Crystallography News

British Crystallographic Association

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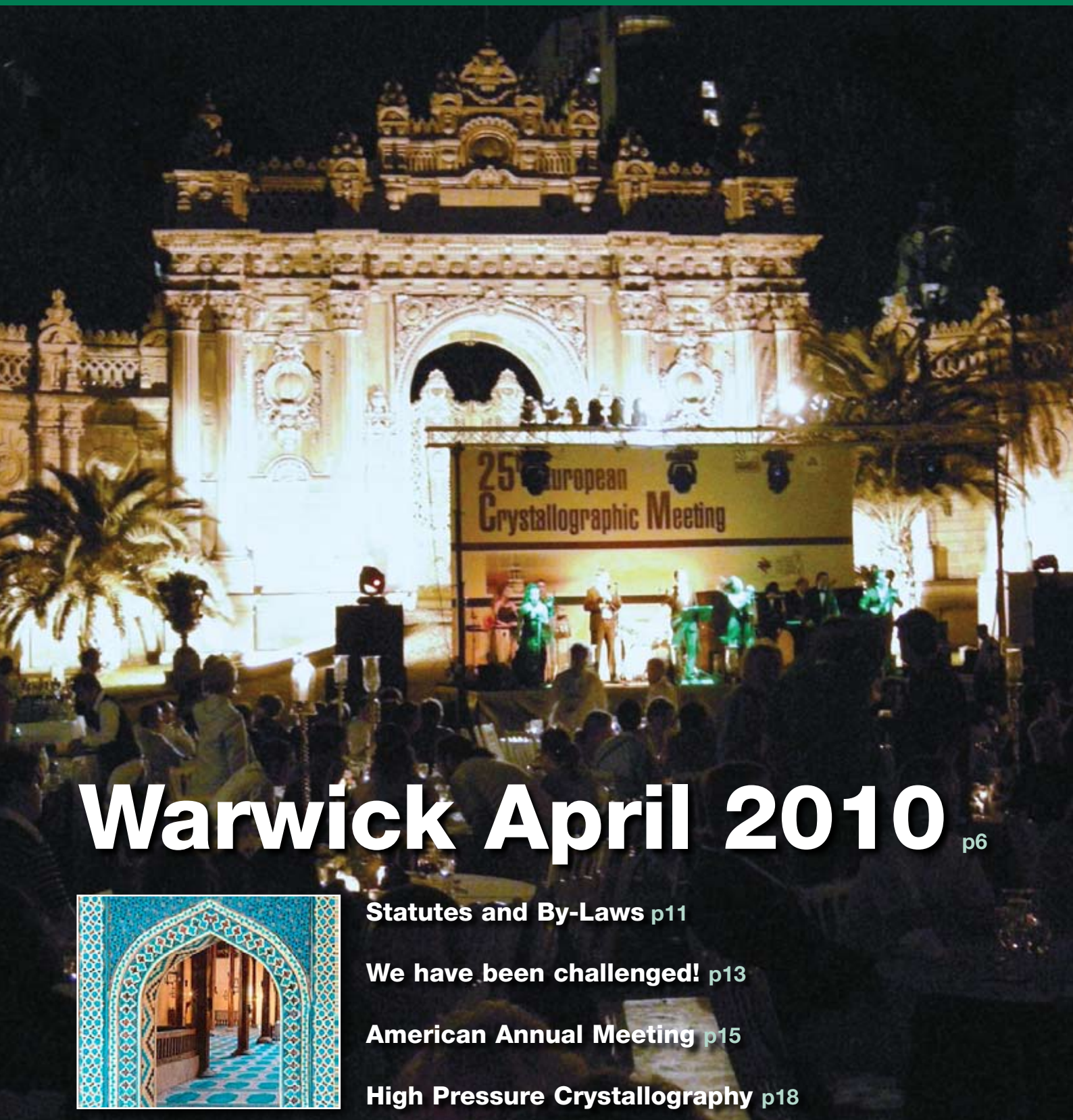

Warwick April 2010 p6

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Crystallography News December 2009

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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 2010 issue are sent to the Editor to arrive before 25th January 2010.

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This month's cover:

Banquet at the Dolmabahce Palace; Beysehir Esrafoglu Mosque

From the Editor

STARTING with the cover, this issue has a strong emphasis on the memorable 25th European Crystallographic Meeting that was recently held in Istanbul. The surprises started with the location. We have grown used to meetings held in university buildings or in convention halls, but this was the first site I have encountered that combined the functions of a conference centre and a military museum. Lectures were held in a grand building that resembled a small palace. To get from there to the exhibition and posters we walked through beautiful gardens along paths lined with rows of cannons facing each other. When it proved difficult to decide between the countries bidding to host the 2013 ECM, there would have been plenty of ordnance available if it had come to a duel! Fortunately, peace prevailed.

The powerful peacemaking ability of crystallography was brought out in a progress report on SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East). When the BESSY-1 synchrotron in Germany was undergoing replacement by its more up-to-date successor, **Herman Winick** and **Guss Voss**, an American and a German, suggested re-installing it in the Middle East. This idea was welcomed by scientists from the Middle East and by the German government. UNESCO supported the project and provided the initial direction, while Jordan provided the site near Amman and the building. Further donations ensured that the facility would not re-create a worn-out old banger but would become state-of-the-art. The injector complex comprises the original 22.5 MeV Microtron and 800 MeV Booster from BESSY-1 with new power supplies, vacuum pumps and control system, but it would feed a new 2.5 GeV Main Storage Ring. The donation of beamlines from Daresbury will enhance the available applications. Although worrying budgetary constraints surfaced in 2008, on July 14, 2009, the refurbished Microtron produced its first beam. In an amazing display of collaboration among scientists from often feuding countries the SESAME Council includes delegates from: Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, the Palestinian Authority and Turkey.

This issue also includes a vivid account of this year's summer school in Erice, Sicily, held in June under the title "High Pressure Crystallography: from Novel Experimental Approaches to Applications in Cutting-Edge Technologies". These courses provide a stimulating combination of intensive science with culture and scenery. Next summer's course, the 42nd, is entitled "Structure and Function from Macromolecular Crystallography: Organisation in Space and Time". It will run from June 3-13, 2010.

Stimulating science can also be enjoyed at our own Group Meetings. Although the Chemical, Industrial, Physical and YC meetings will have already taken place in November, there should still be time to attend the Biological Structures Group Winter Meeting at the Royal Free Hospital, London, on Friday 18th December 2009. The title, "Pathological Proteins", is intended to encompass structural studies of proteins involved in a wide range of disease processes including neurological disorders, amyloid disease, infection and immunity. Our lives may depend on an understanding of these protein structures! Another alluring prospect is the next CPOSS Open Meeting, "Control and Prediction of the Organic Solid State - Characterisation and Computational Modelling of Complex Behaviour", to be held on Monday, 19 April 2010, at University College London. For a while it may have appeared that our ability to predict crystal structures had reached a plateau, but the results of the most recent Blind Test show that dramatic progress has been made. International speakers and a free lunch further enhance the appeal of this meeting.

This issue contains updated information about the BCA Spring Meeting from 13-15 April 2010 and the satellite meeting of the Young Crystallographers just before it. The overarching title "Data Matters" reminds us that the superiority of crystallography as a method for structure determination rests on the excellence of our data. The conference will show us how to collect data faster and better, treat our data well and extract the maximum amount of information.

I remind our readers that the provision to BCA members of an issue of *Crystallography Reviews* covering topics from the Spring Meeting has now ceased. Although this issue gave us a wonderfully lucid resumé of important lectures, the arrangement had the drawback of telling us about lectures that many of us had attended while leaving us in ignorance about the enlightening reviews published in the "non-BCA" issues. Starting from 2010 BCA members can receive a complete set of reviews for the heavily discounted price of £25. Now would be a good time to take out a subscription.

I join Elspeth in offering our congratulations to the three crystallographers who shared this year's Nobel Prize in Chemistry. I got to know laureate **Tom Steitz** when we were both postgraduate students in "Colonel" Lipscomb's laboratory at Harvard. Although Tom was working on macromolecules while I was part of the boron hydride group, it was clear to all of us that Tom was a high-flier. Talk about keeping the Nobel Prize in the family: Prof. Lipscomb won his in 1976 for elucidating the structure and bonding of boron hydrides, and his supervisor Linus Pauling was a laureate in 1954 for his work on DNA. This sequence provides compelling evidence that crystallography is one of the most dynamic fields of science, where Nobel-quality research can be carried out over three scientific generations.

I am aware that recent Puzzle Corners have dealt with words rather than numbers or symmetry, and it is time to redress the balance. To accompany the reports in this issue on the recent ECM-25 in Turkey, I am pleased to welcome **Didem Rodoplu** from Hacettepe University as our guest puzzle-setter. At ECM-25 she delighted us with an eye-catching presentation on symmetry in Seljuk Turkish ornamentation, convincing us that these people had a deep intuitive understanding of symmetry the best part of a millennium ago. Our puzzles are based on this work. Didem also supplied the spectacular cover picture of the Beysehir Esrafoglu Mosque. I also am happy to report that I have already lined up a distinguished puzzle-setter for the March issue.

Carl Schwalbe

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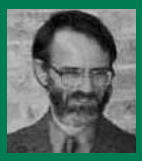

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(The dates in parentheses indicate the end of the term of office).

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,

We are now deep into the new academic year and I hope those of you who teach have an enthusiastic new cohort of students!

The last three months have brought both sad and glad news for the global crystallographic community.

At the Council Meeting in September, we were informed of the death of one of our Members, Professor **John S. Rutherford**. John graduated in Chemistry from Glasgow University, then gained his PhD at McMaster University, Canada, before working as a post-doctoral research fellow at Birkbeck College. He then held increasingly senior academic appointments in Oman, Zimbabwe and South Africa. John was a Member of the IUCr Commission on Mathematical and Theoretical Crystallography and had specific interests in chemical bonding, particularly in solids, and discrete mathematics applications. After retirement he collaborated with colleagues at Southampton University and succeeded in solving some highly complex and difficult crystal structures.

It was with deep shock that we learned of the untimely and sudden passing of Professor **Louis Delbaere** of the University of Saskatchewan who was a very active macromolecular crystallographer and variously served as the Canadian Rep to the ACA from 1999-2001, a member of the ACA Communications Committee from 2003-2006, and as President of the ACA in 2005. He was the current President of the Canadian National Committee for Crystallography, a member of the IUCr Executive Committee, and led the successful Canadian bid to host the 2014 IUCr Congress in Montreal. In the mid 1990s, he was a key figure in establishing the Canadian Macromolecular Crystallography Facility (CMCF) at the Canadian Light Source, the national synchrotron research facility at the University of Saskatchewan. I had the great pleasure of sharing an office with Louis during his sabbatical time in Oxford during 2003, and as we got to know one another, I grew to greatly appreciate both his quiet humour and his calm and wise approach to problems, as well as his broad knowledge of structural biology. He will be sorely missed and we send our sympathy to his family.

On a much happier note, it was very good to learn that Dr **David Watkin**, an Honorary Member of the BCA, has been awarded the 2010 Fankuchen Award by the American Crystallographic Association. David has worked at the University of Oxford's Chemistry Department for many years, and is prominent in the Chemical Crystallography community worldwide. The award recognizes contributions to crystallographic research by one who is known to be an effective teacher of crystallography. The Award will be presented at the Chicago ACA Annual Meeting, to be held from July 24 to the 29th, 2010 at which David will also be delivering a Plenary Lecture. I very much look forward to being present at the ACA to hear it.

Talking of Honorary Members, this is the first time that as President I have had the very enjoyable task of inviting nominations for new Honorary Members of the BCA. Honorary Membership is the highest membership accolade of the BCA, and is awarded to a small number of colleagues who have contributed significantly to crystallography and to the work of the BCA. Last year **Frank Allen** and **David Watkin** became our most recent Honorary Members, taking the total number to 19. In the coming year we anticipate electing one or two new Honorary Members.

Please send your nominations, together with a short supporting case to me at president@crystallography.org.uk by 31st January, 2010. For information, a list of our 19 current Honorary Members is now available at **http://crystallography.org.uk/honorary-members** (thanks to **Richard Cooper** our WWW Master and **Sandy Blake**, our indefatigable Vice-President).

It was also wonderful news to hear of the award of the 2009 Nobel Prize for Chemistry to **Venki Ramakrishnan** (MRC-LMB, Cambridge), **Tom Steitz** (Yale University, U.S.A.) and **Ada Yonath** (Weizmann Institute, Israel) for their work towards solving the structure of the ribosome. Those of you who heard Venki's inspiring Plenary lecture entitled "Induced Fit: a Common Strategy Used by the Ribosome in Decoding, Peptdiyl Transferase and Termination" at the BCA SM 2009 will appreciate and laud the crystallographic tour de force of this achievement. Many congratulations to all three Laureates!

The 2010 Warwick Spring Meeting planning is now well advanced, and details can be found later in this issue. I encourage all members to bring as many of their group as is feasible to the meeting, since it promises to deliver some interesting and enlightening science. The Young Crystallographers will again hold their pre-meeting event on Monday 12th April and the morning of Tuesday 13th, with their last lecture being the first lecture of the full Spring Meeting. The BCA is very grateful to the EPSRC for funding the YCs event to the tune of £2,000. Talking of funding, the BCA was also pleased to receive over £800 from **Graham Bushnell-Wye** (STFC), who very kindly arranged the transfer of residual funds from the European Synchrotron Radiation Society (ESRS). After discussions with Graham representing the ESRS, these funds have been earmarked to assist young scientists who are going to present work carried out at synchrotrons at a European event (e.g., at an ECM or at the IUCr meeting in Madrid in 2011).

Despite concerted efforts from a number of quarters, the issue of bouncing BCA e-mails has not yet gone below the horizon. We have now tracked down all but 30 or so members whose e-mail addresses bounce the general BCA circulars. I would be grateful if Members would check the "Emails from the BCA" section of the website (URL: **http://crystallography.org.uk/emails**) and tell us

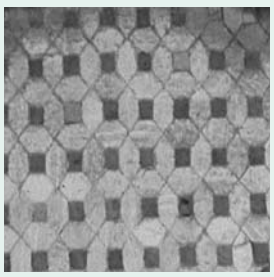
their current email address (e-mail it to president@crystallography.org.uk) if they are not receiving these emails. There is also still a pressing necessity to update the Group e-mail listings, and this is currently being addressed. I am particularly grateful to the Chair of our biggest group, **Andrew Bond**, who has taken on pushing this forward for the CCG, in conjunction with Northern Networking.

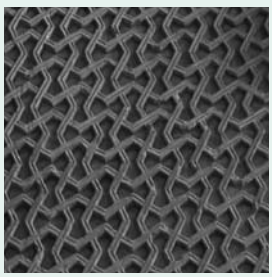
Lastly, the option to make payment of Membership dues for 2010 onwards by Direct Debit has now been set up, and it would be a big step forward in simplifying the administration of the Association if as many as possible of you would avail yourselves of this. The option to pay by Standing Order is no longer available, and those of you who pay by this method will have to make alternative arrangements. By the time you read this, I will have had the pleasure of attending 3 out of 4 of the day autumn Group meetings where I will have mentioned this issue. Apologies to the Industrial/YC Groups that I could not get to St. Helen's on November 5th due to undergraduate lecturing commitments!

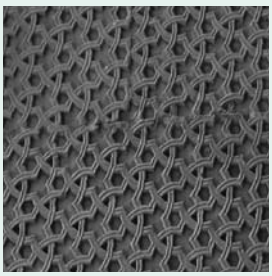
Wishing you all a Merry Christmas and Happy 2010

Puzzle Corner

COMPLEMENTING our coverage of ECM-25 in Istanbul, this month's puzzle has been contributed by **Didem Rodoplu**. What is the symmetry of each of the following three examples, provided from the Art History Department of Hacettepe University, of 13th or 14th century Seljuk Turkish stone ornamentations?







Ref. 1: Y. Özbek, Osmanlı Beylişi Mimarisinde Taş Süsleme (1300- 1453), Ankara 2002
Ref. 2-3: N.Ş. Doǵan-E. Bilget Arşivi

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BCA AGM 2010

Scientific Programme: Data Matters

PLENARY LECTURES

THIS meeting is packed with Plenary, Named and Prize lectures, with the inaugural Parkin Lecture as the YCG plenary and link from the satellite to the main meeting. Some details of session lectures are not available at the time of writing, but a full programme will be published on the meeting website (http://crystallography.org.uk/bca-spring-meeting-2010) by the time you are reading this article!

Hodgkin Lecture (BSG): Prof **Dame Louise Johnson** FRS (University of Oxford) *'Forty years of structural biology: where have we come from and where might we be going?'*

Bragg Lecture (CCG): Prof **Sir John Meurig Thomas** FRS (University of Cambridge) *'The essence and promise of 4D electron microscopy'*

Teaching Plenary (IG): Prof **Simon Billinge** (Columbia University) *'Title: to be confirmed'*

Physical Crystallography Group: Dr **Lynne McCusker** (ETH Zürich) *'Polycrystalline materials, powder diffraction, electron microscopy and charge flipping - a remarkable brew'*

Parkin Lecture (YCG): Prof **Simon Parsons** (University of Edinburgh) *'Phase Transformations in Simple Molecular Solids'*

Alun Bowen Lecture (IG): Dr **David Taylor** *'Title: to be confirmed'*

Additionally the PCG Thesis Prize, the CCG CCDC Young Scientist Prize and the Young Crystallographers Industrial Group Prize Lecture will all be announced and presented at the meeting.

SESSION LECTURES

At the time of writing invited and confirmed contributed talks, with titles where available, will be given by the following speakers:

Data; what goes in (IG)

Chair: **Matthew Johnson**
Ross Harrington (University of Newcastle) *'Traps and Pitfalls in Single Crystal Diffraction (and how to avoid them!)'*
Sarah Barnett (Diamond Light Source) *'Rough Guide to Synchrotron Diffraction'*
Contributed Talk: TBC

Data; what comes out (IG)

Chairs: **Brett Cooper** & **Cheryl Doherty**
Trevor Rayment (Diamond Light Source) *'Food, formulation, foams, and fabrication - modern applications of Synchrotron Radiation for industry'*
Klimentina Pencheva (Pfizer) *'Crystal surface modelling of pharmaceutical compounds'*
Young Crystallographer Prize Presentation: To be announced at the meeting

Complementary non ambient techniques (IG)

Chair: **David Beveridge**
Tim Hyde (Johnson Matthey) *'Catalyst Studies using Complementary and Non-Ambient Techniques at Johnson Matthey'*
Lynn Gladden (Cambridge University) *Title: TBC*
Simon Watson (GSK) *'Running Hot and Cold: understanding crystal structure phenomena with variable temperature Solid-State NMR'*

Unpublished Data and Almighty Blunders (CCG / IG)

Chairs: **Luca Russo** & **Richard Morris**
William Clegg (University of Newcastle) *'To publish or not to publish'*
Simon Coles (University of Southampton) *'eCrystals: Management and publication of small molecule data'*
Contributed Talk: TBC

Electron diffraction (PCG)

Chair: **Kirsten Christensen**
Chris Gilmore (University of Glasgow) *'The electron crystallography of zeolites'*
Sven Hovmöller (Stockholm University) *'Single Crystal Diffraction from powders using electrons'*
Wuzong Zhou (University of St. Andrews) *'Electron Diffraction of Some Beam Sensitive Materials'*

Resonant X-ray diffraction (PCG)

Chair: **Peter Hatton**
Invited Talk: TBC
Invited Talk: TBC
Contributed Talk: TBC

New approaches to structure solution (PCG)

Chair: **David Keen**
Sarah Lister (Durham University) *'The use of complementary techniques in structure solution from powders'*

Maryjane Tremayne (University of Birmingham) *'Title: to be confirmed'*
Paul Midgley (Department of Materials Science and Metallurgy, University of Cambridge) *'Towards Routine Structure Solution using Precession Electron Diffraction'*

PDF: Local Structure (PCG)

Chair: **Matt Tucker**
Joseph Hriljac (University of Birmingham) *'PDF studies of the pressure-induced amorphisation of zeolites'*
Daniel P. Shoemaker *(University of California) 'Local structure and the search for polar ordering in geometrically frustrated oxides'*
Samantha Chong (University of Liverpool) *'Investigating disorder in a pure bismuth A site perovskite using total scattering and RMC modeling'*

Structure and Property Prediction (CCG)

Chair: **Stephen Moggach**
Graeme Day (University of Cambridge) *'Lattice Energy Landscapes for Predicting Crystal Structures and Anticipating Solvate Formation'*
Caroline Mellot-Draznieks (UCL) *'Title: to be confirmed'*
Peter Galek *(CCDC) 'Truly Prospective H-bond Predictions: Linking Free Energy and Structural Stability'*

Databases & Data Mining (CCG)

Chair: **Hazel Sparkes**
Peter Wood (CCDC) *'Hydrogen Bonds: Energy Matters Too'*
Anna Stevenson (University of Bath) *'Knowledge Mining Studies on Gas Storage Materials using the CSD.'*
Gordon Barr (University of Glasgow) *'Data mining & data visualisation using cluster analysis and related technique'*

Data & Structure Validation (CCG)

Chair: **Ross Harrington**
Tony Linden (University of Zurich) *'Structure validation: automation versus vigilance'*
Ian Bruno (CCDC) *'From deposition to application: use of the CSD for crystal structure validation'*
Roy Copley (GSK) *'Structure validation: an industrial perspective'*

Dealing with Difficult Data (CCG)

Chair: **David Watkin**
Matthias Meyer (Oxford Diffraction) *'Optimal Data Collection Strategies for Area Detector Diffractometers'*
Aire Van der Lee (Université de Montpellier II) *'Charge Flipping versus Direct Methods: Tips and Tricks'*
Christopher Serpell - Oxford University *'Refinement of large supramolecular structures'*

High Throughput Membrane Proteins (BSG)

Chair: **Steve Prince**
Liz Carpenter (SGC) *'Title: to be confirmed'*
Jon Haddon (Heptares) *'Title: to be confirmed'*
Contributed Talk: TBC

High Throughput & Screening (BSG)

Chair: **Bill Hunter**
Graeme Winter (Diamond Light Source) *'Automated MX at Diamond'*
Robbie Joosten (Netherlands Cancer Institute) *'PDB_REDO: an automated re-refinement method to keep the PDB up-to-date'*
Gerard Kleywegt (EBI, Hinxton) *'Model validation'*

Data Management (BSG)

Chair: **Keith Wilson**
Rob Esnouf (Oxford) *'Title: to be confirmed'*
Invited Talk: TBC
Contributed Talk: TBC

Dynamics (BSG)

Chair: **Mark Sansom**
Adrian Mulholland (University of Bristol) *'Title: to be confirmed'*
Phil Fowler (University of Oxford) *'Extracting more information from the structure: computer simulations of membrane proteins'*
Contributed Talk: TBC

Hot Structures (BSG)

Chair: **Steve Smerdon**
Chris Oubridge (LMB, Cambridge) *'Structure determination of human spliceosomal U1 snRNP'*
Dale Wigley (CRUK) *'Title: to be confirmed'*
Leo Sazanov (MRC-MBU) *'The architecture of bacterial respiratory complex I'*

Membrane Structures (BSG)

Chair: **Liz Carpenter**
Simon Newstead (Imperial College) *'Recent progress on the crystal structure of a new family of membrane transport proteins'*
Bonnie Wallace (Birkbeck College London) *'Structure and Function of Voltage-Gated Sodium Channels'*
Gebhard F. X. Schertler (Paul Scherrer Institute Switzerland) *'Structural insights into G Protein Coupled Receptor activation'*

New Techniques (BSG)

Chair: **Robin Owen**
Invited Talk: TBC
Invited Talk: TBC
Contributed Talk: TBC

As usual there will be an Exhibitors Forum (*Chair:* **Elspeth Garman**) and this year there will be a Software Fayre running throughout the meeting. The latter will be organised by **Horst Puschmann** and **Simon Coles** – please register your interest (email **s.j.coles@soton.ac.uk** or **horst.puschmann@durham.ac.uk** by Jan 18th 2010) if you would like to demonstrate software, conduct a problem-solving session or run a drop-in session. The Fayre will be aimed at small groups and a timetable will be published in advance of the meeting via the March edition of Crystallography News and the conference website.

	Mon April 12th	Tuesday April 13th			
9:00		LT3			
9:15		YC 4			
9:30					
9:45					
10:00			Registration/Exhibition 10:00-11:30		
10:15					
10:30		LT3 Parkin Lecture: Simon Parsons			
10:45					
11:00					
11:15					
11:30		LT3 Hodgkin Lecture: Prof. Dame Louise Johnson FRS Chair: Elspeth Garman			
11:45					
12:00					
12:15					
12:30		Lunch/Registratio/Exhibition 12.30-13.30			
12:45					
13:00	PLT				
13:15	YC 1				
13:30		Sessions 13.30-15.00			B207
13:45		LT4	LT5	PLT	
14:00		Resonant X-ray Diffraction PCG	Structure & Property Prediction CCG	New Techniques BSG/YCG	ICDD Workshop IG
14:15					
14:30					
14:45					
15:00	Coffee 15.00-15.30	Coffee 15.00-15.30			
15:15					
15:30	PLT	Sessions 15.30-17.00			B207
15:45	YC 2	LT 1	LT2	LT3	
16:00		New Approaches to Structure Solution PCG	High Throughput 1 BSG	Alun Bowen Lecture David Taylor IG	ICDD Workshop IG
16:15					
16:30					
16:45					
17:00	Break	Break			
17:15	PLT	LT3			
17:30	YC 3	Exhibitors Forum 17.15-18.45 Chair: Elspeth Garman			
17:45					
18:00					
18:15					
18:30					
18:45	YC Dinner	Dinner, Exhibition and Posters			
19:00					
19:15					
19:30					
19:45					
20:00					
20:15					
20:30					
20:45					
21:00					

<table>
<tr><th colspan="3">Wednesday April 14th</th><th colspan="3">Thursday April 15th</th></tr>
<tr><td colspan="3">LT3
PCG Plenary: Dr Lynne McCusker
Chair: David Keen</td><td colspan="3">LT3
IG Teaching Plenary: Prof. Simon Billinge
Chair: Matt Johnson</td></tr>
<tr><td colspan="3">Coffee 9.45-10.15</td><td colspan="3">Coffee 9.45-10.15</td></tr>
<tr><td colspan="3">Sessions 10.15-11.45</td><td colspan="3">Sessions 10.15-11.45</td></tr>
<tr><td>LT4</td><td>LT5</td><td>PLT</td><td>LT4</td><td>LT5</td><td>PLT</td></tr>
<tr><td>Dealing with Difficult Data
CCG</td><td>Dynamics
BSG</td><td>Electron Diffraction
PCG</td><td>Complementary & non-ambient techniques
IG</td><td>High Throughput 2
BSG</td><td>Data & Structure validation
CCG</td></tr>
<tr><td>IG AGM
11.45-12:30</td><td>BSG AGM
11.45-12.30</td><td>PCG AGM
11.45-12.30</td><td colspan="3">Break</td></tr>
<tr><td colspan="3" rowspan="2"></td><td colspan="3">Sessions 12.00-13.30</td></tr>
<tr><td>LT4</td><td>LT5</td><td>PLT</td></tr>
<tr><td colspan="2" rowspan="2">Lunch, Exhibition 11.45-13.30
12.30-1.30</td><td rowspan="2">CCG AGM
12.30-1.15
LT1</td><td rowspan="2">PDF: Local Structure
PCG</td><td rowspan="2">Hot Structures
BSG</td><td rowspan="2">Unpublished Data & Almighty Blunders
CCG/IG</td></tr>
<tr><td colspan="3"></td></tr>
<tr><td colspan="3">Sessions 13.30-15.00</td><td colspan="3">Close 13.30</td></tr>
<tr><td>LT4</td><td>LT5</td><td>PLT</td><td>Location TBA</td><td colspan="2" rowspan="15"></td></tr>
<tr><td>PCG Prize
Chair D. Keen</td><td rowspan="2">Data; what goes in
IG</td><td rowspan="2">Membrane Structures
BSG</td><td rowspan="14">PDF Workshop</td></tr>
<tr><td>CCDC Prize
Chair A. Bond</td></tr>
<tr><td colspan="3">Coffee 15.00-15.30</td></tr>
<tr><td colspan="3">Sessions 15.30-17.00</td></tr>
<tr><td>LT4</td><td>LT5</td><td>PLT</td></tr>
<tr><td rowspan="2">Databases & Data Mining
CCG</td><td rowspan="2">Data Management
BSG</td><td>Data; what comes out</td></tr>
<tr><td>YC Prize
IG Sponsored</td></tr>
<tr><td colspan="3">Break</td></tr>
<tr><td colspan="3">LT3
Bragg Lecture: Prof. Sir John Meurig Thomas FRS
Chair: Elspeth Garman</td></tr>
<tr><td colspan="3">LT3</td></tr>
<tr><td colspan="3">BCA AGM 18.00-19.00</td></tr>
<tr><td colspan="3">Comfort Time</td></tr>
<tr><td colspan="3">Conference Dinner 19.30 for 20.00</td></tr>
</table>

Posters are always an important and vibrant aspect of any Spring Meeting and we want this year to be no exception! Abstracts should be submitted through the meeting website (http://crystallography.org.uk/bca-spring-meeting-2010) on the template format available there – it should be noted that, due to the poster boards that will be available, dimensions are to be landscape 1m x 2m.

WORKSHOPS AND SATELLITES

THERE will be an ICDD Workshop (*Chairs:* Cyrus Crowder & Timothy Fawcett) during the conference.

After the meeting **Matt Tucker** will chair a Workshop on data correction for PDF (Pair Distribution Function) and total scattering analysis. This workshop will follow on from the PDF and Reverse Monte Carlo analysis workshop held before the 2007 BCA spring meeting. The aim will be to enable people to produce data suitable for the analysis tools demonstrated in the last workshop. If you would like to attend this workshop or would like further information please email the organizer, Matt Tucker (**matt.tucker@stfc.ac.uk**), so the level of interest can be gauged.

CCDC will host a "Cambridge Structural Database Discussion Forum" at the end of the Meeting. The session will provide an opportunity for expert and non-expert CSD users to share problems and solutions. The aim is to enable users to get the maximum benefit from their use of the CSD. Attendees will be encouraged to identify problems or limitations they have found in their use of CSD, from depositing data, through data content of CSD entries, to getting what they want when searching. CCDC editorial staff, software developers and research and applications scientists will be on hand, but discussions between users as well as CCDC staff will be encouraged so we can all learn from each other. The session will take place at 1.30 p.m. on Thursday 15th April and last a maximum of 2 hours. Refreshments will be provided and there is no charge for attendance.

We look forward to seeing you all in Warwick!

On behalf of the Programme Committee,

Simon Coles (Chair)

Young Crystallographers 2010

FOLLOWING the tradition of the previous years the Young Crystallographers Satellite Meeting (YC2010) is going to precede the next BCA Spring Meeting. These gatherings of Young Crystallographers are a fantastic opportunity to present and discuss your work in a friendly and relaxed environment. Of course, more senior crystallographers are also welcome in the audience, provided difficult questions are kept at bay. A special highlight this time is the establishment of the Parkin Lecture, which will be linking the YC2010 and the main meeting.

The YC2010 will take place in the afternoon of 12th April and in the morning of 13th April 2010 at the University of Warwick. In good old fashion there will be three sessions of oral presentations and a poster session on Monday evening together with a buffet dinner and drinks. Accommodation, dinner and registration for the YC2010 will be free for those who have registered for the whole Spring Meeting (if you haven't done so, then see the BCA website **http://www.crystallography.org.uk** for further details). If you only want to attend the YC2010 and not the main meeting then you are welcome to do so, but a fee of £67 will be charged. There are a limited number of bursaries available for people presenting a poster or talk and applications have to be made online on the BCA webpage.

So submit your abstracts now! Deadline for abstracts to be considered for oral presentations is 15th January 2010 and deadline for poster abstracts is 2nd February 2010. Submission should be made through the main meeting abstract submission webpage using the template available there.

The preliminary programme is as follows and once all speakers are confirmed the full programme will be available on the YCG website (**http://yc.crystallography.org.uk/**).

YC1 PLENARY (CHEMICAL)

Stephen Moggach (University of Edinburgh) – *"Putting the Squeeze on Porous Materials"*

YC2 PLENARY (PHYSICAL)

Andrew Goodwin (University of Cambridge) – "*The atom's perspective: crystallography in real-space"*

YC3

AGM
1 minute poster flash presentations
Poster Session with dinner and wine

YC4 PLENARY (BIOLOGICAL)

Elspeth Garman (University of Oxford) – *"From hot to cool and more for less: New developments for structural biology"*

FOUNDATION PARKIN LECTURE

Simon Parsons (University of Edinburgh) – *"Phase Transformations in Simple Molecular Solids"*

Furthermore elections will be held at the AGM in order to fill YCG Committee vacancies, which include the officer positions. For more details on how to become a committee member have a look on the YCG website.

See you all in Warwick!

Susanne Coles (née Huth), YCG Chair

Statutes and By-Laws

FROM THE VICE PRESIDENT

Proposals for Changes to the BCA Statutes and By-Laws

THE current BCA Statutes and By-Laws are on the Web at http://crystallography.org.uk/statutes. If you are unable to access these please contact the Vice President – see page 3.

1. Changes to Statutes

Note: Any amendment to the Statutes requires a quorum of thirty and the affirmative vote of at least two-thirds of those present and entitled to vote.

Proposal 1. Amend Statute B (Membership)
The purpose of this group of amendments is (a) to formally recognise the category of "*Student Member*"; (b) to acknowledge the change in the name of the Physical Crystallography Group within the Institute of Physics; (c) to replace the upper limit on the number of Honorary Members with a limit on the number of people who may be accorded this status in any one calendar year.

Amend Statute B as follows:
(a) Add B.2(f): "*Student Members*".
Add a new Statute B.8 (Student Members):
"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."

(b) In B4 change "Physical Crystallography Group of the Institute of Physics [hereinafter referred to as the Joint Group], on whose behalf the Group pays an annual subvention fixed by the Council."
to "Structural Condensed Matter Physics Group of the Institute of Physics [hereinafter referred to as the Joint Group and identified within the Association by the name Physical Crystallography Group]."

(c) The former Statute B.8 (Honorary Members):
"*Honorary Members*: the Officers of the Association shall from time to time recommend the name(s) of person(s) deserving of Honorary Membership of the Association, and such recommendations must be ratified by Council. The number of Honorary Members shall normally be limited to twenty persons at any one time. Honorary Members shall be absolved from paying annual subscriptions but in all other contexts the expression Ordinary Members shall include Honorary Members."
is renumbered as Statute B.7 and will read:
"*Honorary Members*. The Officers of the Association shall from time to time recommend the name(s) of person(s) deserving of Honorary Membership of the Association; such recommendations must be ratified by Council. Honorary Membership shall normally be accorded to a maximum of two persons in any one calendar year. Honorary Members shall be absolved from paying annual subscriptions but in all other contexts the expression Ordinary Members shall include Honorary Members."

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."

2. 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 proposed amendment to By-Law E.2 is:

"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 ~~two~~ **four** days before the Annual General Meeting."

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

1. ~~The Physical Crystallography Group of the Institute of Physics is to be regarded as a Joint Group of the Association and the other organisation [Statute B.4]. Similar Joint Groups may be set up by the Association~~

~~with other organisations, but will not confer Joint Membership of the Association.~~ The Structural Condensed Matter Physics Group of the Institute of Physics is to be regarded as a Joint Group of the Association (under the name Physical Crystallography Group) and of the other organisation [Statute B.4]. Similar Joint Groups may be set up by the Association with other organisations, but membership of the other organisation will not confer Joint Membership of the Association.

2. Ordinary Members of the Association have the right to become members of ~~one Joint Group or other~~ 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.
3. The Council shall determine what additional subscription, if any, shall be paid by ~~an Ordinary or Joint Member~~ **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.**

Proposal 5. Changes to By-Laws G (Groups and Joint Group) and I (Financial Arrangements with Joint Groups under Statute B.4):

(a) I propose 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."

(b) I believe that, over time, By-Laws I.4 and I.5 have become wrongly placed and I propose moving these to appear under By-Law G as G.4 and G.5, thereby referring to all Groups. By-Laws I.4 and I.5 read:

4. 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.
5. Each Group shall submit an annual financial statement to the Treasurer of the Association, giving details of its income and expenditure during the year.

Proposal 6. Minor change to the wording of By-Law H (Reduced Subscriptions)
This proposal is 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 ~~no longer~~ **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.

Proposal 7.
All text from "Version 5, 26 April 2000" onwards shall be removed.

These amendments, if accepted by the AGM, will take effect immediately and the revised Statutes and By-Laws will appear on the BCA website within seven days.

Sandy Blake
Vice President
25 October 2009

Reminder about Crystallography Reviews for BCA Members

BCA members will no longer receive the special "BCA Issue" of Crystallography Reviews by default; however there is no need to miss out! We are pleased to announce that members will now be entitled to the entire volume (Issues 1-4) of Crystallography Reviews for just £25 by taking up the new special and greatly reduced 'Members' Subscription' rate. Please go to www.tandf.co.uk/journals/gcry and click on News & Offers for more details.

The Editors of Crystallography Reviews would like to commend the BCA for its excellent Annual Conference programs and remain committed to publishing reviews arising from these. We hope that many BCA members take up this new arrangement and we look forward to serving the crystallography community further with our review journal.

John R. Helliwell & **Moreton Moore**
(Editors of Crystallography Reviews)

We have been challenged!

FOLLOWING consultation with the academic community and its Strategic Advisory Teams, EPSRC is highlighting four new Grand Challenges in chemical sciences and engineering.

The Grand Challenges are:

- Utilising CO_2 in Synthesis and Transforming the Chemicals Industry
- 'Dial-a-Molecule' - 100% Efficient Synthesis
- **Directed Assembly of Extended Structures with Targeted Properties**
- Systems Chemistry: Exploring the Chemical Roots of Biological Organisation

Grand Challenges are defined as significant problems that need a long-term, coordinated approach from researchers to overcome. They serve as a mechanism being used by EPSRC in a number of different research areas.

Fresh from his success in keeping the extended structure of the BCA orderly and solvent, and its properties targeted, our own **Paul Raithby** has been designated team leader for the third of these challenges. The teams responsible for championing each of these areas are now putting together network proposals to build communities of researchers around each challenge. These networks will set the research agenda, develop new research strategies and address the societal and economic impact of the Grand Challenge. If you wish to become involved in or kept informed of the progress of the third network please contact Paul (p.r.raithby@bath.ac.uk). The statement describing the definition and impact of this Grand Challenge follows:

The aim of this 'grand challenge' is to be able to control the assembly of matter with sufficient certainty and precision to allow preparation of materials and molecular assemblies with far more sophisticated and tunable properties and functions than are accessible in materials synthesised using current methods.

Vision: Our control over the assembly of atoms into molecules and materials, and the controlled assembly of molecules into both solid-state and solution aggregates, remains very limited in scope, setting limits on the ability of chemists and materials scientists to design materials with desired properties even in cases where the underlying material requirements for a particular property are understood. Control of covalent bond formation in conventional synthesis of molecules with strong bonds is good and remarkably complex molecules can be prepared with confidence in multi-step (and increasingly in single-pot) syntheses. In contrast, much more limited control is possible in the preparation of solid-state materials, by chemical vapour deposition techniques for infinite structures, crystal engineering (employing non-covalent intermolecular interactions and utilising molecules as the basic building blocks) for molecular solids, or solution-phase assembly of molecular components using non-covalent interactions. Covalent bond formation in small molecules can be seen as the first step in an exploration of chemical assembly that now needs to be extended, by the incorporation of the use of molecular synthons and non-covalent interactions, to drive the assembly of more complex systems with the same degree of certainty and control that is already achievable for molecular synthesis. By achieving this goal, biological levels of complexity and function could be imposed on artificial materials.

Essentially, this Grand Challenge can be split into two parts: (1) The ability to "design" a material, which may be a solid, a liquid, a gel or a non-Newtonian fluid, with a desired function; this implies a thorough understanding of structure/property relationships in molecules, materials and multi-component assemblies. (2) The ability to "engineer" that material, which implies control over the assembly of matter on scales ranging from molecular, through meso, micro, macro to manufacturing and market-scale and mastery of all of the strong and weak forces that are involved in chemical processes across all the length scales. This, it can be argued, is really the ultimate 'Chemical Grand Challenge' which eclipses all others: the goal is to establish complete control over the preparation, properties and functions of condensed matter over the complete range of length scales. Achieving all of this within the timescale of a few decades is very unlikely, but substantial progress is realistic and will underpin developments across all of chemistry as well as related sciences. This Grand Challenge is essential to permit other Grand Challenge activities requiring specific functions from currently unidentified or inaccessible materials to succeed. Such progress does, however, require a paradigm shift in our approach to materials design and synthesis. In realising this Grand Challenge we must move beyond synthetic approaches to single molecule design (traditional synthesis), and beyond recently attempted Combinatorial methods, which have shown much success but have also emphasised the complexity of the molecular phase space that is accessible in synthetic chemistry, to a fully rational and sophisticated "one-pot" methodology in which the complex sets of reactions being carried out in that pot are understood, designed and controlled. This way lies the next generation of chemical synthesis.

State of the Art: Many useful functions of matter are associated with molecular properties (e.g. pharmaceuticals; many homogeneous catalysts; single-molecule magnets; fluorescent markers, labels and sensors; liquid crystalline and polymeric materials, electron donors or acceptors… etc.), and such functions are accessible using incremental advances based on the current state of the art. However, more sophisticated functions are often based on assemblies

containing many types of molecular component. These assemblies, and the associated rich variety of controllable properties are common in biological systems, but in general are currently synthetically inaccessible. In contrast, many useful functions arise from bulk electronic, magnetic, ferroelectric, mechanical and thermophysical properties of solid assemblies, but capability is limited by the extent to which assembly of the solid materials can be controlled, particularly in the creation of anisotropic structures. Currently it is not even possible to control reliably polymorphism in simple molecular crystals. Looking at naturally occurring systems, a good illustration is the photosynthetic reaction centre, in which a large number of molecular components are combined in a spatially precise array that permits correct interfacing of their individual properties, so that light can be converted into an electrical potential. Synthesis of this complexity is completely beyond our current abilities. In like vein, complex bulk properties based on multi-component (>2) systems, such as photoactivated ferromagnetic ferroelectrics for information storage and room-temperature superconductivity, are currently inaccessible.

Research Challenges and Barriers to Progress: Addressing this Chemical Grand Challenge will require the following capabilities:

1. 'Reverse engineer' a target from its desired function, so that the function can be used as a starting point for defining the components that need to be included and how they should be combined. This could be a catalyst assembled from a mixture of molecular components which between them will recognise a substrate, absorb light, and trigger the photoinduced decomposition or conversion of the substrate.
2. The prediction of the outcome of a combination of weak, non-covalent interactions acting together. Currently genuine control of self-assembly in solution and the solid state is limited to simple one-or two-component systems that assemble through relatively strong, directional and predictable interactions. Extension of this to controlling the outcome of a large number of weak interactions will require a much more detailed understanding of, and computational models for, a wide range of weak interactions (dispersion, hydrophobic, π-π interactions, etc).
3. Many functional assemblies of the forms described above are not in a thermodynamic minimum or at equilibrium. It will be necessary to control the course of an assembly process such that it can be pushed into a desired local minimum, so that we can select one end state from a multiplicity of accessible structures. It may also be necessary to maintain a non-equilibrium state by introducing an external potential, thereby introducing a "metabolic" component to a process. One example is to control crystallisation of a polar molecule such that it forms a polar crystal with 2nd order NLO properties, rather than the more thermodynamically stable non-polar crystal in which neighbouring molecules alternate in orientation, leading to the cancellation of the NLO effect. In solution the equivalent would be to directly assemble the components in a virtual combinatorial library along one kinetically desired pathway. This is currently challenging for an assembly based on one or two molecular components: it is beyond our reach in more elaborate assemblies. It could be achieved by
   (i) Pre-programming the reagents with sufficient information to self-assemble reliably (these processes should be reversible to allow error-correction, which means extending reversible bond formation to as many bond types as possible). This amounts to control of assembly via final structural stability and can be enabled by informatics approaches to build on existing knowledge.
   (ii) Intercepting the assembly process at the critical stage ("nucleation" of the complex structure) with directing action, e.g. light, temperature, chemical potential changes, or the delivery of reactive species.
   The ability to achieve goal (3) successfully and reliably will necessitate the development of new fast, time-resolved spectroscopic and analytical techniques that allow real-time monitoring of all stages of an assembly process, from the first combination of two components to the finished product, at all stages of a process from laboratory to plant. This will allow intervention in an assembly process at a particular point to push it in the desired direction. New modelling techniques and the development of new theories to control and analyse the equilibrium and dynamical properties of the systems are also essential.
4. We will need to be able to control the combination of functions of components as well as their assembly. For example, combination of molecules displaying the properties of a 'molecular wire', a 'molecular switch' and a 'molecular motor' (all known individually) will be of no use unless their functions are also correctly combined and interfaced: the switch must switch on/off electron flow through the wire, which in turn will activate or deactivate the motor. Again inspiration comes from biological systems. Furthermore, it will be necessary to not only control and monitor the chemical state but also the temporal and spatial state of the material at all stages of a process from laboratory to plant.

Involvement: This is a wide ranging multidisciplinary challenge that will involve chemists, chemical engineers, material scientists, systems engineers, computer scientists, physicists and, potentially, life scientists. Because of the breadth of the project and its many potential applications to modern industry, we would anticipate that industrialists will become involved at an early stage and play a significant role in the development, progress and implementation of this Grand Challenge for the next 20-40 years as the socioeconomic impact is realised.

Since the appearance of the Call for the Networks a proposal has been assembled with the help of about 100 active researchers from across the scientific disciplines, both in academia and industry (Many of whom are BCA members) and, at the time of writing the Grand Challenge Network proposal has been submitted. Paul expects to hear whether or not the bid has been successful by mid-November. If the Network goes ahead further information on it and ways to participate will be available early in 2010. It is hoped to hold the first meeting as part of the "Control and Prediction of the Organic Solid State (CPOSS)" Meeting to be held at UCL in April, 2010.

Annual Meeting of the American Crystallographic Association, July 2009

THE 2009 meeting was held in the hospitable and exciting city of Toronto. Spectacular views from the CN Tower, still the world's tallest free-standing tower, as well as baseball games that can never be rained out in a stadium with a retractable roof, fascinating exhibits at the Royal Ontario Museum and luminous paintings of Canadian scenery by the Group of Seven artists complemented a very stimulating meeting. The conference name badge had a clever design feature. Participants' names were printed on adjacent pieces of card stock. When folded over and inserted into the badge-holder, they ensured that one's name could be read whichever way the badge was facing. It must be an exception to the laws of probability; but it seems to me that when wearing a conference badge printed on one side only, I display the blank side to the world about 2/3 of the time. If the YC's can confirm this doesn't happen to them, perhaps it is a consequence of middle-age spread.

The centerpiece of any ACA meeting is the Transactions Symposium, which this year dealt with the topic of Phase Transitions. In the key role of giving the first lecture of the symposium was our own **Simon Parsons**. After describing the design of a diamond anvil cell that can apply pressure up to 10 GPa, Simon presented results obtained with the cell. At ambient pressure crystalline serine has N-H…O hydrogen bonds about 2.9 Å in length. It was thought that extreme pressure might squeeze these contacts to super-short values. Indeed, at 4.8 GPa the distance is reduced to 2.69 Å, at the short end of the distribution found for such hydrogen bonds in the CSD. However, above 5 GPa a phase transition occurs, filling voids and allowing the N-H…O distance to revert to 2.85 Å. Salicylaldoxime also exhibits a phase transition near the "magic" 5 GPa. However, calculations with Gavezzotti's PIXEL method show components of the interaction energy falling on different parts of the energy versus volume curve in these two compounds.

The next talk changed our entire view of protein crystallography. **Chae Un Kim** pointed out that many protein crystals contain >50 % water. Therefore it is logical, if unorthodox, to regard the protein as a mere receptacle holding water, and to concentrate on the phase changes of the water upon cryo-cooling. When bulk water is cooled below its glass transition temperature too rapidly for it to form crystals, it exists in one of two metastable amorphous phases: high density amorphous (HDA) with a density of 1.17 g cm^{-3} at 80 K or low density amorphous (LDA) with a density of 0.94 g cm^{-3} at 170 K. Rapidly freezing a sample to 80 K under pressure, followed by release of pressure and gradual warming, led to the sequence HDA›LDA›cubic ice› hexagonal ice, each with a characteristic diffraction pattern. When thaumatin crystals, which contain 60 % water, are subjected to the same treatment, superimposed on the Bragg peaks is the same sequence of water diffraction. Surprisingly, the unit cell volume only increases by 2.5 % between 120 K and 170 K. Since the volume increase is 23 % for the HAD›LDA transition of the water alone, a volume increase amounting to 60 % of 23 % would be expected. The counter-intuitive conclusion that water is being lost seems inescapable.

ACA meetings often feature some very worthwhile lunchtime and evening sessions. So it proved this time, too, with a discussion one evening entitled "Would You Publish This?" Perhaps aided by the availability of good Canadian beer at the poster session preceding it, a series of eminent crystallographers unveiled the skeletons in their closets. **Joseph Tanski** reported on pyrazine bridged Ru(III)-Pt(II) complexes. One salt yielded a good refinement (R = 0.038), but another suffered from intractable non-merohedral twinning. Since these salts have relevance to the discovery of anti-cancer drugs, they should be published; but can one trust the second structure at R = 0.105, or how could one improve it? The next contribution, from **Carla Slebodnick**, reported on the frequent disorder affecting host-guest interaction that occurs in crown-ether based crystals, along with strategies adopted to deal with it. **Amy Sarjeant** described her tribulations with metal-organic frameworks that have large voids and a high degree of disorder, leading to weak data. **Gary Enright** reported the successful structure determination of an important intermediate in the synthesis of bioactive compounds. As well as the typical experimental problem of small flexible needles (0.02 x 0.02 x 0.40 mm), the molecule was chiral and the space group was hexagonal with Z = 6. In presenting a series of isosteric quasiracemates **Gregory Ferrence** raised thought-provoking questions about the boundaries of isosterism, their greatest difference between "isosteric" components being 3 carbon atoms. Continuing the theme of non-centrosymmetric structures with pseudo-inversion symmetry, **Victor Young** showed us some enantiopure or enriched materials whose packing implies a (nonexistent) inversion centre that can be used in remarkably successful refinement. The most spectacular confession came from **Frank Fronczek**, who owned up to

a small-molecule structure with R no less than 0.258! His troublesome crystals come from collaboration with chemists who synthesize porphyrins and phthalocyanines that bear large and frequently flexible appendages and that usually incorporate much solvent in the crystals, if any crystals grow at all. Structure determinations from such unpromising material yield little more than the molecular connectivity, but this information alone is of immense value to the chemists.

Lunchtimes were enlivened not only by presentations from equipment suppliers featuring descriptions of their exciting new offerings but also by their tasty free lunches. In addition, we had the chance to see films: one entitled "Naturally Obsessed" describing the trials and eventual triumphs of a newly minted macromolecular crystallographer, and another, "H. M. Hauptman, Portrait of a Laureate".

There always is a significant strand at ACA meetings that is devoted to education. This year's topic, "Educational Outreach", concentrated on bringing crystallography to non-crystallographers or fledgling crystallographers. We heard how the Research Collaboratory for Structural Bioinformatics is working on appropriate ways to tell "molecular stories" to audiences with widely varying background and needs, and how the Cambridge Structural Database is being integrated into undergraduate teaching so that structural chemistry can be taught in 3-D. **Sean Seaver** gave an informal presentation about www.P212121.com, a site he has established for macromolecular crystallography blogs presenting lots of hints and tips and some funny comments.

Bernhard Rupp recounted the agony and ecstasy of writing a graduate-level macromolecular crystallography textbook that makes students go beyond learning and applying techniques and also think about the validity of their model by hypothesis testing. The most astonishing educational development was a series of presentations by "Pied Piper" **Bill Duax** and his troop of high school students. Awarded summer internships at the Hauptman-Woodward Medical Research Institute in Buffalo, NY, they had carried out data mining in genomics, providing evidence that the bacterium *Anaeromyxobacter dehalogenans* primarily uses only the 32 codons ending in G or C. At BCA meetings we have come to expect presentations from our YC's whose fluency matches that of longer-established crystallographers, and we are not disappointed. Still, it was an eye-opener to witness these high school students giving their presentations with such clarity and confidence. A flyer was distributed with brief biographies of 13 interns. Their thirst for knowledge is phenomenal. Alongside crystallography their interests span the range from Anglo-Saxon runes to chess to Chinese culture to the stock market. Two of them suffer from diseases (diabetes and lupus) that motivate them to strike back by carrying out medical research, and all of them showed keenness that inspired the rest of us.

Carl Schwalbe

THE American Crystallographic Association (ACA) meeting 2009 was held in Toronto, Ontario, Canada from the 25th-30th of July. This meeting is held annually for the association's 2000+ members to meet and discuss their work and current ideas. World leaders in crystallography and crystal engineering are attracted to this meeting and many presented their current thinking on important topics.

The meeting featured 623 presentations (including both oral and posters) from a range of 47 topics. My oral presentation was featured in the Supramolecular section chaired by Prof. **Christer Aakeroy**. Within this section a number of other presentations and posters were highly relevant to my research and general interest in this field. I will discuss the highlights of some of these presentations in this report.

Prof. **G. Desiraju**'s talk discussing additive induced polymorphism was an interesting way of thinking of a problem we regularly encounter. While my work does not directly use polymorphism, it is an issue that affects the work of all crystallographers. He considered whether polymorphic structure can be correlated with that of the additive and linked this to the logical but mostly ignored point, that crystallographers should be documenting cases of this they find while forming salts and cocrystals. After this presentation I will certainly be considering this more carefully.

Safiyyah Forbes, supervised by Christer Aakeroy, presented her work on using cocrystals to improve the aqueous solubility of anti-cancer drugs. She used the even-odd rule for straight chain dicarboxylic acid solubility to show how, when using hexamethylene bisacetamide (HMBA), the solubility of the drug could be increased with the acid. Also, again using HMBA, a plot was displayed showing a linear correlation between cocrystal melting point and that of the dicarboxylic acid. Therefore, the thermostability could be manipulated in a controlled way. This was all very interesting to me as at the beginning of my PhD I had tried doing something similar with ephedrine and a range of acids forming salts. I had concluded that no correlation existed, but after hearing this presentation I intend to go back and revisit my data. Due to my interest in this work I asked the presenter whether she had any evidence of this working with other systems. Another system investigation has apparently commenced and is looking promising.

My presentation was entitled 'The Formation of Molecular Salts Using both Solution and Non-solution Methods' and focussed on the case study of one salt, ephedrine pimelate. Within the presentation I discussed my work forming the salt through both grinding and solution methods, then my subsequent studies of binary phase diagrams (both experimental and ideal). The comparison between the ideal and experimental phase diagrams led into my work using infra-red microscopy and eventually the conclusion that potentially a 2:1 salt is also present in the system.

Prior to attending I had hoped my presentation would stimulate discussion with other researchers working in the same field. After my presentation I was approached by **Dmitriy V. Soldatov**, an associate professor from the University of Guelph, who wanted to learn more about the theoretical phase diagram aspect of my talk, which I happily expanded upon. To provide further information I provided a number of references of publications from colleagues at the University of Manchester. X-Ray crystallographer Dr. **John Warren** from the University of Bath, UK, also showed interest in my presentation, suggesting a new approach to the formation/ positive identification of the 2:1 salt I mentioned I was struggling to isolate. If this works it will be a major step forward in my PhD, as the issue has been holding back progress in this direction.

Thanks to this travel grant I have been able to raise my profile within the crystallisation community by presenting at my first international conference. My PhD research has been enhanced by new ideas and perspectives and I have made a number of key contacts.

Claire Cooke

Puzzle Corner...

...SEPTEMBER ANSWER

THE winning entry came from Jim Trotter, who answered as follows. "My own eldest son (Martin) fitted the bill, as did your own Spanish equivalent (Carlos). Then try a site like www.babynames1000.com/six_letters, and you get 983 boys' and 1165 girls' names (only some of which have c-v-c-c-v-c, of course), e.g. Baxter, Benson, Carmen, Cedric, Conner, Conrad.....etc.

Then, there are lots of crystallographer surnames; among the more-well-known are: Bernal, Donnay, Germer, Harker, Hughes, Kasper, Lipson, Miller, Warren, Wilson.....etc."

The only thing I have to add is that two distinguished crystallographers from our own ranks (Garman and Watkin) also satisfy the criterion, and the great fibre diffractionist Watson Fuller is a true son of the CSD.

International School of Crystallography 41st Course 4-14th June 2009 in Erice, Sicily

High Pressure Crystallography: From novel experimental approaches to applications in cutting-edge technologies

THE Ettore Majorana Foundation and Centre for Scientific Culture in Erice has been hosting "International Schools" across multiple disciplines since 1963. The first International School of Crystallography course was held in 1974 and has since been held annually; with the last course focusing on High Pressure Crystallography held in 2003. This course was attended by 120 participants across 20 different nationalities.

The setting for this course was the gorgeous town of Erice, located at the top of Mount Erice some 750 meters above sea level overlooking the town of Trapani; this little town is steeped in history, displaying both ancient and medieval architecture. Every turn leads to a new wonder from tiny cobbled streets to impressive churches and castles. If buildings are not your thing then the spectacular views could easily win you over: from the balcony of the lecture hall you could see the sparkling blue of the Mediterranean, the impressive Sicilian countryside and mountains in the distance. It was a very pleasant way to spend a coffee break, and to set the mind ready for another set of lectures.

The accommodation in the echoing halls of St Francesco was well appointed and spacious. Stepping out of your room was like going back in time (a common theme for Erice), exemplified by large wooden doors with their massive iron keys.

The course consisted of three elements, lectures, workshops and poster sessions. The lectures were timetabled so that each session was devoted to a particular theme.

The first block of talks focused on experimental techniques, kicking off with an introduction to high pressure science by **Przemak Dera** and highlighting some of the work done in the different areas of chemistry, physics, geophysics, material sciences and engineering, biology and energy science. This talk was followed by the history of the Diamond Anvil Cell (DAC) from its origins in the 1950s to the present by **Moshe Paz-Pasternak**. Experiments that could be performed at synchrotrons were discussed by **Dera, Mohamed Mezouar**, **Anatoly Balagurov**, **Jennifer Jackson** and **Leonid Dubrovinsky**.

The first workshop of the course, on DAC handling and high pressure crystallography, was given by **Colin Pulham**, **Kamil Dziubek** and **Giovanni Hearne**. As novices at working with high pressure, we were most looking forward to this workshop, and it didn't disappoint, with practical advice from experts in the field. There was even an opportunity to get a hands-on chance at growing a crystal within the diamond anvil cell. (It's difficult to tell if I actually managed it from the microscope we were using.) The day ended with a welcoming buffet and entertainment by a local performance group, a folk show and dance.

The second day focused on phenomena that occur at high pressure starting examples with the simplest case: compression without phase transitions and chemical transformations. **Tiziana Boffa-Ballaran** introduced us to the Equation of State, an empirical method for describing the functional relationship between pressure, volume and temperature in a material. **Robert T. Downs** talked about the systematic compression observed with minerals and perovskites.

Elena Boldryreva and **Andrzej Katrusiak** gave talks on the understanding of intermolecular interactions. Boldryreva showed how compression should be treated anisotropically in all systems except cubic. Katrusiak showed some examples from his work on phases crystallized at high pressure and how they could be used to understand intermolecular interactions.

The afternoon block introduced the theoretical aspects of phase transitions. This was a workshop on the treatment of powder diffraction data and the implementation of the Equation of State calculation.

The next block of lectures focused on the treatment of computer simulations and calculations. From this block of lectures **Artem Oganov** demonstrated the use of USPEX, an evolutionary algorithm for the prediction of crystal structures. This evolutionary algorithm tries to find the global minimum by retaining knowledge on previous good solutions. After each cycle the next generation of solutions

should be getting better as offspring solutions retain some of the positive traits found in the parent.

High pressure structures of various solids formed from simple molecules or elements were covered in another block. From this block of lectures there were a couple of lectures that I could relate directly to the sort of research into intramolecular geometry I carry out myself.

There was a block of lectures dedicated to the topic of high pressure synthesis and superhard and advanced materials. In this block **Colin Pulham** gave a lecture on energetic materials (i.e., explosives) at high pressure. He showed how these high pressure techniques could be used to study how these compounds behave during detonation.

The final block of lectures looked at systems of biological importance. **Francesca Fabbani** explained the importance of developments in these high pressure techniques to the pharmaceutical industry for maximizing the experimental space in the search for polymorphs.

In total the course stretched over nine days with more than 50 lectures on a range of topics and five separate workshops allowing more relaxed and practical applications of structure solution, equation of state calculations, quantum mechanical calculations and *ab initio* crystal structure prediction.

We were given an opportunity to show off our work to the wider scientific community in the form of a very rushed 3 minute presentation. The accompanying poster session allowed for a more relaxed discussion where we got some nice interest and feedback.

It wasn't just all work and no play, however: there were opportunities to take in some of the sights of Sicily. We visited the Mozia Island, just 0.4 km^2 in size. The history of Mozia is very ancient: as a shipping centre and staging post, and due to its presence near the coast of an important trade city, it was one of the most important Phoenician and Carthaginian settlements in the Mediterranean area. The Phoenicians transformed the inhospitable island, which they called *Motya*, into one of the most affluent cities of its time, naturally defended by the lagoon as well as high defensive walls. The island has no roads, no cars and very few modern buildings (apparently only a small coffee shop and museum) and being a good distance from the coast, you quickly found yourself lost out of time again, with nothing but the smell of flowers and the sea air. Phoenician ruins were impressive, as was the local wildlife such as wild lizards and snakes which we found crawling around the sun-drenched ruins.

We also had a chance to visit the Greek temples at Selinunte, which according to our tour guide was the largest archeological site in Europe. Split between two hills, the site includes six temples, a walled-in closed upper city with the lower city yet to be uncovered. All of these temples have collapsed in the years since their construction but two of them were rebuilt in the 20th century. The whole site is visually stunning, with ruins and architecture everywhere you look. On the same day we also visited the Theater at Segesta, a city of the Elymian people. We were the first group to arrive at the site and we decided not to wait for the tour bus to drive up the hill to the temple but to walk instead. After an invigorating climb of some 400 m up the mountain, the view of both the Theater and the surrounding countryside in the Sicilian afternoon was well worth the effort.

This was our first international meeting and it was a thoroughly worthwhile experience. We would like to thank the BCA and the Erice committee for funding in order to attend.

Henry Wong and **Daniel Bailey**,
The University of Nottingham

News from the Groups

Biological Structures Group Winter Meeting 2009

THE Biological Structures Group winter meeting will be held on Friday December 18th 2009 at the Royal Free Hospital in Hampstead (north London) starting at 11.00 am in the Atrium lecture theatre.

The theme of the meeting is 'Pathological Proteins' ...which should be interpreted in its broadest context. The aim is for the conference to encompass structural studies of proteins involved in a wide range of disease processes including neurological disorders, atherosclerosis, amyloid disease, infection and immunity, and prospects for therapy.
Invited speakers include:

Prof. Salam Al-Karadaghi, Department of Molecular Biophysics, University of Lund, Sweden. 'Insights into the molecular mechanism of Friedreich's ataxia from X-ray crystallography and electron microscopy studies of frataxin.'

Dr Kate Brown, Department of Life Sciences, Imperial College London. 'Scraping the surface of C. difficile: structural characterisation of SLPs and toxin B.'

Dr Carien Dekker, The Institute of Cancer Reseach, London. 'The crystal structure of the eukaryotic chaperonin CCT.'

Dr Leo James, MRC Laboratory of Molecular Biology, Cambridge. 'Cyclophilin A: HIV co-factor or antiviral?'

Dr Simon Kolstoe, UCL Department of Medicine (Royal Free Campus). 'Targeting transthyretin - X-ray crystallography and rational drug design.'

Dr Paul McEwan, Centre for Biomolecular Science, University of Nottingham. 'Loosening the grip on von Willebrand factor by breaking the thumb of GPib.'

Dr Arefeh Seyedarabi, School of Biological and Chemical Sciences, Queen Mary, University of London. 'Structural and functional studies of IpaH9.8 from Shigella flexneri'.

Dr Ian Taylor, National Institute of Medical Research, Mill Hill, London. 'The retroviral capsid and restriction factors.'

Prof Gabriel Waksman, ISMB, Birkbeck / UCL. 'Structural Biology of Type IV Secretion Systems.'

The Royal Free Hospital is situated close to leafy Hampstead Heath and is a short walk from Belsize Park tube station which is about 10 - 20 minutes on the underground from most London main line rail terminals. More details about the meeting are available via the BCA / BSG website. The meeting is being generously sponsored by Bio-Rad, Bruker-AXS, Douglas Instruments, GSK, Molecular Dimensions, Oxford Diffraction and Rigaku. Enquiries should be made to the organiser: **Jon Cooper** by e-mail to **jbcooper@medsch.ucl.ac.uk**

10th Biennial Conference on High Resolution X-Ray Diffraction and Imaging

XTOP 2010, the 10th Biennial Conference on High Resolution X-Ray Diffraction and Imaging, will take place from Monday September 20th to Thursday September 23rd 2010 at the University of Warwick, UK. The conference runs from Monday afternoon and finishes with lunch on Thursday 23rd. En-suite accommodation on the University of Warwick's award-winning central Campus has been reserved for the nights of 20th-22nd September (further nights can be arranged on request) together with breakfast, buffet lunch and dinner on each day. There will be a conference banquet on the evening of Wednesday 22nd September.

Lectures and poster exhibitions will be held in the Physics Lecture Theatre and on the Physics concourse just 5-10 minutes walk from the accommodation. Details of the pricing structure and the first circular will follow shortly together with abstract submission and registration information. Please register the dates in your diary and reserve the time to come and join us in Warwick for XTOP 2010.

XTOP will bring together scientists from the fields of X-ray diffractometry, coherent and conventional X-ray diffraction imaging and topography, as well as X-ray phase contrast imaging (radiography and micro-tomography). XTOP is thus one of the central scientific platforms concerning methods and instrumentation in synchrotron-based high-resolution X-ray diffraction methods, phase contrast imaging, and microtomography.

For more information see
http://www2.warwick.ac.uk/go/XTOP2010

ECM, Istanbul

Twenty-fifth European Crystallographic Meeting, Istanbul

TOPICS covered in the presentations were allocated to one of five focus areas, and then to one of up to around a dozen microsymposia. Often it was difficult to choose between two (or more) very interesting parallel sessions, but I thought there was particular strength in the observation, analysis and prediction of intermolecular interactions. Most of my report will cover this field. For additional perspectives I am grateful to Georgina Rosair and Stefanie Schiffers.

The microsymposium on "Weak Interactions in Chemical Processes or Properties" attracted strong interest. The first speaker, **Susan Bourne**, demonstrated that the charge-assisted hydrogen bonding between substituted ammonium and carboxylate ions created a robust supramolecular synthon in the form of columns. She explored the influence of chirality on the nature of the columns. Homochiral salts form columns around a 2_1 axis ("2_1-columns"). Racemates can do the same or build columns through the action of successive inversion centres ("i-columns). Examination of 126 primary ammonium carboxylates in the CSD, both chiral and achiral, showed 2_1-columns in 75 structures and i-columns in 26. Implications were explored for Wallach's Rule (1895), which states that racemic crystals generally have higher density and greater stability than crystals of the corresponding pure enantiomers. In the ensuing lively discussion **Sally Price** made the important point that while the racemic crystals may benefit from low-energy packing arrangements not available to their homochiral counterparts, a term for the entropy of mixing is appended to the Gibbs free energy change when they melt. Thus, if the racemic and enantiopure crystals have the same melting point, the racemic crystal is the more stable.

Georgina Rosair managed to create some order in the disorderly world of supraicosahedral metallacarborane cages. Carborane cages typically are icosahedral. Much recent synthetic effort has gone into expanding the number of vertices, and a maximum of 15 is now known. Unfortunately, disorder detracts from our ability to verify the location of carbon atoms crystallographically. One strategy is to tag the C atoms with methyl or phenyl substituents. However, this requires an extra synthetic step, introduces an extra variable to interpret and may result in steric interference. An alternative strategy is to use lower-symmetry capping ligands such as *p*-cymene instead of benzene. Often the result is an ordered structure with Z' > 1.

In the next talk the focus shifted to liquid crystals, which lack translational order in at least one dimension but retain orientational order. **Alessandra Crispini** showed that liquid crystals could be obtained not just by the classical approach of assembling rod-shaped molecules side by side or piling disc-shaped molecules into columns, but more generally from association phenomena and molecular self-assemblies. **Nourredine Benali-Cherif** introduced a systematic study of the structural properties of hybrid anilinium compounds, in which an acidic substituent is located in the ortho, meta or para position. Finally, **Vera Vasylyeva** discussed the weak intermolecular interactions of fluorinated benzenes and pyridines. While benzene and perdeuterobenzene form similar crystals, perfluorobenzene is very different. The drastic change is not attributable to hydrogen bonding since fluorine in C-F, unlike F^-, is not a strong hydrogen bond acceptor. In pyridine derivatives carrying 2-fluoro, 2,6-difluoro or 2,4,6-trifluoro substitution, only the latter shows F…F and C-H…F interactions; and these are weak.

In his keynote lecture **Andrzej Katrusiak** took us into the strange world of seriously high pressures. For reference, the

pressure at the bottom of the Marianas Trench is about 0.1 GPa. Unusual things happen to common elements: at 10 GPa oxygen forms a red magnetic crystalline phase, and up to 240 GPa nitrogen becomes a non-molecular semiconductor (results from the Carnegie Institution in Washington). The range of elements in the Periodic Table that can superconduct broadens out at high pressure. Lithium forms hydrogen-like diatomic molecules, and above 199 MPa sodium becomes transparent. Carbon forms a super-hard monoclinic polymorph. Andrzej concluded by reporting effects on organic molecular crystals, showing the utility of Hirshfeld surfaces in their interpretation.

In a session entitled "Multicomponent Crystals" **Len Barbour** described the behavior of Dianin's compound (DC) as a host. Upon sublimation of a racemic mixture, 3 copies of the R enantiomer and 3 of S associate around a hexagon; these hexagons form columns with a central aperture 2.5 Å in diameter. Crystal growth from a suitable solvent leaves solvent molecules in the channels. The racemic thia analogue of DC forms a similar clathrate with wider solvent-filled channels when grown from CCl_4 solution. However, sublimation leads to spontaneous resolution. Len proceeded to play fascinating games by combining various enantiomers of DC and the thia analogue.

László Fábián introduced rationality into cocrystal screening. A promising approach when a pharmaceutical compound has valuable medicinal properties but unsatisfactory bioavailability is to incorporate it in a cocrystal. However, unguided attempts to screen for cocrystal formation only have a 20% success rate, and even homologous compounds behave differently. László introduced descriptors of polarity based on the fraction of N and O atoms, and of molecular shape based on the ratios of edge lengths in a box model. Complementarity of these descriptors between two molecules brought a much improved chance of cocrystal formation.

Lynne Thomas convinced us that diffuse scattering is not just a nuisance detracting from the intensity of Bragg peaks, but as "structured diffuse scattering" it may provide information about local correlation. Among the examples cited was phoroglucinol dehydrate, which exhibits a "domino effect" whereby the H atom position in the hydroxyl group affects the water H atom position.

On a related topic, though in a different microsymposium, "Crystal Energy Landscapes: Computation and Uses" **Graeme Day** addressed the prediction of solvent inclusion, i. e. stoichiometry and structure of solvates and the existence of inclusion compounds. A search for the global lattice energy minimum supported by calculation of 3-D molecular structure with density functional theory took a lot of computer time but successfully predicted the observed structure for carbamazepine plus acetic acid and urea plus acetic acid. Graeme concluded by inviting submission of crystal structures for the next Blind Test. Contributions should be addressed to **bardwell@ccdc.cam.ac.uk**. **Jacco van de Streek** outlined the method based on dispersion-corrected density functional theory that had achieved so much success in the most recent Blind Test. It is essential to consider dispersion; without it, the unit cells of molecular crystals expand by ca. 20%. The emphasis of this talk, however, was not on doing well in structure prediction contests, but rather the thoroughly practical application of this methodology to make sense of otherwise uninterpretable low-quality experimental data. In a validation test, of the 249 organic structures downloaded from the August 2008 issue of *Acta Cryst., Section E*, 215 could be energy-optimised.

Emiliana D'Oria discussed the computational prediction of spontaneous resolution. Once again the method involved sophisticated procedures to generate low-energy crystal structures. Such calculations for racemic and enantiopure crystals of test compounds yielded all known crystal structures and reasonable-looking alternatives with only small energy differences between them. For the *ab initio* prediction of hydrogen bond energy and geometry **Paola Gilli** introduced a pH/pKa slide rule to assess donors and acceptors.

Martin Schmidt concluded with a fine example of using new techniques to obtain a trial structure for powder diffraction data, achieving hard-won success in determining the structure of the technologically important but insoluble Pigment Yellow 213. With recrystallisation ruled out, it has to be analysed by powder diffraction. Attempts to obtain a trial structure by lattice energy minimization initially failed. Only when an unusual hydrogen bond was made to an ester group involving the ester O atom instead of the usual O=C did a viable structure emerge, leading to satisfactory Rietveld refinement.

Crystallography in pharmaceutical sciences was well represented. In "The Trouble with Hydrates" **Norbert Nagel** pointed out the steps in the manufacturing process for solid drugs that could form hydrates (e. g. wet granulation) or drive off the water (drying). Further changes, which blister packs cannot always prevent, may occur upon storage in very humid or very dry climates. An understanding of the phase diagram, gained by X-ray powder diffraction allied to other techniques, is essential to anticipate and avoid problems. As a particularly challenging example, the sodium salt of a drug with molar mass ≈550 showed 4 hydrates and 16 solvates. **Rosanna Rizzi** reported that EXPO2009, which includes enhancements designed for the automatic solution of structures from X-ray powder diffraction data, was successful with paracetamol.

William Jones discussed multicomponent pharmaceutical crystals and gave three convincing examples where the formation of cocrystals had improved properties. (1) Bioavailability. Crystalline itraconazole is poorly water-soluble. It is marketed as the amorphous solid, which offers increased solubility but causes concern about instability. As a coformer succinic acid creates a sandwich with two molecules of itraconazole. This cocrystal is stable and nearly as soluble as the amorphous drug. We were reminded that

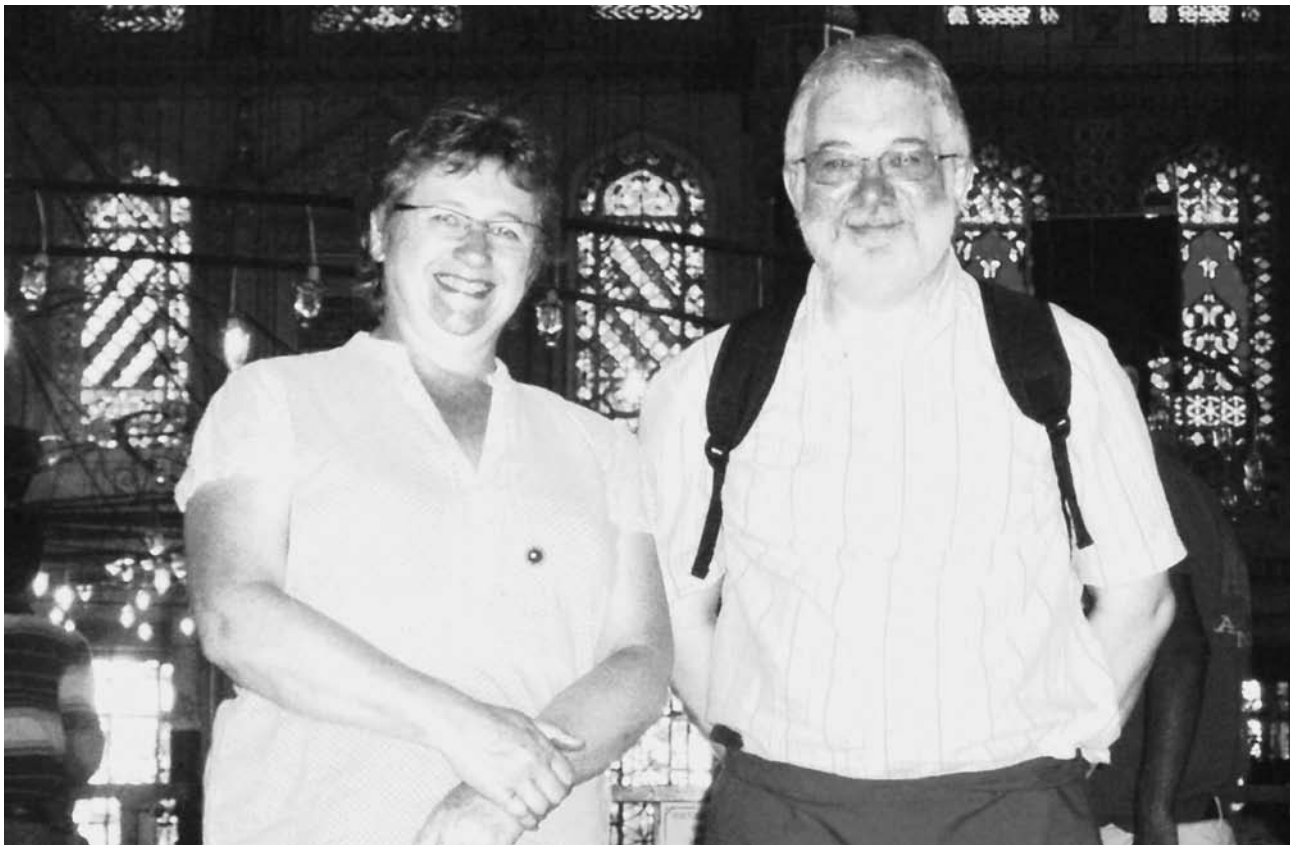
recrystallisation from solution is not the way to obtain a cocrystal with improved solubility since the pure drug would come out first. (2) Avoidance of hydrate formation. Above 75% relative humidity solid caffeine converts to hydrates. A 2:1 caffeine:oxalic acid cocrystal is stable up to 98% R.H. (3) Mechanical properties. The stable polymorph of paracetamol has corrugated layers, to the detriment of its behaviour under compression. The flat layers in Form 2 facilitate compression, but this form is metastable. A suitable coformer can stabilize the flat layers.

Eric Chan investigated diffuse scattering from a combined experimental and theoretical perspective. The stable monoclinic form and metastable orthorhombic form of benzocaine both show broad diffuse streaks with synchrotron radiation. Monte Carlo calculations of displacive disorder in model crystals provide insight into local structure and intermolecular interactions. Finally, **Tatiana Timofeeva** described improvements in photodynamic therapy (PDT), which involves the irradiation of a photosensitiser concentrated in harmful cells. In its excited state the sensitizer converts oxygen to reactive species which kill the cells. PDT currently relies on porphyrin derivatives which respond to single-photon excitation. Tatiana and coworkers have characterized about 20 arylidenepiperidinones that can be efficiently excited in a two-photon process. The lower energy per photon reduces damage to normal tissues, and the longer wavelength increases penetration under the skin to 5-7 cm; in addition, these fluorescent compounds can be used to image themselves.

A microsymposium entitled "The Future of Small Molecule Software" actually included perceptive commentary about old software as well as the excitement of the new. **Luc Bourhis** paid tribute to the excellent algorithm design and clever FORTRAN programming in traditional software. The ease of incorporating such routines into new software varies. For instance, the prevalence of comment lines ranges from 3.3% in SHELXL to 24.8% in Crystals, with the much newer Superflip coming in at around 15%. Choices made in widely used software can have an impact on studies carrying out data mining. The automatic positioning of secondary H atoms in SHELX depends on the X-C-Y angle; as that angle increases, H-C-H decreases. A plot of these angles taken from the CSD has a well-populated descending diagonal surrounded by scatter. Is this natural or a consequence of SHELXL?

Arie van der Lee compared approaches for automatic structure solution. The traditional sequence is: data > space group > solve by direct methods > refine. However, charge-flipping follows the route: data > solve in P1 > space group > refine. SHELXS, SIR2004 and Superflip all have a fine record, achieving success rates around 90% on the test structures, which rises to ≈98% when the methods are combined. Superflip does have the advantage that it is immune to a wrong choice of space group. This comment nicely closed the circle of the meeting, since **Lukáš Palatinus**, the lead author of Superflip, was awarded the 2009 Lewy-Bertaut Prize for his significant contribution to the solution of the phase problem and gave a very lucid lecture describing his work.

Carl Schwalbe



Focus Area 4 – Microsymposium 5. Structure and Reactivity in Molecular Crystals by Crystallographic, Spectroscopic and Computational Methods

THIS microsymposium consisted of talks spanning a wide range of contemporary chemical crystallographic topics. Stefanie Schiffers, a PhD student in Prof Paul Raithby's group in Bath, UK kindly stepped in to present her supervisor's talk on work she and co-workers had conducted in photochemical reactions in single crystals of complexes containing the NO_2 ligand which take up different coordination modes on irradiation. The relative populations were estimated from occupancy factors. She explained how they use an array of white LED lights rather than more expensive lasers to induce these changes in coordination mode.

The second speaker Prof **Maria Calhorda** from the University of Lisbon, Portugal, described the diverse packing arrangements of Mo(allyl)complexes and complemented these with DFT calculations. Her group also tested the biological activity of these species against cancer cell lines. Next **Julia Bakcowicz** from Wroclaw, Poland, talked about organic solid state reactions involving cyclisation in a related group of organic compounds some of which were inert and others which became amorphous. Electronic and vibrational spectroscopic studies on compounds for display applications were presented by **Pančе Naumov**, based at Osaka University. These complemented both single crystal and powder diffraction studies to build up a more complete picture of what happened to these species under photochemical reactions. Finally **Susanne Huth** at Southampton University UK brought a more theoretical flavour with her descriptions and knowledge based classifications of hydrogen bonding patterns in closely related pharmaceutical acylanilines, these were also complemented by lattice energy calculations which aimed to rank the relative energies of different packing arrangements.

Georgina Rosair
Heriot Watt University

ECM Review

THE 25th European Crystallographic Meeting in Istanbul was overall a great success in a stunning location. The social programme was well chosen and nicely made. The impressive opening ceremony started with a really good prize lecture from Dr. Lynne B. McCusker about charge flipping for powder solutions; then the lecture theatre wall moved away dramatically and we wandered out into the garden for a pleasant social evening. And then there were a classical concert in the church of St. Irene at the Topkapi palace, a conference dinner in another palace garden and a cruise along the Bosporus sparkling in the sunshine, near to but unfortunately not quite into the Black Sea.

The meeting itself was equally well organised, although not having a keyboard in front of oneself during a presentation did make speakers' lives more complicated then necessary. Another small annoyance was that the location of the poster session and the exhibitors wasn't ideal, firstly because they were in a different building from the lectures and secondly on different floors in that building.

A personal anecdote was that I went for the student package, which meant that you would share a room with another person. To my surprise, it turned out that you not only had to share the room, but the bed and the blanket as well. Luckily my bed mate was very nice and we didn't have fights about the blanket.

My personal highlights during the conference were definitely the software fayre and a great keynote lecture about solid-state reactions from **Menahem Kaftory**. He was showing some excellent results that his group had obtained: about 1,3 sigmatropic shifts at higher temperatures, producing different ring sizes depending on the host molecules and chiral [4+4] cycloaddition reactions.

It was nice to see not only new programmes being shown during the software fayre, but also some which are used (or could be being used) by everyone during a normal working day; for example PLATON.

Another interesting morning was the charge density session; with some great talks, for example the one from **Frederica Bertolotti** about Cu-Cu bonds within bridging ligand complexes. Also it was quite funny that it wasn't possible to see the speaker behind the lectern, as she was too small.

I want to mention as well that as a result of this meeting a new general interest group was established. This is the young crystallographers GIG, from where we hopefully will hear some lectures at the next ECM in Darmstadt.

Steffi Schiffers

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. The help of the IUCr listing is gratefully acknowledged.

13 December 2009
Nature's Treasures II: the Wonder of Minerals and Gems, Natural History Museum, London
http://www.minersoc.org

3-5 March 2010
Dynamics in Confinement, Grenoble, aFrance
http://www.ill.eu/news-events/events/confit2010/

3-5 March 2010
EMBO Workshop on Visualizing Biological Data, Heidelberg, Germany
http://www.embl.de/training/courses_conferences/conference/2010/VIZ10-01/

8-12 March 2010
International Collaboration on Advanced Neutron Sources (ICANS-XIX), Grindelwald, Switzerland
http://www.iucr.org/news/notices/meetings/meeting_2009_127

11-13 March 2010
Sixth International Workshop on X-ray Radiation Damage to Biological Crystalline Samples, Stanford Synchrotron Radiation Laboratory, Stanford, USA
http://smb.slac.stanford.edu/news/workshops/rd6/index.shtml

11-19 March 2010
31st Berlin Neutron Scattering School, Helmholtz Centre, Berlin, Germany
http://www.helmholtz-berlin.de/events/neutronschool/

15-17 March 2010
Polymorphism & Crystallisation 2010, London, United Kingdom
http://www.polyandcrys.com/Event.aspx?id=244544

15-17 March 2010
High-Resolution X-ray Spectroscopy: Past, Present, and Future. Symposium, Utrecht The Netherlands
http://www.sron.nl/index.php?option=com_content&task=view&id=2156&Itemid=1986

15-19 March 2010
International Centre for Diffraction Data, Spring Meeting, Newtown Square, PA, USA
http://www.icdd.com/

17-19 March 2010
NOP2010. International Workshop on Neutron Optics, Alpe d'Huez, France
http://www.ill.eu/news-events/events/nop2010/

18-20 March 2010
Discussions in Structural Molecular Biology, Nove Hrady, Czech Republic
http://www.structbio.eu/Current_Meeting.html

21-25 March 2010
American Chemical Society Spring 2010 National Meeting & Exposition, San Francisco, CA, USA
http://www.acs.org/meetings

27-31 March 2010
Small-Angle Scattering Short Course 2010, "Beyond RG", Argonne, IL, USA
http://small-angle.aps.anl.gov/courses/short_course_2010.html

7-10 April 2010
POLYCHAR18. World Forum for Advanced Materials, Siegen, Germany
http://www.uni-siegen.de/fb8/polychar18/

12-13 April 2010
Young Crystallographers satellite meeting, University of Warwick
http://www.chem.gla.ac.uk/yc/

13-15 April 2010
BCA Spring Meeting: Data Matters, University of Warwick
http://www.crystallography.org.uk/

18-22 April 2010
PCG Rietveld School, Durham
http://www.crystallography.org.uk/

18-23 April 2010
Adsorption, Absorption and Crystal Growth, Gargnano, Italy
http://www.imem.cnr.it/deptecpro.html#cg

19 April 2010
CPOSS: Characterisation and Computational Modelling of Complex Behaviour
http:// www.cposs.org.uk/

21-25 April 2010
International Workshop DyNano 2010 "Structure and Dynamics of Nano-objects using short wavelength radiation ", Corsica, France
http://www.synchrotron-soleil.fr/Soleil/ToutesActualites/Workshops/2010/DyNano2010

26 April - 7 May 2010
School on Synchrotron and Free-Electron-Laser Sources and their Multidisciplinary Applications, Trieste, Italy
http://cdsagenda5.ictp.trieste.it/full_display.php?ida=a09142

28-29 April 2010
Data Analysis for Quasielestic Neutron Scattering with FRIDA, Garching, Germany
http://www.jcns.info/DataAnalysis2010

2-7 May 2010
European Geosciences Union. General Assembly 2010, Vienna, Austria
http://meetingorganizer.copernicus.org/EGU2010/sessionprogramme

2-7 May 2010
3rd ILL Annual School on Advanced Neutron Diffraction Data Treatment using the FullProf Suite, Grenoble, France
http://www.ill.eu/news-events/events/fpschool-2010/

12 May 2010
BCA Industrial Group XRF users' meeting, British Geological Survey. Keyworth, Nottingham
http://ig.crystallography.org.uk/ig.htm

13 May 2010
BCA Industrial Group minerals meeting, Between the Sheets! British Geological Survey. Keyworth, Nottingham
http://ig.crystallography.org.uk/ig.htm

24-28 May 2010
ISC. 2nd Granada International School of Crystallization: Foods, Drugs and Agrochemicals, Granada, Spain
http://www.iscgranada.org/

24-30 May 2010
Diffraction at the Nanoscale Nanocrystals, Defective & Amorphous Materials, PSI Villingen, Switzerland
http://user.web.psi.ch/powder2010/

25-28 May 2010
ISDSB 2010. 3rd International Symposium on Diffraction Structural Biology, Paris and Orsay, France
http://www.synchrotron-soleil.fr/Workshops/2010/ISDSB

3-13 June 2010
International School of Crystallography. 42nd Course: Structure and Function from Macromolecular Crystallography: Organisation in Space and Time. Erice, Sicily
www.crystalerice.org/erice2010/2010.htm

6-11 June 2010
Gordon Research Conference in 'Crystal Engineering', Waterville Valley, NH, USA
http://www.grc.org/programs.aspx?year=2010&program=crystaleng

7-11 June 2010
Fundamentals of X-ray Powder Diffraction, ICDD Headquarters, Newtown Square, PA, USA
http://www.icdd.com/education/xrd.htm

7-11 June 2010
Graduate Course - Neutron Scattering techniques in Structural Biology, Oak Ridge National Laboratory, TN, USA
http://neutrons.ornl.gov/conf/gcnb2010/

8-11 June 2010
COHERENCE 2010. International Workshop on Phase Retrieval and Coherent Scattering, Rostock-Warnemünde, Germany.
https://indico.desy.de/conferenceDisplay.py?confId=2327

14-18 June 2010
Advanced Methods in X-ray Powder Diffraction, ICDD Headquarters, Newtown Square, PA, USA
http://www.icdd.com/education/xrd.htm

21-24 June 2010
IWPCPS12. Twelfth International Workshop on Physical Characterization of Pharmaceutical Solids, Lille, France.
http://www.assainternational.com/workshops/iwpcps_12/iwpcps_12.cfm

21 June - 2 July 2010
MathCryst Summer Schools: Topological Crystal Chemistry & Irreducible representations of space groups, Nancy, France
http://www.crystallography.fr/mathcryst/nancy2010.php

26-28 June 2010
ECRS-8 - the 8th European Congress on Residual Stresses, Riva del Garda, Italy
http://events.unitn.it/en/ecrs8

4-9 July 2010
IZC16 and IMMS7. 6th International Zeolite Conference and 7th International Mesostructured Materials Symposium. Engineering of New Micro- and Meso-Structured Materials, Sorrento, Italy.
http://www.izc-imms2010.org/index.php

5-8 July 2010
MOLMAT2010. IVth International Conference on Molecular Materials, Montpellier, France
http://www.molmat2010.fr/

5-8 July 2010
PNCMI2010: 8th international workshop on Polarised Neutrons in Condensed Matter Investigations, Delft, The Netherlands.
http://www.tnw.tudelft.nl/live/pagina.jsp?id=3f2f14d1-c18b-4276-aa94-90d5d52fc337&lang=en

5-9 July 2010
Combined Analysis Using X-ray and Neutron Scattering, Caen, France.
http://www.iucr.org/news/notices/meetings/meeting_2009_222

11-14 July 2010
7th International Conference on Synchrotron Radiation in Materials Science (SMRS-7) and 6th International Conference on Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation (MEDSI), Oxford.
http://www.diamond.ac.uk/Home/Events/MEDSI.html

11-16 July 2010
Gordon Research Conference in 'Electron Distribution & Chemical Bonding', South Hadley, MA, USA
http://www.grc.org/programs.aspx?year=2010&program=elecdist

18-23 July 2010
Gordon Research Conference in `Diffraction Methods in Structural Biology', at Bates College, Lewiston, Maine, USA. Chair: Andrew Leslie. Co-chair: Ana Gonzales.
http://www.grc.org/programs.aspx?year=2010&program=diffrac

24-29 July 2010
American Crystallographic Association Meeting, Chicago, Illinois, USA
http://www.amercrystalassn.org//meetingspg_list/futuremeetings.html

21-27 August 2010
20th General Meeting of the International Mineralogical Association, Budapest, Hungary
http://www.ima2010.org/

22-26 August 2010
240th ACS National Meeting & Exposition, Boston, MA, USA
http://portal.acs.org/portal/acs/corg/content

23-27 August 2010
FEL 2010. 32nd International Free-Electron Laser Conference, Malmö, Sweden
http://fel2010.maxlab.lu.se/

27-30 August 2010
EPDIC12. 12th European Powder Diffraction Conference, Darmstadt, Germany
http://www.epdic12.org/

27-29 August 2010
MaThCryst Satellite Conference of ECM26, Darmstadt, Germany
http://www.crystallography.fr/mathcryst/darmstadt2010.php

29 August - 2 September 2010
26th European Crystallographic Meeting, Darmstadt, Germany
http://www.ecm26.org/

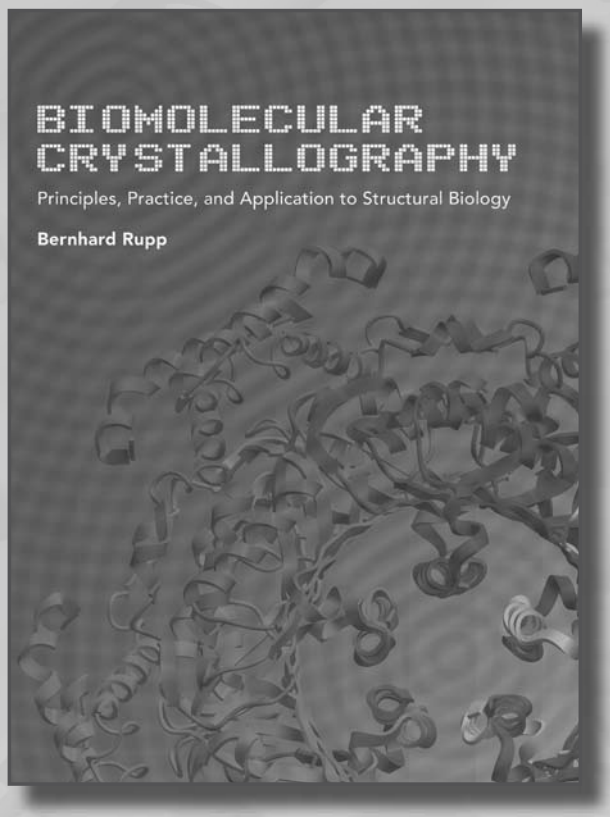
5-10 September 2010
BCA/CCP4 Summer School XV, Oxford.
http://crystallography.org.uk/bca-ccp4-summer-school-2010

20-23 September 2010
XTOP2010, the International Conference on High-resolution X-ray Diffraction and Imaging. University of Warwick, UK
http://www2.warwick.ac.uk/go/XTOP2010

3-4 November 2010
BCA Industrial Group Autumn Meeting, Diamond Light Source, Harwell
http://ig.crystallography.org.uk/ig.htm

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

NEW FROM GARLAND SCIENCE



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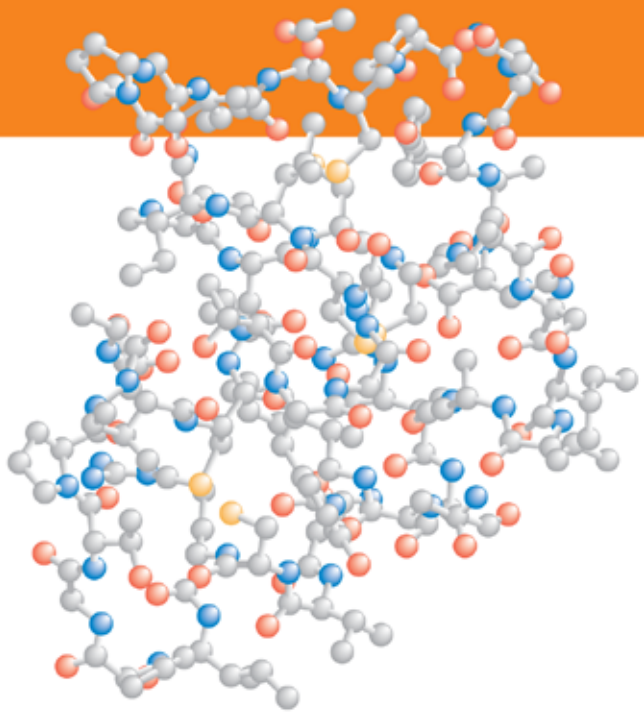

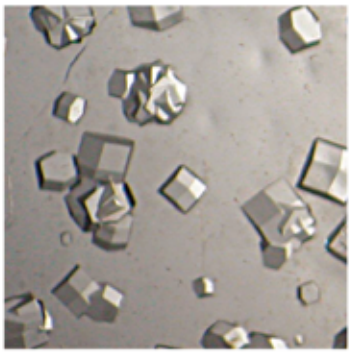

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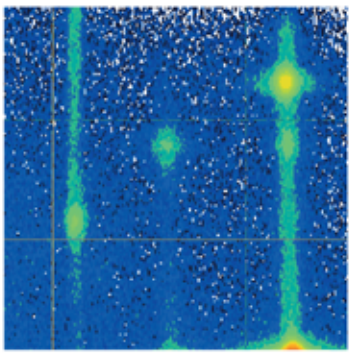

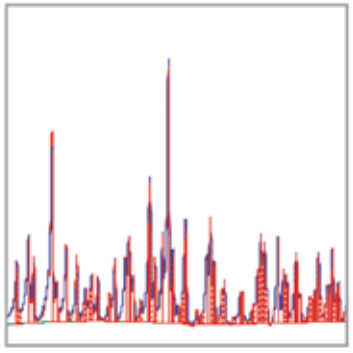

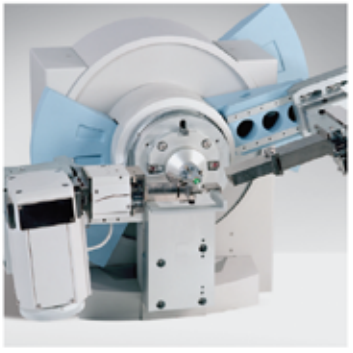

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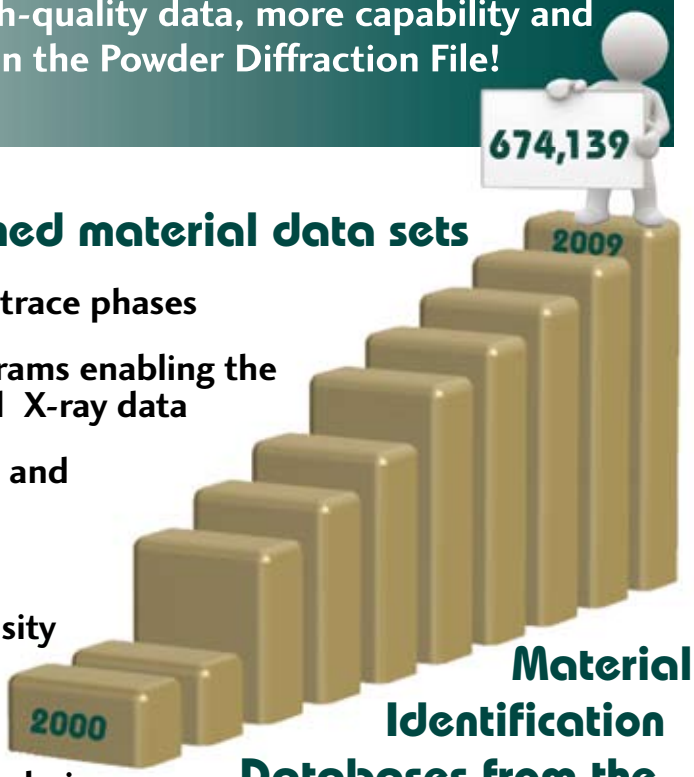

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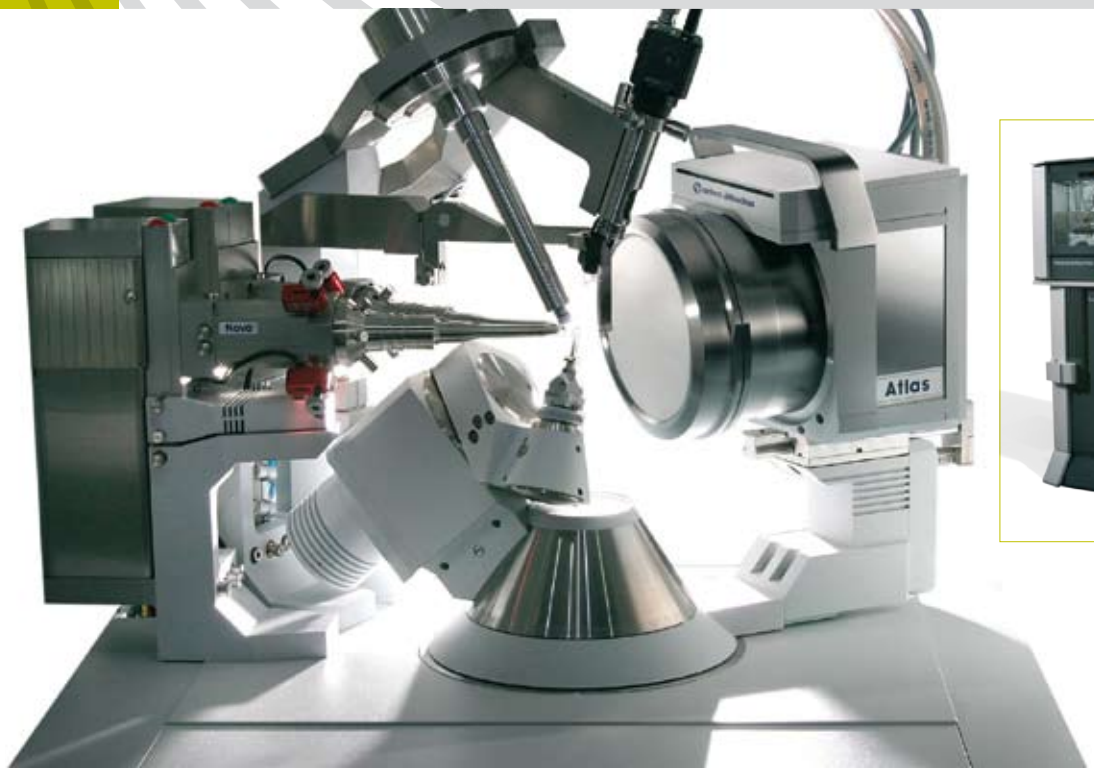

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