cnrs.fr/

13-26 June 2011
Zürich, Switzerland.
The Zürich School of Crystallography 2011. Bring Your Own Crystals.
http://www.oci.uzh.ch/group.pages/linden/zsc/

19-24 June 2011
Liquid Crystals, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2011&program=liqucryst

20-21 June 2011
XDL 2011 Workshop 3: Ultra-fast Science with "Tickle and Probe", Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

20-23 June 2011
I W P C P S® 13 Thirteenth International Workshop on Physical Characterization of Pharmaceutical Solids, Indianapolis, IN, USA.
http://www.assainternational.com/workshops/iwpcps_13/iwpcps_13.cfm

20-24 June 2011
XVII International Conference on Crystal Chemistry, X-ray Diffraction and Spectroscopic Studies of Minerals, St Petersburg, Russia.
http://onlinereg.ru/ccxrds

23-24 June 2011 XDL 2011 Workshop 4: High-pressure Science at the Edge of Feasibility, Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

25-30 June 2011
36th Federation of European Biochemical Societies Congress, Turin, Italy.
http://www.febs2011.it/

26-30 June 2011
5th International Workshop on Crystal Growth Technology, Berlin, Germany.
http://iwcgt5.ikz-berlin.de/

27-28 June 2011
XDL 2011 Workshop 5: Materials Science with Coherent Nanobeams at the Edge of Feasibility, Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

29-30 June 2011
XDL 2011 Workshop 6: Frontier Science with X-ray Correlation Spectroscopies using Continuous Sources, Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

30 June - 1 July 2011
European Lab Automation, including Advances in Protein Crystallography, Hamburg, Germany.
http://www.selectbiosciences.com/conferences/APC2011/

3-7 July 2011
iWoRID2011. International Workshop on Radiation Imaging Detectors, Zurich, Switzerland.
http://indico.psi.ch/conferenceProgram.py?confId=29

4-8 July 2011
Workshop on Combined Analysis Using X-ray and Neutron Scattering, Caen, France.
http://www.inel.fr/news/page.asp?n=39http://www.inel.fr/news/page.asp?n=39

4-8 July 2011
AIC International School 2011 Crystallography Beyond Diffraction, Camerino, Italy.
http://www.unicam.it/geologia/AICS2011/

4-13 July 2011
High throughput methods for protein production and crystallization, Marseille, France.
http://events.embo.org/11-HTP/

9-19 July 2011
Layered mineral structures and their application in advanced technologies, Rome, Italy.
http://www.emuschool2011.unimore.it/

10-12 July 2011
British Association for Crystal Growth (BACG) 2011 Annual Conference held jointly with the Dutch Association for Crystal Growth (DACG) and in partnership with the British Crystallographic Association (BCA) Industrial Group, London.
http://www.bacg.co.uk/index.php/2011-bacg-conference

10-15 July 2011
9th International Conference on Nitride Semiconductors, Glasgow.
http://www.icns9.org/

16-17 July 2011
Hydrogen-Metal Systems, Easton, MA, USA.
http://www.grc.org/programs.
aspx?year=2011&program=grs_hydrm

17-21 July 2011
ECNS 2011. 5th European Conference on Neutron Scattering, Prague Czech Republic.
http://www.ecns2011.org/joomla_15/

17-22 July 2011
Thin Film and Crystal Growth Mechanisms. Gordon Research Conference, Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2011&program=thinfilm

22-23 July 2011
S&S@ess conference, Prague, Czech Republic.
http://ess-scandinavia.eu/s-and-s

24-29 July 2011
Clusters, Nanocrystals & Nanostructures, South Hadley MA, USA.
http://www.grc.org/programs.aspx?year=2011&program=clusters

31 July - 5 August 2011
18th American Conference on Crystal Growth and Epitaxy in conjunction with the 15th US Biennial Workshop on Organometallic Vapor Phase Epitaxy, Monterey, CA, USA.
http://crystalgrowth.us/accge18/index.php

1-5 August 2011
DXC 2011. 60th Annual Denver X-ray Conference, Denver, CO, USA.
http://www.dxcicdd.com/

1-5 August 2011
THERMEC-2011 - Neutron Scattering & X-Ray Studies of Advanced Materials, Quebec, QC Canada.
http://www.thermec2011.ca/

7-12 August 2011
X-ray Science. Gordon Research Conference, Waterville, ME, USA.
http://www.grc.org/programs.aspx?year=2011&program=xray

22-29 August 2011
IUCr2011. XXII Congress and General Assembly, Madrid, Spain.
http://www.iucr2011madrid.es/

13-16 September 2011
ISIC18. 18th International Symposium on Industrial Crystallization, Zürich, Switzerland.
http://www.isic18.ethz.ch/

25-29 August 2013
28th European Crystallographic Meeting, University of Warwick.
http://www.crystallography.org.uk/

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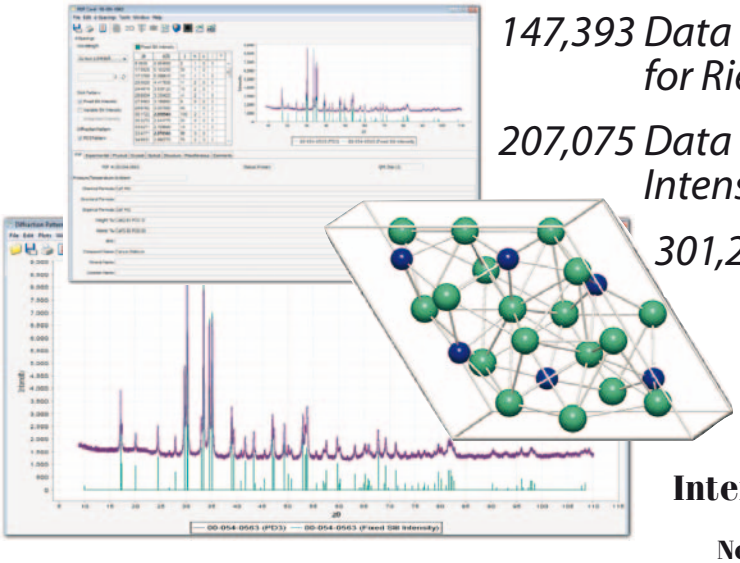

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