Crystallography News

British Crystallographic Association

Issue No. 120 March 2012
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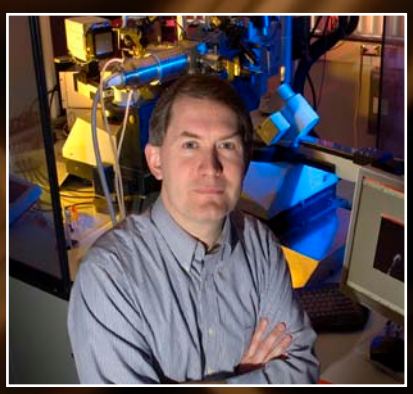
X RAY DIFFRACTION

THEN & NOW



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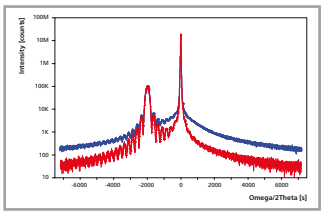
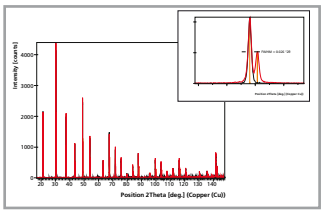
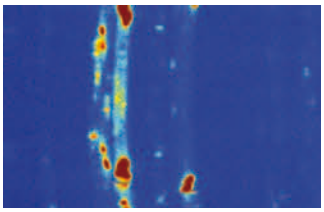
0D



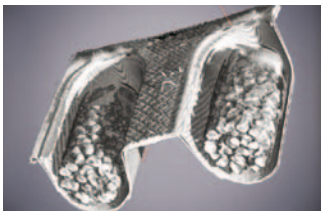
1D



2D



3D



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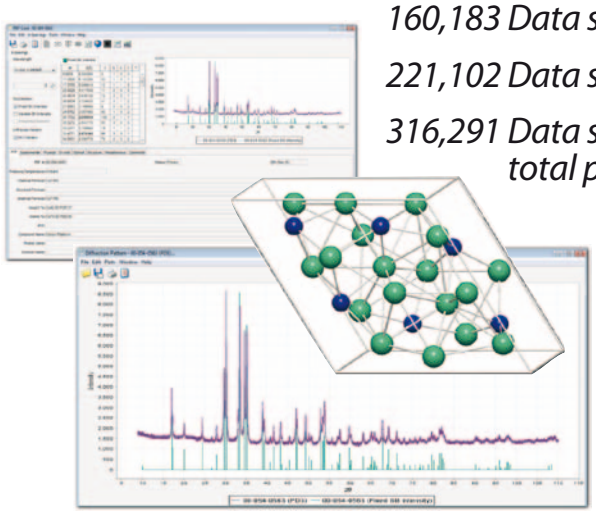

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Crystallography News March 2012

Contents

We would like to take this opportunity to thank the BCA officers and members who we have enjoyed a close working association with for over a decade.

You will be much missed on our list of clients.

"Fare Thee Well"

Best regards
Northern Networking Events

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 2012 issue are sent to the Editor to arrive before 25 January 2012.

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This month's cover:

Laue and Spring Meeting Plenary Lecturers at Munich and Warwick

From the Editor

OUR cover shows the discoverer of X-ray diffraction, Max von Laue, and the institution where his discovery in collaboration with the experimentalists Walter Friedrich and Paul Knipping took place 100 years ago, the University of Munich. Our picture of Laue is from the Bundesarchiv, and we thank **Werner Kunz**, www.werner-kunz.com, for the unusual panoramic photo of the Court of the Main Building of the University. Beside and below these images are pictures of three outstanding speakers who will be giving Plenary Lectures at our forthcoming BCA Spring Meeting at the University of Warwick, along with some of the architecture on the Warwick campus.

This is the issue where we publish the full and final details of this BCA Spring Meeting. I am confident that anyone who is still uncertain about attending will be convinced that this meeting is unmissable! Even sooner, I am looking forward to a trip to Munich, not just for the beer but mainly for a meeting that is a double celebration. This is the 20th annual meeting of the German Crystallographic Society (the BCA woz 'ere first) and the 100th anniversary of the discovery of X-ray diffraction by Laue. Even though the hatred between nations that led to World War I was steadily worsening, scientists from many nations immediately hailed and put to use Laue's discovery. Later, Laue received an honorary degree from Manchester while **William Lawrence Bragg** was Langworthy Professor of Physics there. A review of these developments, fittingly authored by Manchester academics Helliwell and Blunden-Ellis along with Blake, Moore and Schwalbe, has recently appeared in *Crystallography Reviews*.

There are more meetings coming up that are well worth attending. Already on the 3rd of April the 2012 Open Meeting of CPOSS will take place. Within the theme "Crystal or Not, Where Do We Go From Here?" a set of highly regarded experimentalists and computational crystallographers will give talks, and there will be an opportunity to present posters. Even better, thanks to sponsorship by the CPOSS Industrial Alliance, this meeting proves that there is such a thing as a free lunch. In May at the University of Leicester our Industrial Group will hold another in its successful series of joint XRF/XRD meetings. Further details are given in this issue. Then, from July 28 to August 1, the American Crystallographic Association will be meeting in Boston. On Saturday the 28th there will be four workshops, covering Refmac/Coot, OLEX2, Modeling Refinement of Nanoparticle Structures from Diffraction Data and "Crystallography – World of Wonders" for schoolteachers from kindergarten to high school. This year's Transactions Symposium is on the topic of "Transformations and Structural Oddities in Molecular Crystals." It is in honour of **Bruce Foxman**, a renowned expert in this field. Some British people who go to Boston complain that New England seems so similar to Old England that they hardly feel that they have left home. Of course, this brings a number of advantages. The numerous cultural attractions, excellent restaurants and lively pubs are within easy walking distance or accessible by the excellent public transport system. So, too, is Fenway Park, the iconic home of the Boston Red Sox baseball team. The weather may well be warm and sticky, but Boston does not turn into a bake-oven very often. If you haven't experienced an ACA meeting before, this could be a good one to try. The shortness of the distance from the U.K. makes flying less expensive and less stressful than to most places in the USA, and the switch to a 4-day format for the main meeting saves on hotel and subsistence costs. The deadline is March 31, both for the submission of abstracts and for applications for Student and Young Scientist travel grants. Oh, by the way, the 2013 ACA meeting will be in Honolulu!

Looking east instead of west, and about a week later, the European Crystallographic Meeting will take place in Bergen, Norway, from August 6-12. Along with the excellent science always on offer at the ECM, this will provide an excellent opportunity to get to know a picturesque part of Scandinavia. Bergen has a spectacular natural harbour and a well-preserved district of merchants' houses, the Unesco World Heritage site of Bryggen. With a population of about a quarter of a million, Bergen is able to offer big-city attractions in a format that is not too large. In addition, Bergen was the home of that great Scottish composer **Edvard Grieg** (our Norwegian friends may disagree with this attribution, but I expect that **Alex Salmond** will concur with me). Namely, Grieg's great-grandfather **Alexander Greig** was a merchant from Cairnbulg, Scotland, trading dried fish and lobsters. As trade between England and Scotland became impaired after the Battle of Culloden, Greig concentrated his efforts in Norway, settling in Bergen in 1770 and changing the family name from Greig to Grieg. There are regular concerts both in central Bergen and at Grieg's home on the outskirts, Troldhaugen.

I draw your attention to a block of items from our friends at the International Centre for Diffraction Data. Of particular importance to our student members and their supervisors, the Robert L. Snyder Student Travel Awards have been made available to support students, also from outside the USA, to attend the Annual Denver X-ray Conference.

Carl Schwalbe

BCA Council 2011

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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

It is snowing here in Oxford today and winter has finally arrived in earnest as I gather some thoughts to write my last letter to the BCA membership at the end of my term as President.

In musing on what has and has not been achieved in the last three years by and for the Association, I am minded of my 'hustings' presentation in 2009, in which I mentioned a number of ideas on how to build the BCA into a stronger educational and supportive organisation. Some of these have come to be, but as an incurable optimist in life, I now find that my three years is up and that I was rather ambitious in my vision: regrettably I have not succeeded in expediting them all, although some major challenges have been fruitfully addressed.

Notably, with the help of Northern Networking Events, we tendered for and won ECM 2013 for the UK during the 100th anniversary of the year in which the Braggs (father and son) solved the structure of sodium chloride. This meeting will be a wonderful opportunity for us to showcase all areas of UK crystallography. The International Year of Crystallography, IYCr 2014, will be another high profile event in which the BCA could take a leading role. As mentioned in my last letter, we now have an education representative from each of the groups, who are ready to put time and effort into planning for both of these. Our move to the CAF Bank and more membership subscriptions being paid by Direct Debit has considerably simplified the administration of the Association, and we have worked hard to update and correct our membership database. I have very much enjoyed meeting quite a number of you on my visits to the Autumn meetings. I am grateful to Crystallography News readers for displaying the new posters we have produced to encourage membership, and which were sent to you with your last issue. It is only by drawing on and including more of the UK crystallography community that we will be in a position to do justice to the two events mentioned above. It is particularly important that our younger crystallographers are involved, and while I have been BCA President, it has been tremendously encouraging to witness the enthusiasm and liveliness of our YC group. There is still time to take part the 'Member get a Member' challenge, the prize for which is a free registration for ECM2013, the winner of which will be announced at the next AGM in Warwick.

This autumn I only managed to visit one of the annual one day BCA Group Meetings: that of the CCG at the Research Complex at Harwell (RCH), but I took with me the 'written off as an accountable asset' bag of BCA ties, and I am happy to say that we found takers for them all. This means that there are no more ties in store and thus the one you have in your cupboard is now a collector's item! By all reports the other autumn meetings were also very successful, particularly that of the BSG on 'From Macromolecular to Supramolecular' at Diamond Light Source and RCH, which was a sell-out.

The BCA contract with Northern Networking Events (NNE) expires on 30th March 2012, and in 2011 Council put out a tender for Administrative services for the next approximately 5 year period. Three tenders were received by the 31st August 2011 deadline, and after an extraordinary Officers meeting in October, HG3 of Harrogate was selected as the successful tenderer. They will take over the Membership Administration from 30th March 2012, and the meeting organisation from 1st April 2013 (to organise the 2014 Spring Meeting). The contracts for both roles will expire at the same time, on 31st July 2018. I would like to express my thanks to **Dave Allan**, our Vice-President, for producing the very comprehensive tender documents. These benefitted enormously from his eye for detail, born out of wide tendering experience at Diamond. The BCA is most grateful to NNE for all their help and care over the last 12 years, and for graciously agreeing to run the Spring Meeting in Warwick from 16-19th April 2012 after the end of their formal contract. NNE will also be the conference organisers for the 2013 ECM in Warwick for us, so we will be continuing our valuable relationship with them and look forward to continuing to work with them on this exciting meeting.

As President, I would particularly like to thank **Gill Moore**, **Jennifer Kirkcaldy** and **David Massey** for their assistance with the running of the BCA, both before and during my tenure.

From 30th March 2012, the contact details for the BCA Membership Administrative services will be:

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Fax +44 (1) 1423 855999

For the information of our new members, of which I am happy to say there are now over 80 since last April, we are now offering an electronic version of Crystallography News to members as a pdf file instead of a paper copy. This will assist in keeping our costs down and is also better for our planet. If any member who has not already done so wishes to take up this offer please email the BCA Secretary **Georgina Rosair**: secretary@crystallography.org.uk

The BCA Spring Meeting at Warwick is fast approaching,

and so I end by wishing the next President a productive term in office, and by thanking the current Officers (**Dave Allan, Georgina Rosair** and **Andrea Mulholland**), and the previous Officers with whom I worked (**Sandy Blake** and **Harry Powell**) for their care and hard work, as well as the current and past members of Council for their enthusiasm, particularly **Richard Cooper**, our Webmaster for his continuous updating, and **Carl Schwalbe**, our wonderful CN Editor. Lastly, I am grateful to the (increasing number of) BCA members for their continued support. I have very much enjoyed working with you all to help build a strong future for the BCA.

Best wishes and adieu,

Elspeth

P.S. I thought you might like to see that the 2009-2012 President took seriously the remit to spread the word about the BCA: this is a photo of our Haflinger Puch, made in Graz, Austria in 1964 and given the name 'Hettie' by our daughters. These small four wheel drive vehicles were designed for troop carrying across Austrian terrain! See http://en.wikipedia.org/wiki/Haflinger_(vehicle)

BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
- A 10% discount on exhibition stands on the annual BCA Spring Meeting, OR - A promotional poster at the annual BCA Spring Meeting.
- Free insert in the annual Spring Meeting delegate bag.
- Two free full registrations to the annual Spring Meeting.
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BCA Spring Meeting Scientific Programme

Challenges in Crystallography

PLENARY LECTURES

PL1: **BSG Plenary**
Professor **Laurence Pearl** (Sussex)
Structural Biology of the DNA Damage Response

PL2: **BCA Prize Lecture**
Dr **Robin Taylor**
(Taylor Cheminformatics Software)
Predicting Low-Energy Conformations of Small Organic Molecules: Is Crystal-Structure Data Redundant?

PL3: IG Plenary
Professor **Dan Shechtman** Nobel Prize 2011
(Technion, Haifa, Israel)
Quasi-Periodic Materials – Crystals Redefined

PL4: Teaching Plenary (PCG)
Professor **Branton Campbell**
(Brigham Young University)
Symmetry Modes: Nature's Favoured Description of Structural Distortions

YCG Satellite Plenaries

Dr **Kenneth Shankland** (Reading)
Downhill All the Way: an Optimisation View of Crystal Structures from Powders
Dr **Robin Owen** (Diamond Light Source)
Seeing the Full Picture: Combining Crystallography with Tomography and Spectroscopy at I24

HIGHLIGHTS

S06: Young Scientist Award Ceremony
Winner of the CCG CCDC Young Scientist Prize:
Dr **Gareth Lloyd** (Cambridge).
Phase changes of crystalline and soft materials
Award of the Physical Crystallography Prize and the Young Crystallographers Industrial Group Prize Lecture will be announced and presented at the meeting.

S05: Interdisciplinary Forum
Bridging the Gap Between MX and Small Molecule Crystallography
Introduced by **Arwen Pearson** and **Amber L. Thompson**
As small molecules get larger, the challenges they pose increasingly approach those associated with macromolecular crystallography. However, with the divergence of the two fields, we now talk different languages as well as have different scientific backgrounds. This forum is intended to help break down these barriers through the medium of questions with a panel of experts. Possible questions for discussion include, "What is Rfree?"; "How do you judge data quality?"; "How do you prevent solvent loss?" and "What do you do to prevent radiation damage?". The session is short and intended to promote discussion; if successful it could be a prototype for a longer event next year, so suggestions and feedback are greatly encouraged.
Chair: **Kirsten E. Christensen**

SESSION LECTURES

S01: Multidimensional Materials
(PCG & CCG)
This session will cover the use of crystallographic and imaging methods to understand the structure and properties of low-dimensional materials: zero-dimensional clusters, nanotubes, layered materials and frameworks.
Chair: **Andrew Goodwin**
Mark Weller (Southampton)
Transition Metal Fluorophosphates: New Structural Motifs and Crystallographic Challenges
Valeria Nicolosi (Oxford)
Atomic Resolution Imaging of Two-dimensional Nanomaterials
Paul Saines (Cambridge)
Facile Synthesis and Structural Diversity of Nanosheets of Inorganic-Organic Frameworks
Elena Marelli (Reading)
The Structure of CuNi(CN)4: A Simple Cyanide Containing Cu(II) in a Square-Planar Environment

S02: Proteases in Disease (BSG)
The session is themed around protease structure, mechanisms of proteolysis and understanding the regulation of complex processes such as blood coagulation and innate immunity.
Chair: **James Huntington**
Piet Gros (Utrecht, Nederlands)
Proteases in Complement and Innate Immunity
Vilmos Fulop (Warwick)
Oligopeptidases in Peptide Processing Memory Disorders and Pathogen Virulence
James Huntington (Cambridge)
Thrombin Structure and Dynamics

S03: Piecing Together the Puzzle – Multidimensional Approaches
(CCG, YCG & PCG)
This session will cover investigations where a number of techniques are required in order to see the full picture. Sometimes we are so focussed on diffraction that we fail to see the added value of viewing the problem from a different angle. This session will show the benefits and extra information one can obtain by using a multi-dimensional approach.
Chairs: **Iain Oswald** and **Anna Warren**
Lynne Thomas (Bath)
Beyond the Structure: Investigating Physical Properties in Molecular Materials
Andrew Goodwin (Oxford)
Frameworks, Flexibility and Frustration
Mark Eddleston (Cambridge)
A Novel Approach to Crystal Structure Determination Combining Crystal Structure Prediction and Transmission Electron Microscopy.
Christopher H. Woodall (Bath)
An Investigation in the Luminescent Behaviour of Gold(I) Trimers at Variable Temperature and Pressure.

S04: Protein Crystallography in Drug Discovery: Binding Sites in the Spotlight (BSG)
The session will cover aspects of protein crystal-lography in a drug discovery setting, including issues arising during ligand fitting, as well as new structure-guided inhibitor design possibilities opened up with the structure elucidation of G-Protein Coupled Receptor structures.
Chair: **Robert Van Montfort**
Judit Debreczeni (Structural Genomics Consortium)
Practical Considerations in Ligand Substructure Validation
Andy Dore (Heptares Therapeutics)
Structure Based Drug Design for the Human A2a G-Protein Coupled Receptor
David Robinson (University of Dundee)
Structural Biology in Academic Drug Discovery – Perspectives from the Dundee Drug Discovery Unit

S07: Software Workshop (BSG)
Development of computational methodology underpins the basis of all crystallographic analysis. In this software session there will be two lectures (1) developments in the popular molecular graphics program Coot will be described. Coot is used for macromolecular model building, model completion and validation, particularly suitable for protein modelling using X-ray data and is currently being developed for structure based drug design.
(2) Developments of the X-ray data processing program CrysAlisPro will also be described including the fully integrated unit determination work bench for standard, twin and incommensurate samples allowing an easy and intuitive unit cell finding especially for demanding cases.
Paul Emsley (Oxford)
New Ligand-Based Tools in Coot
Mathias Meier (Agilent)
CrysAlisPro – The New EwaldPro Tool and Data Reduction Improvements

S08: H-bonding: From Water to Supermolecules I (PCG & CCG)
The session will give an overview of recent theo-retical and experimental studies on the condensed phases of water. Specific topics will range from supercooled water and the nucleation of ice at sur-faces to stacking disorder in ice.
Chair: **Christoph Salzman**
Benjamin Murray (Leeds)
The Structure of Ice Crystallised from Supercooled Water
Angelos Michaelides (UCL)
Ice Nucleation at Surfaces
Dominic Fortes (UCL)

S09: Hot Structures and Hot Methods (BSG)
This session consists of talks selected from abstracts reflecting late breaking topics, reports of new structures and updates on new methods.
Chair: **Jon Cooper**
Gabor Bunkóczi (Cambridge)
Phaser.MRage: a Scaleable and Extendable Molecular Replacement Pipeline.
Tom Burnley (Utrecht, Netherlands)
Ensemble Refinement of Protein Crystal Structures in PHENIX.
Jose E. Jimenez-Roldan (Warwick)
From Crystal Structure to Conformational Changes via Rapid Simulations.
Stephane Mouilleron (London)
Molecular Analysis of a G-actin Sensor.
Peter J. Watson (Leicester)
The Mechanism of Activation of HDAC3 by the SMRT Corepressor. A Key Role for Inositol Tetraphosphate.
Wyatt W. Yue (Oxford)
A New Look at Glycogen Biogenesis – Conformational Plasticity of Glycogenin and Its Maltosaccharide Substrate During Catalysis.

S10: SAXS (IG & BSG)
The technique of Small Angle X-ray Scattering, in particular biological SAXS, has become increa-singly popular in recent years, complementing high resolution structural studies by crystallography, NMR and electron microscopy. Sensitive to length scales in the nanometre range, SAXS can be applied to a wide range of different types of samples including polymers, lipids, nanoparticles, proteins and biomaterials. This session will high-light some recent advances in the field.
Chair: **Elizabeth Shotten**
Clair Baldock (Manchester)
Combining SAXS and Biophysical Techniques to Investigate the Nanostructure of Extracellular Matrix Proteins
Nick Terrill (Diamond Light Source)
Small Angle Scattering -
The Last Resort of the Desperate?
Briony A. Yorke (Leeds)
New Approaches to Time-Resolved Structural Studies of Macromolecules
Allan Pang (London)
Cracking the Shell of Metabolosome

S11: H-bonding: From Water to Supermolecules II (CCG & PCG)
This session focuses on the Crystal Engineering aspects of the hydrogen bond. Intermolecular interactions mediated by hydrogen are frequently structure-defining in organic and metal-organic structures from hydrates, polymorphs and co-crystals right through to highly complex supra-molecular systems. The session will touch on the importance of the hydrogen bond in analysis, design and prediction of small molecule crystal structures.
Chair: **Peter Wood**
Doris E. Braun (UCL)
Contrasting Organic Hydrate Structures Generated in Silico to in vitro
Laszlo Fabian (UEA)
Cocrystal Design: Interactions and Properties
Miren Ramirez (Birmingham)
Hydrogen Bonding and Conformation in Salts of Diclofenac

S12: Crystallography and Cancer (BSG)
High throughput structural biology approaches can play a pivotal role in the target validation, hit identification, hit-to-lead and lead-optimisation phases of drug discovery. In this session, two pioneers of these approaches will discuss high value and high throughput approaches to unlocking the potential of anti-kinase and anti-chaperone drug targets.
Chair: **Jane Endicott**
Chris Murray (Astex Therapeutics, Cambridge)
The Application of Fragment-Based Drug Design to Drug Targets in Oncology
Stefan Knapp (Oxford)
Structure based design of protein interaction inhibitors that target acetyl-lysine recognition domains
Pierre J. Rizkallah (Cardiff)
Adaptive Immune System Response to Melanoma
Richard Bayliss (Leicester)
An Atypical - propeller Directs Tubulin Binding in the EML Family of Proteins

S13: Process Analytical Technology (PAT) for Online Monitoring of Material Quality in Manufacture (IG)
Industrial group session covering the application of PAT for monitoring and controlling the quality of a product during manufacture, as used in the Pharma-ceutical and Aggregate/ Cement industries.
Chair: **Brett Cooper**
Ali Saleemi (Loughborough)
The Role of PAT in Crystallisation Process Monitoring and Control
Paolo Avalle (Merck Sharp & Dohme)
Preliminary Development of PAT Methods for Controlled Release Pellets Coating

S14: Phase Transitions I: Distortion Mode Analysis (PCG & CCG)
The session will connect the fundamentals with the topical materials research and provides the basis for a state-of-the-art diffraction data analysis approach.
Chair: **Ivana Evans**
John S. O. Evans (Durham)
Symmetry Mode Analysis of Functional Materials
Mark Senn (Edinburgh)
The Verwey Structure of Magnetite: Charge Order and Three-Site Distortions
Philip Lightfoot (St. Andrews)
New Twists on the Perovskite Theme: The Elusive Phases R and S of NaNbO3

S15: Membrane Protein Crystallography (BSG)
Protein crystallographic analysis of membrane proteins is critical to understanding structure-function relationships and important to understand-ding disease processes and for the development of new medicines. Only a small subset of independent structures of integral membrane proteins have been reported so far and in this session the technological challenges and recent breakthroughs of research in this important area are explored.
Chair: **Jonas Emsley**
So Iwata (Imperial College)
Structural Studies of Integral Membrane Proteins
Andrew Leslie (Cambridge)
Crystallography of G-protein Coupled Receptors
Elizabeth Carpenter (SGC Oxford)
High Throughput Structural Studies ofHhuman Membrane Proteins Leading to the First Structure of a Human ABC transporter, ABCB10

S16: Coatings (IG)
Coats of many colours: Probing and understanding surfaces and the coatings interacting with them, is a science that continues to grow as technology becomes more specifically focused on this interesting environment. This session will present lectures from speakers picked across a number of industrial sectors, showing how these surfaces and coatings are important to each and the techniques used to understand the associated challenges.
Chair: **Judith Shackleton**
Bob J. Cernik (Manchester)
Raja Khan (Birmingham)
Evaluation of Residual Stresses in Coatings by X-ray Diffraction
Mark Farnworth (NSG)

S17: Phase Transitions II:
Transformations in the Solid State
(CCG, IG & PCG)
This session is concerned with the transformation of one crystalline form into another as a result of a stimulus such as a change in temperature. The primary tool to monitor such processes is the monitoring of structure before and after transition by diffraction-based techniques. However the field is now increasingly turning to other techniques to probe the kinetics, dynamics and mechanisms of these transitions and complementary techniques such as Calorimetry, Solid State NMR and computational-based calculations are now being employed to further our understanding of these complex processes. The session will draw on all these complementary approaches in presentations outlining examples from different areas of academia and particularly pharmaceutical relevance.
Chairs: **Simon Coles** and **Cheryl Doherty**
Kenneth Harris (Cardiff)
Structural and Dynamic Aspects of Phase Transitions in Solid Inclusion Compounds
Spoorthi Dharmayat (Pfizer)
Solid Form Transformations of Pharmaceutical Compounds
Mateusz B. Pitak (Southampton)
Patterns in Aliphatic Amino-acid Phase Transitions

S18: Protein Crystallisation:
Magic Versus Logic (BSG)
This session will focus on non-standard methods for obtaining and optimising macro-molecular crystals using "logic" (i.e. chemical and physico-chemical prior knowledge, crystallisation diagnostic techniques and further means) to counter balance the "magic" ingredient which many regard as essential for producing diffracting crystals.
Chair: **Naomi Chayen**
Terese Bergfors (Uppsala, Sweden)
Highways, Biways and Detours: the IspD Story
Emmanuel Saridakis (Demokritos, Greece)
Discovering Crystallisation Conditions Using Dual Polarization Interferometry
Lesley F. Haire (London)
A Combinatorial Approach to the Optimization of Protein Crystallization
James Hall (Reading & Diamond)
Room Temperature Crystals Are Not Rigid – The Dynamic Nature of a Crystal System Shown by Humidity Control

	Monday 16 April 2012	Tuesday 17 April 2012		
9:00		Lecture Theatre 3		Lecture Theatre 3
9:15		Young Crystallographers Session 4: 09.00 - 10.30		9.00 - 9.45 PL2: *BCA Prize Lecture F* *Molecules: Is Crystal-Stru* *Chair:* **Elspeth Garman**
9:30				
9:45				Refreshments 09.45 - 10.
10:00				Sessions: 10.00 - 11.45
10:15				
10:30		Break 10.30 - 10.45		Lecture Theatre 3
10:45		Young Crystallographers Session 5: 10.45 - 11.30 Science Outreach		S06: CCDC/CCG Prize Lecture PCG Prize Lecture IG/YCG Prize Lecture
11:00				
11:15				
11:30				
11:45				PCG AGM 11.45 - 12.30
12:00		Registration, Lunch and Exhibition From 12.00		
12:15		Lecture Theatre 3		
12:30		12.15 - 13.00 PL1: BSG *Plenary Structural Biology of the DNA Damage Response* Professor **Laurence Pearl** *Chair:* **Elspeth Garman**		CCG AGM 12.30 - 13.15
12:45				
13:00	Lecture Theatre 3	Break 13.00 - 13.30		
13:15	Young Crystallographers Session 1: 13.00 - 15.00			
13:30		Sessions: 13.30 - 15.00		Sessions: 13.30 - 15.00
13:45		Lecture Theatre 3	Lecture Theatre 4	Lecture Theatre 3
14:00		S01: *Multidimensional Materials* PCG/CCG *Chair:* **Andrew Goodwin**	S02: *Proteases in Disease* BSG *Chair:* **James Huntington**	S08: *Hydrogen-bonding: From Water to Supermolecules* PCG/CCG *Chair:* **Christoph Salzm**
14:15				
14:30				
14:45				
15:00	Refreshments 15.00 - 15.30	Refreshments 15.00 - 15.30		Refreshments 15.00 - 15.30
15:15				
15:30	Lecture Theatre 3	Sessions: 15.30 - 17.00		Sessions: 15.30 - 17.00
15:45	Young Crystallographers Session 2: 15.30 - 17.00	Lecture Theatre 3	Lecture Theatre 4	Lecture Theatre 3
16:15		S03: *Piecing together the puzzle - Multidimensional Approaches* CCG/YCG/PCG *Chairs:* **Iain Oswald & Anna Warren**	S04: *Protein crystallography in drug design: binding sites in the spotlight in drug discovery* BSG *Chair:* **Rob Van Montfort**	S11: *Hydrogen-bonding: From Water to Supermolecules* CCG/PCG *Chair:* **Peter Wood**
16:30				
16:45				
17:00	Break 17.00 - 17.30	Break 17.00 - 15.15		Break
17:15		Lecture Theatre 3		Lecture Theatre 3
17:30	Lecture Theatre 3	17.15 - 18.15 S05: *Bridging the gap between MX and Small Molecule crystallography Forum by* **Arwen Pearson** and **Amber L. Thompson** *Chair:* **Kirsten E. Christensen**		17.15 - 18.00PL3: IG *Pler* **Professor Dan Shechtr** *Chair:* **Judith Shackleto**
17:45	Young Crystallographers Session 3: 17.30 - 19.00			
18:00				Lecture Theatre 3
18:15		Exhibitors Forum, Buffet Dinner and Posters From 18.15		BCA AGM 18.00 - 19.00
18:45				
19:00	Young Crystallographers' Buffet Dinner & Poster session From 19.00			Comfort time
19:15				
19:30				Conference Dinner From Ceilidh Dancing After Dinr
20:00				

Wednesday 18 April 2012			Thursday 19 April 2012		
			Lecture Theatre 3		
Predicting Low-Energy Conformations of Small Organic ucture Data Redundant? **Dr. Robin Taylor**			09.00 - 09.45 PL4: PCG *Teaching Plenary Symmetry modes: Nature's favoured description of structural distortions* Professor **Branton Campbell** *Chair:* **Ivana Evans**		
00			Refreshments 09.45 - 10.15		
			Sessions: 10.15 - 11.45		
	Lecture Theatre 4		Lecture Theatre 3	Lecture Theatre 4	Lecture Theatre 5
	S07: Software Workshop BSG	Lecture Theatre 5	S14: *Phase transitions: Distortion Mode Analysis* PCG/CCG *Chair:* **Ivana Evans**	S15: *Membrane Protein Crystallography* BSG *Chair:* **Jonas Emsley**	S16: *Coatings* IG *Chair:* **Judith Shackleton**
	BSG AGM 11.45 - 12.30	IG AGM 11.45 - 12.30	Break 11.45 - 12.00		
			Sessions: 12.00 - 13.30		
	Lunch and Exhibition 12.30 - 13.30		Lecture Theatre 3	Lecture Theatre 4	
			S17: *Phase transitions: Transformations in the Solid State* IG/CCG/PCG *Chairs:* **Simon Coles** and **Cheryl Doherty**	S18: *Protein Crystalllisation: Magic versus Logic* BSG *Chair:* **Naomi Chayen**	
			Conference Close: 13.30		
	Lecture Theatre 4	Lecture Theatre 5			
an	S09: *Hot Structures and Hot Methods* BSG *Chair:* **Jon Cooper**	S10: SAXS IG/BSG *Chair:* **Elizabeth Shotton**			
	Lecture Theatre 4	Lecture Theatre 5			
	S12: *Crystallography and Cancer* BSG *Chair:* **Jane Endicott**	S13: *PAT-Online Processing* IG *Chair:* **Brett Cooper**			
17.00 - 17.15					
nary Quasi-Periodic Materials – Crystal Redefined **man**, 2011 Nobel Prize Winner **n**					
19.30 ner					

A Fevered Sleep & Fuel production

Stilled

A photographic performance marathon
Created by Fevered Sleep

Stilled is a performance piece for adults, created in a collaboration between Fevered Sleep and an advisory team of X-ray Crystallographers. Weaving together dance, light, music and photography, Stilled creates a meditative cross-artform event exploring perception, movement and stillness.

Accompanied by a live sound and light score, the piece is performed for both for a human audience and for a bank of silent, all-seeing pinhole cameras. Throughout the performance, images are exposed, developed and displayed, to show glimpses of bodies moving slowly in the light. Each image bears witness to dances that have already been and gone, durations of time captured in a single image.

Join us at Warwick Arts Centre on Tuesday 17 April as part of the BCA's spring conference.

Entrance is free, and audiences can enter and leave the performances as often as they please.

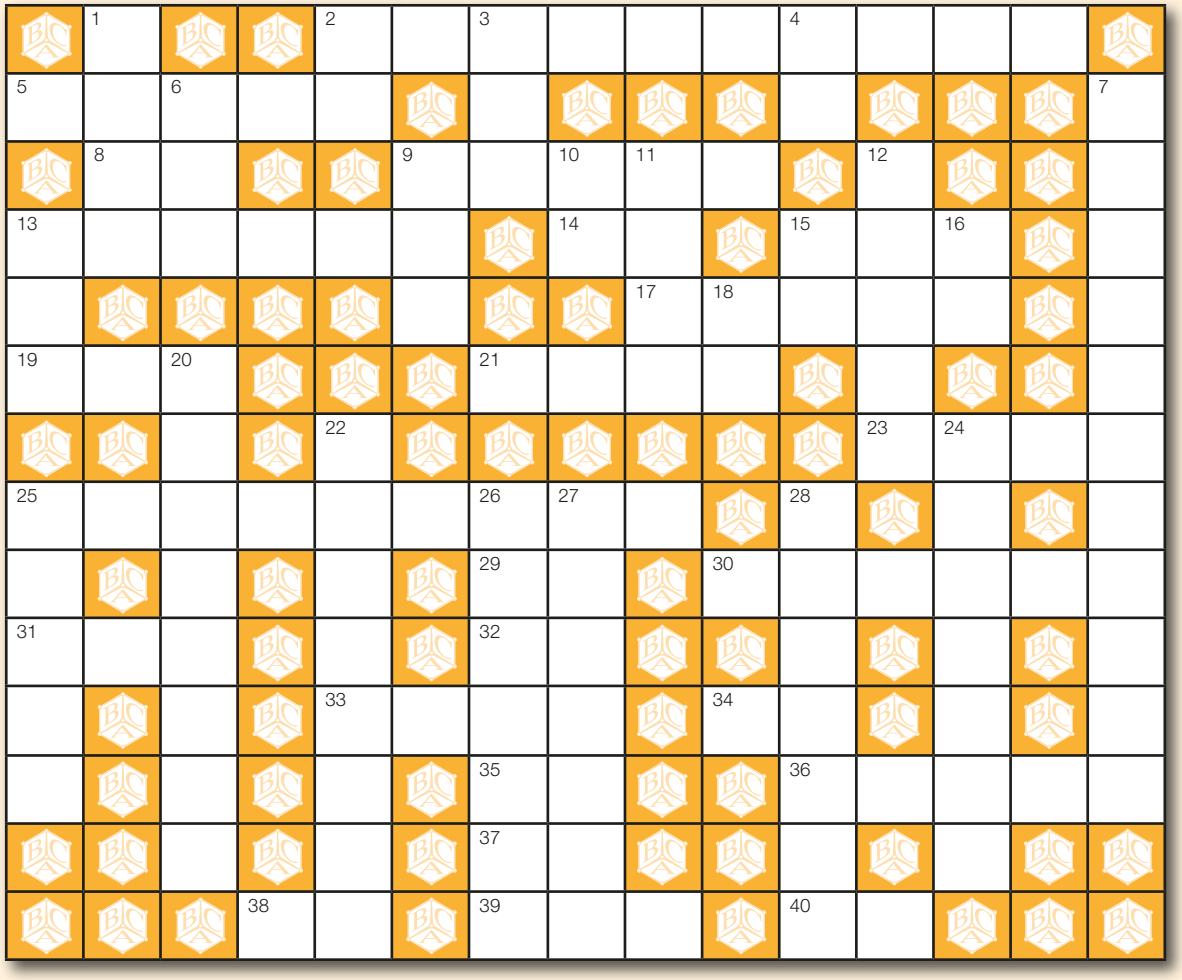
Originally commissioned for Wellcome Collection
Supported by the Wellcome Trust and Grants for the Arts.

Fevered Sleep's work is produced in association with Fuel.

www.feveredsleep.co.uk

Puzzle Corner

CROSSWORD: pioneers of X-ray diffraction and a bit of chemistry



ACROSS

2. Laue's boss
5. Braggs' employer, pt. I
8. Iron
9. Laue's award, pt. II
13. Laue's city
14. Nickel
15. Braggs' and Nishikawa's drink?
17. Laue's award, pt. I
19. Fertiliser components
21. Braggs' sample, pt. I
23. Braggs' sample, pt. II
25. Laue's co-author
29. Gallium
30. Keeps constant acidity (2-4)
31. Braggs' food?
32. Neodymium
33. Smallest unit of element
34. Osmium
35. Bismuth
36. Shroud tested by XRF
37. Europium
38. Helium
39. London Metal Exchange
40. Rhodium

DOWN

1. Nishikawa's food?
2. Senior Lecturer
3. Useful for proteins
4. Francium
6. Nishikawa's money
7. Braggs' employer, pt. II
9. What Knipping got later
10. Indium
11. Element 30
12. W H Bragg's first chair here
13. With 28, W L Bragg was here
15. Terbium
16. Aluminium
18. Satisfactory
20. Laue's co-author
22. W L Bragg's birthplace
24. Followed Bragg in Yorks
25. DNA sample for XRD
26. Opposite of Laue's award?
27. Element 48
28. IUCr site

BCA AGM 2011/2012

2011 Annual General Meeting of the BCA

THE Annual General Meeting of the British Crystallographic Association was held on Wednesday 13 th April 2011 at 6.00 p.m. at the University of Keele. 84 members were present.

1. Approval of Agenda
The agenda was approved by **Mike Glazer** and **Chris Gilmore**.

2. Apologies for absence
Paul Raithby

3. Minutes of the last AGM (published in March 2011 Crystallography News)
These were approved by **Moreton Moore** and seconded by **John McGeehan**.

4. President's Report
The President thanked **Arwen Pearson** for her excellent chairing and organisation of the programme committee for this Spring meeting. There are 99 delegates registered for the YCM on Monday. **Susanne Coles** is retiring as Chair of the YCG and **Duncan Sneddon** is her successor. The President thanked Prof. **John Helliwell** for giving the Lonsdale lecture. Next year's Spring meeting will be held on 16-19 April in Loughborough [note added 26/1/12: this is now Warwick due to the Olympic athletes' training schedule in Loughborough] and **Kirsten Christensen** is the Programme Chair. **Sandy Blake** will speak about ECM2013 under AOB and 2013 will be the International Year of Crystallography [note added 26/1/12: this is now 2014] for which UNESCO approval is being sought by the IUCr. At the IUCr Congress in Madrid, the UK requires five delegates at the General Assembly. Three BCA Council members will take part but two more BCA members are needed. Anyone who can take part was asked to contact the President. She will email the whole membership, offering a pdf version of Crystallography News soon. She thanked Carl Schwalbe, who was applauded for his excellent work as Editor. The President explained that we were not electing any new Honorary members this year. She thanked **Richard Cooper** for his work and prompt updating of the BCA website. The President expressed her thanks to **Harry Powell** who has served as Treasurer for the past 3 years who has done sterling work in changing the bank account and membership payment methods. She also thanked the two other officers for their assistance.
There were no questions on the President's report.

5. Secretary's Annual Report
The Secretary announced that a new Treasurer and new Ordinary member of Council will be elected at this AGM. She has passed on nominations for the following IUCr commissions to **Mike Dacombe**, the executive Secretary of the IUCr; These were for the Computing Commission: **Harry Powell**, Cambridge (LMB, Chair), **Amber Thompson** (Oxford) and **Martin Lutz** (Utrecht, Netherlands) and for the Crystallographic Teaching Commission: **David Watkin** (Oxford) and **Gary Battle** (CCDC Cambridge UK).
The IUCr have sent the Secretary the UK entries for the World Directory of Crystallographers and Council has been working on updating these entries.

At the 2010 ECM in Darmstadt, the Secretary was informed that BCA crystallography Schools could apply for ECA funding. The application needs to be made in February and August of the preceding year. The details are on the ECA website. The Fourth Erwin Felix Lewy Bertaut Prize is to be awarded to a young European scientist for notable contributions to science using crystallographic or neutron scattering methods. The call for nominations was open until 20th April 2011. To publicise the International Year of Crystallography (IYCr2013 [now 2014]) the IUCr are holding a logo competition. The closing date for entries will be 1 July 2011 and details appeared on the IUCr website. The prize is an Apple iPad.

Various proposals for the European Crystallography meeting in 2013 in Warwick have been put forward, such as an exhibition on the development of crystallography and we hope UK departments can contribute to this. Durham has already offered to be involved.
She thanked the President **Elspeth Garman** for her inspiration, energy and enthusiasm over the past year. She also thanked **Harry Powell**, our hardworking and retiring treasurer and **Dave Allan**, our vice President for his valuable work on Council.
There were no questions on the Secretary's report.

6. Northern Networking Events Report
David Massey presented his report stating that the BCA has 444 members, split as follows according to interest group: 93 (BSG), 167 (CCG), 65 (PCG), 48 (IG),38 (Unspecified) and 33 (Corporate), According to category this breaks down as: 212 (Ordinary), 74 (Student/retired/unemployed), 33 (Corporate), 38(Term/overseas), 25 (Life), 27 (Honorary) and 35 (unspecified). He listed all 10 corporate member companies and thanked them for their support of the BCA and said that just under 300 people were registered for this meeting. The commercial exhibition sites were all sold out and he thanked all 23 companies individually. There were 75 posters. He also thanked **Harry Powell** as outgoing Treasurer for his assistance with administration. Following feedback from previous Loughborough meetings, better signposting has been requested by NNE for Loughborough 2012.
Mike Glazer asked why the membership had dropped by half. The President replied that contributing factors included the fact that most corporate members do not take up all 10 memberships, and that the membership forms from the BSG Autumn meeting had not yet been processed.

7. Report of the Treasurer to include Presentation of the Accounts for 2010 and the Examining Accountant's Report

The Treasurer **Harry Powell** said that funds had dropped by £5K but the £12K income surplus from the 2010 Spring meeting in Warwick had assisted greatly with offsetting this. He thanked the exhibitors for enabling us to keep costs down for registrants and for their vital role in assisting the BCA. He emphasised that the attendance cost to participants for our Spring meetings has decreased over the past few years contrary to perception. The decrease in BCA funds arose from the very significant decrease in interest paid on bank accounts, the drop in membership, fewer advertisers in Crystallography News and a drop in donations. Expenditure on grants and sponsorship increased but decreased for bursaries as two cheques were sent out but not cashed. No bursary applications for ECM2010 in Darmstadt were received and he reminded everyone that the IUCr meeting was taking place this summer. The BCA accounts had been posted on the Spring Meeting noticeboard.

Mike Glazer asked about the drop in donations. The President replied that the BSG donate their bank interest every year which has been over £1K in the past but now no interest is being paid on accounts. **John Helliwell** noted the move into investments from cash. The Treasurer replied that cash was moved into investments because interest income was so low, therefore money from IUCr fund was put into medium term (2 yr) investment bonds as suggested by our advisors. Previous IUCr meetings did not want the offered money and it will not be required until 2017 (if then). The funds are not restricted for use by the IUCr Congress and it has been established from those who set up this fund that it could be used for the ECM in Warwick.

Judith Howard asked whether it was possible for Crystallography News to be produced more economically. The President said the pdf option was one move in reducing costs.

The Treasurer thanked **David Massey** and **Jennifer Kirkaldy** of Northern Networking and the group treasurers for getting their accounts in on time.

8. Acceptance of the Accounts

The accounts were accepted.
Proposed by **Arwen Pearson**
Seconded by **Pierre Rizkallah**

9. Appointment of Examining Accountant for 2011

Young and Company of Huntingdon, Cambridgeshire were reappointed as the examining accountants for the BCA
Proposed by **Susan Lea**
Seconded by **Sandy Blake**

10. Raising of membership fee for 2012 from £20 to £30 (ordinary) from £35 to £50 (student 4 year term).

The price of membership had not been increased since 2006 and with the drop in membership numbers, the increase was necessary for the well-being of the BCA. The support from the floor was unanimous. The rise in membership fees was accepted.
Proposed by **Mike Probert**.
Seconded by **Mike Glazer**.

11. Elections to Council

Alex Griffin will stand down as Ordinary member for one year and be co-opted. **Amber Thompson** was elected as an Ordinary member for 3 years unopposed.
Harry Powell is retiring as Treasurer. **Andrea Mulholland** was elected unopposed as Treasurer.

12. Co-option of Mike Probert for a further year as Education rep.

Susanne Coles asked if this post could be open to election.
Helen Maynard asked if someone could be allocated to Outreach.
An open vote took place as to whether the Education officer should be an electable post and most were in favour with one against and four abstentions. The President said that **Mike Probert** had made great efforts in convening an Education Committee but there had been little response to his request.
Ivana Evans said that one reason for a lack of response was the lack of clarification in what the role involved.
Judith Howard said such an electable post would have to be in the Statutes and would have to be voted on at the AGM in 2012. The President replied that the vote was information gathering rather than committing to an electable post.
David Beveridge suggested that we co opt **Mike Probert** for one year, then elect an Education rep. at the AGM in 2013.
Mike Probert was co-opted for one year.
Proposed by **Arwen Pearson**
Seconded by **David Beveridge**

13. "Member recruit a new BCA member"

In order to boost membership numbers, the President announced that the prize for recruiting the most new members from now until Spring Meeting 2012 will be free registration for the ECM in Warwick in 2013. Every member who encouraged someone to join the BCA should ask them to put the BCA member's name on their form. Ten new members is the minimum recruited number to be eligible for the competition. The President recounted the benefits of belonging to the BCA, in particular eligibility of student members for bursaries to attend meetings. She wanted to initiate and encourage BCA networking within a university so that BCA members from different departments and sections can assist each other with crystallographic advice and contacts but this had not been organised yet.
The big drop in membership numbers mainly arose from the many members who were still paying standing orders at outdated rates and when the BCA Bank account was closed, they did not renew. **Harry Powell** added that there were many standing orders without proper identification and many dormant members had probably forgotten or ignored their subscription, so it is possible we have only had 500 active members for many years.
Judith Howard mentioned that there used to be free registration for students and a huge effort was made to keep student numbers high. It seems that the fee differential between Ordinary "grown up" members and students has diminished over the years. The President disagreed that the Student and Ordinary Meeting fees had become closer in cost, since Students pay half the Ordinary member Spring meeting fee.
Judith Howard said that research group incomes have gone down significantly and she suggested that there should be a temporary suspension or significant reduction to meeting fees as incentive to encourage students to join.
The President expressed concern about this idea since the BCA had made a loss on the York meeting but had then

managed to claw back the losses from the subsequent meetings.
Mike Glazer suggested that ECM2013 would be a great opportunity for recruitment and we should consider BCA membership for attendees. The President considered this possible for UK attendees.
John Evans spoke to clarify the reasons as to why the York meeting made a loss. This was because of an administrative error which was not in the hands of the organiser or Council. The President concurred with this and said the loss was not due to lack of attendees either. York charged a premium for a late booking arising from a requirement to change from the previously arranged venue.
Jeremy Cockcroft asked about using Internet banking to pay BCA membership fees and said that some possible members were put off by direct debits. He also mentioned that membership records were inaccurate. The President said Council would consider internet banking and that considerable efforts had been made by Council to track bounced emails and correcting them, but she agreed that there was still room for improvement.
Edward Bilbe asked whether the meeting could be moved to a more central location since all recent meetings appear to have been in the "north". The President said that north was a relative concept in that Durham is south of where she was from in England. However this raised a key point in that suitable Spring meeting venues are becoming more limited in number. The few universities who have not yet gone over to the semester system were still available and she asked members to notify her if they knew of any suitable Spring meeting locations.
Jamie Gould said he couldn't find his membership records on the website and was not sure that he was a member. The President asked him to get in touch with herself or the Secretary who would ask NNE to correct any errors.
Since the BCA's contract with Northern Networking is due to expire at the end of March 2012, the Association will be tendering for a new 5 year contract. the President said that the Officers are currently writing tenders to make it possible for the keeping of the membership records and the meeting administration to be treated as either separate activities and placed with different providers, or be together and both with one company.
Andrew Goodwin commented that new members will be found amongst students as he expected established academics to be members. He suggested making student membership much cheaper since the BCA will be a secondary membership for many people. **Claire Murray** asked about getting new members, in that how were we to encourage people outside the main established crystallography groups to join us since most of the established groups are represented here at the meeting. The President encouraged older academics to encourage their students to come and join the BCA so that they are eligible for bursaries for subsequent meetings. **Edward Bilbe**, after discussion with other students, mentioned that a small fee decrease would not change the attraction of membership to students.

14.The IUCr computing school
Harry Powell announced that the IUCr Computing school will be held in Oveido in August 2011 and that bursaries are available. He described it as an excellent opportunity to learn how to write crystallographic programs from many key authors of established crystallographic computer programs.

The President reminded members that the deadline for IUCr Congress abstract submission was this week.

15.ECM 2013 organising committee: Secretary, Treasurer and focus area reps.
Sandy Blake has prepared a blue print on how to run this ECM meeting and the President asked for representatives for five focus groups which she listed. These representatives need to be in contact with the relevant ECM2013 program chairs. Interested members were asked to contact **Sandy Blake**, the President or the Secretary.

The meeting closed at 7pm.

Georgina Rosair (Secretary to Council)

2012 Annual General Meeting of the BCA

The Annual General Meeting of the British Crystallographic Association will be held on Wednesday 18th April 2012 at 6.00 p.m. at the University of Warwick.

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

Draft Agenda

1. Approval of Agenda

2. Apologies for absence

3. Minutes of the last AGM (published in Crystallography News)

4. President's Report

5. Secretary's Annual Report

6. Northern Networking Events Report

7. Report of the Treasurer to include Presentation of the Accounts for 2011 and the Examining Accountant's Report

8. Acceptance of the Accounts

9. Appointment of Examining Accountant for 2012

10. Approval to hold the BCA AGM in 2013 at the ECM in 2013.

11. Arrangements for appointing the BCA Education Officer

12. Elections to Council

13. Any other business

Georgina Rosair (Secretary to Council)

ICDD News

Robert L. Snyder Student Travel Awards

THE International Centre for Diffraction Data is pleased to announce the Robert L. Snyder Student Travel Awards, which honor the life and work of Robert (Bob) L. Snyder. These awards offer limited travel support which allows undergraduate and graduate students to attend the Annual Denver X-ray Conference. **Bob** devoted a great deal of energy in cultivating future X-ray analysts, and it is with this award that the ICDD strives to continue his mission.
Students granted the award must participate in the technical program of the conference by submitting an abstract for oral or poster presentation. Grants in the amount of $500 will be awarded to students living in the USA, and those living outside of the USA will receive $1,000. Applications are reviewed on a competitive basis. To apply for a student travel award, students must submit an application, a copy of the abstract for oral or poster presentation at DXC, and a supporting letter from an advisor. The deadline to apply is 1 May each year.
As an outstanding educator and researcher, **Bob** was Professor Emeritus of Ceramic Science at Alfred University, Chairman of Material Science and Engineering at The Ohio State University, and co-chair of the School of Materials Science and Engineering at Georgia Tech. He also served as chairman of both the ICDD and the Denver X-ray Conference. **Bob** was known for his passion for science and life, which was evident in his extensive travel and interactions with scientists from around the world.

Submit an application to:
International Centre for Diffraction Data
12 Campus Boulevard
Newtown Square, PA 19073-3273
dxctravelgrants@icdd.com
Fax: **610 325 9823**
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Sanibel Harbour Marriott Resort & Spa
Fort Myers, Florida, USA
15 – 18 May 2012
Sponsored by the International Centre for Diffraction Data

THE ICDD is pleased to present this unique symposium focusing on cutting-edge topics surrounding the combined fields of Pharmaceuticals and X-ray Powder Diffraction. The symposium includes an optional one-day workshop, and two half-day sessions. Abstracts are currently being accepted for both oral and poster sessions, and the deadline to submit an abstract is 20 February 2012. Visit our web site: www.icdd.com/ppxrd to submit an abstract and view more details regarding the event.

SPECIAL SESSIONS, 16–18 MAY 2012
Subject to change depending upon abstracts submitted. Please check our website regularly for updates.

AMORPHOUS, ACTIVATED AND NANOMATERIALS
Chair: **Peter Varlashkin,** GlaxoSmithKline, Durham, NC
Invited Speaker: **Lian Yu**, University of Wisconsin, Madison, WI

XRPD STRUCTURAL TECHNIQUES (ACQUISITION AND USE OF XRPD DATA, INDEXING, STRUCTURE DETERMINATION, RIETVELD REFINEMENT)
Chair: **Arnt Kern**, Bruker AXS GmbH, Karlsruhe, Germany
Invited Speaker: **Marc Garland**, ICES, Jurong Island, Singapore

FORMULATION & PRODUCT DEVELOPMENT
Chair: **Detlef Beckers**, PANalytical, Almelo, The Netherlands
Invited Speaker: **Peter Wildfong**, Duquesne University, Pittsburgh, PA

CRYSTAL STRUCTURE PREDICTION
Chair: **Tim Fawcett**, ICDD, Newtown Square, PA
Invited Speaker: **James A. Kaduk**, Poly Crystallography, Inc. and Illinois Institute of Technology, Naperville, IL

POLYMORPH & SALT SCREENING
Chair: **Greg Stephenson**, **Eli Lilly** and Company, Indianapolis, IN
Invited Speaker: **Pingyun Chen**, Catalent Pharma Solutions, Morrisville, NC

NEW FRONTIERS IN XRD IN PHARMACEUTICAL R&D
Chair: Cyrus Crowder, ICDD, Newtown Square, PA

COMPLEMENTARY TECHNIQUES
Chair: **Fangling Needham**, ICDD, Newtown Square, PA

REGULATORY AND PATENT ISSUES
Chair: **Shawn Yin**, Bristol-Myers Squibb Company, New Brunswick, NJ
Invited Speaker: **Andrew Raw**, FDA – Center for Drug Evaluation and Research, Rockville, MD

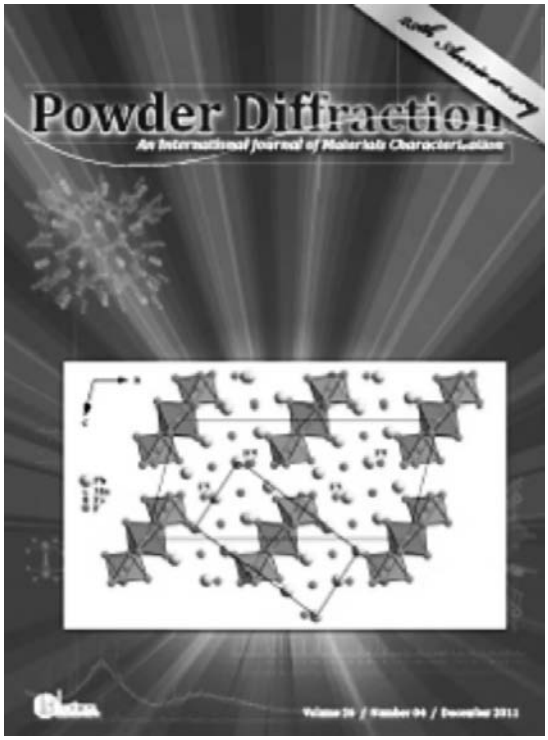
OPTIONAL WORKSHOP, 15 MAY 2012
UNDERSTANDING AMORPHOUS PHARMACEUTICAL MATERIALS—FORMULATION & CHARACTERIZATION
Organizer: **Shawn Yin**, Bristol-Myers Squibb Company, New Brunswick, NJ
Instructor: **Lian Yu**, University of Wisconsin, Madison, WI

POSTER SESSION, 16 MAY 2012
An evening reception and poster session of submitted papers will be held in the exhibit hall. See guidelines for submission of poster abstracts on our web site: www.icdd.com/ppxrd

EXHIBITION, 16 – 17 MAY 2012
Concurrent with the symposium, evening poster session and reception will be a commercial exhibition of analytical instrumentation and related products and services. To learn more about exhibit reservations and sponsorship opportunities, please see complete details about exhibiting in our Exhibitor Open Bid Packet.

Powder Diffraction journal to be published by Cambridge University Press

THE International Centre for Diffraction Data (ICDD) and Cambridge University Press announced that they have formed a new publishing partnership to produce ICDD's flagship journal, Powder Diffraction. *Powder Diffraction* will be published by Cambridge from 2012, in partnership with ICDD, a non-profit scientific organization



dedicated to publishing powder diffraction data for materials identification.

Powder Diffraction, a quarterly journal, brings cutting edge research and new advances to a global community of scientists on behalf of the parent institution, ICDD. The journal has been consistently recognized as the leading international materials science journal most frequently used to aid material identification and analysis. Due to the interdisciplinary nature of its papers, *Powder Diffraction* has wide appeal to a great number of sciences, including materials science, chemistry, geology, environmental science, and biology. Although practice is emphasized, theory is not neglected, especially as its discussion relates to better understanding of technique. The editorial focus will remain on a diverse selection of practical applications of diffraction methods analysis, standard reference materials, search/match methods, the indexing of powder data, and structure solutions from powders.

Together, Cambridge and ICDD will partner to strengthen *Powder Diffraction* in terms of reach and impact. The journal will be hosted on Cambridge's cutting-edge electronic platform, Cambridge Journals Online (http://journals.cambridge.org), and will include increased usability, increased functionality and many new features to enhance and optimize article usage.

Jamie Hutchins, Head of Journals - Americas, said: "By publishing *Powder Diffraction*, Cambridge furthers its position in the physical and materials sciences. As publishing partner, we will assist the ICDD in disseminating their high-quality research to the widest possible audience. We are honored that Cambridge is seen as a worthy home for their journal."

Timothy Fawcett, ICDD Executive Director, said: "The ICDD is very excited to have Cambridge University Press as our new publisher for *Powder Diffraction*. ICDD database products and educational services are currently delivered to thousands of scientists in over 110 countries and we believe Cambridge University Press's global publishing network will enable us to reach scientists in every region of the world."

Cambridge will publish *Powder Diffraction* from March 2012 Volume 27, Issue 1.

Control and Prediction of the Organic Solid State - Crystal or Not, Where Do We Go From Here?

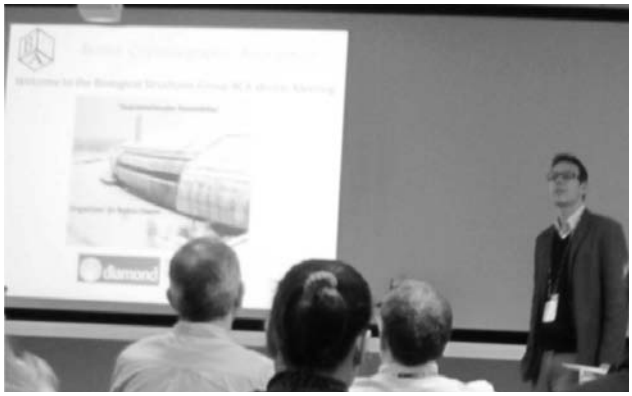
THE 2012 Open Meeting of the CPOSS project will be held at UCL on Tuesday 3rd April 2012. The theme of the meeting will be "Crystal or Not, Where Do We Go From Here?", and will consider what we can learn about the organic solid state from combining a range of experimental and computational methods. Speakers will include **Jon Steed** & **Sharon Cooper** (University of Durham), **Simon Gaisford** (UCL School of Pharmacy), **Sally Price** (UCL), and **Alastair Florence** (University of Strathclyde). **Paul Raithby** and **Chick Wilson** will be presenting the roadmap for directed assembly of organic crystal structures with targeted properties.

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

cposs

BCA – BSG Winter Meeting 2011, Diamond Light Source

THIS year's BSG Winter meeting was organised by Robin Owen with the aid of his three chairmen, Alex Cameron, Simon Phillips and Kostas Beis. The excellent programme attracted over 100 delegates and the topic 'Supramolecular Assemblies' was nicely addressed with a broad range of talks ranging from protein dimers, to large multi-subunit complexes, and finally to whole virus capsids. The presentations embraced the latest technology with some beautiful illustrations and movies revealing how state-of-the-art crystallography can help to unravel complex biological mechanisms. The meeting report below was written by one of our youngest delegates, **Richard Martin**, a PhD student from the University of Portsmouth.
John McGeehan, BSG Secretary



This was the first BSG winter meeting I had attended and I found it very friendly and engaging. The talks were excellent and presented interesting work with a wide array of novel high resolution crystal structures. An introduction was given by **John McGeehan** on behalf of Council and **Elspeth Garman**, highlighting the advantages of membership to the BCA and encouraging attendance at the upcoming Spring meeting. Preparations are now underway for the European Crystallography Meeting in 2013 and the website is now available at ECM28.org.

The first talk was presented by **Gabriel Waksman** who showed the mechanism of bacterial pilus biogenesis through structural biology. The results covered several high resolution protein structures, including the large membrane β-barrel usher complex that acts as an assembly platform for the growing pilus. Co-expression and crystallography of the usher, chaperone and adhesin complex (FimD bound to its cognate FimC-FimH substrate) revealed how donor strand exchange can mediate efficient subunit assembly and translocation across the outer membrane. This talk was a great example of using multiple structures to give an overall mechanism for a much larger system and this was beautifully illustrated in several movies.

Colin Kleanthus spoke on transmembrane signalling through bacterial porins. He revealed a mechanism for epitope delivery whereby an entire soluble protein domain of the bacteriocin ColE9 is inserted in the outer membrane protein OmpF. The structure of the OmpF-OBS1 complex showed the colicin bound within the porin lumen spanning the membrane bilayer and reveals how colicins exploit porins to deliver their epitope signals to facilitate cell killing. Again this talk featured several structures to show an overall mechanism and I found the insertion of a disordered polypeptide into a tight and highly selective membrane pore very interesting.

Leo Sazanov presented a talk on the structure of respiratory complex I, a bacterial homologue of the first protein complex in the eukaryotic mitochondrial electron transport chain. The talk featured electron microscopy models of the complete complex and subsequent crystallisation and structure solution. The talk demonstrated the difficulties in large membrane protein crystallography, including a slide presenting the very large volumes of bacterial culture (1300 litres!) and purified protein (600 mg!) required to yield this high resolution structure. The talk also covered many practical issues such as anisotropy and ways to reduce it. The final structures presented were fascinating

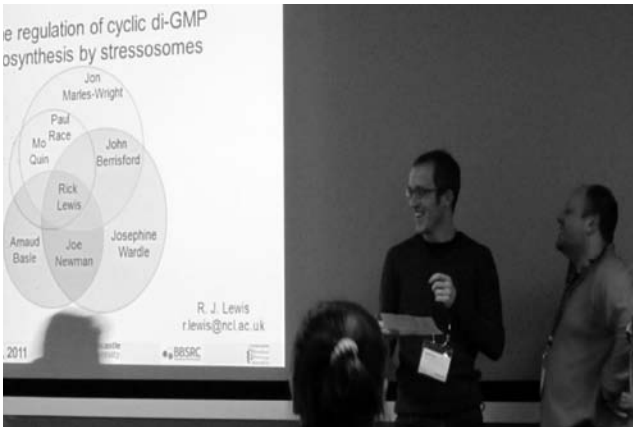
and gave great insight into the mechanisms of proton transport with a nice analogy to the steam engine design by **James Watt**.

Following an excellent lunch in the Diamond atrium, **Rick Lewis** presented a very engaging talk on his work on the stressosome, noting first that the 4% ethanol required to elicit the stress response from *B. subtilis* was clearly lower than that required by some of the delegates in the front row! His talk covered multiple techniques to analyse the structure of these very large protein complexes including electron microscopy and some beautiful three-dimensional immunofluorescence that was able to identify the location of around 20 such complexes per cell. Rick described the multitude of signalling proteins including YtvA and their interactions with the RsbR and RsbS complexes and finished with some structural insights into the resetting of the stressosome complexes via the interaction of the PP2C phosphatase.

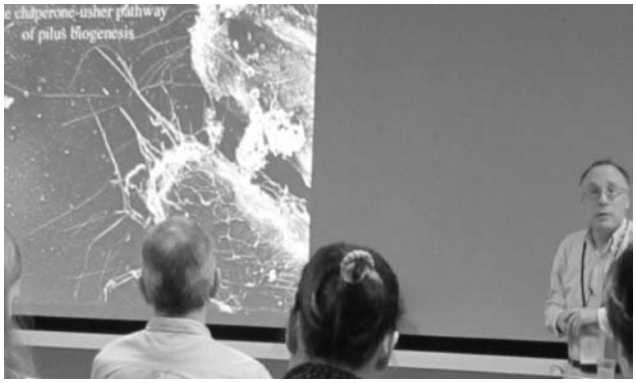
Helen Walden presented a very nice story on the FANCL protein of the Fanconi Anemia pathway. With contributions from 15 genes already identified and several complexes contributing to DNA recognition, ubiquitination and repair, this represents a significant challenge to structural biology. I especially liked Helen's comparison of crystallography to a game of snakes and ladders with sudden jumps ahead and unforeseen setbacks. The protein structure presented a novel fold and turned out to be extremely different to the WD40 propeller prediction. I was also intrigued by her observation of improved resolution with certain heavy atom soaks and this is definitely something I will take away with me. In addition to these crystallography experiments, NMR and site-directed mutagenesis were employed to analyse the binding of ubiquitin, while ITC, size-exclusion chromatography and a cell biology system were used to put the structural studies into a biological context.

The third talk of the second session by **Chang-jiang Dong** was very interesting and presented a structure-function mystery. The structure of a viral genomic RNA protection protein solved by x-ray crystallography was shown to be almost identical to an exonuclease. *In vitro* assays confirmed that the protein did indeed have exonuclease activity and that this is necessary for the inhibition of interferon production. Despite high-resolution x-ray data, significant issues caused by twinning had to be overcome before selenomethionine phasing was successful. This talk was a good example of how knowing the atomic structure of a protein does not necessarily answer all the questions you have about its function.

The final session of the day started with a talk from **Peter Cherepanov** on the structure and function of the retroviral integrase. The structural history of the integrase was based on individual domains of the full length protein, however, even the 2-domain structures did not fully illuminate the mechanism and, importantly, the drug interactions. This was a case of "only the full length protein will do" and significant effort was required, including 32 constructs and 40,000 crystallisation conditions before a suitably well diffracting crystal was produced. I found it very interesting as the final structures included protein-nucleic acid complexes, my own area of research. The structural biology revealed very clearly the mechanism of DNA integration into the host genome. Insights into future drug design were given by comparing various drug-bound structures, revealing a highly rigid active site, and thoughts to the future included further studies on the interaction of the integrase with chromatin.



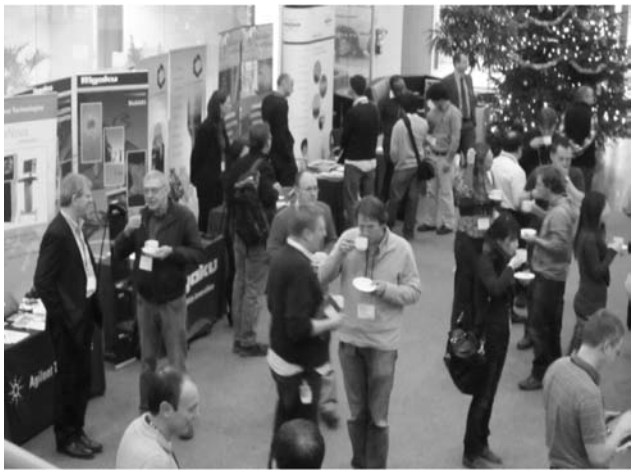
Phil Kerry's talk on the influenza protein NS1 was a good example of a protein that interacts with many other proteins. The part of the talk that stood out for me was that the original structure of this protein was shown to be in a particular dimeric form. However, when other structures were solved, alternative dimeric structures could be proposed as the biological unit. This demonstrates the need for multiple crystal forms where possible to aid in the interpretation of biological interfaces and interactions. The use of multiple structures from a range of viral clades revealed flexibility in the dimeric organisation and may relate to how this central viral protein interacts productively with such a wide range of protein partners.



The final talk of the meeting focused on structural vaccinology with **Dave Stuart** giving an engaging presentation beginning with an introduction to the history of vaccines and diseases such as polio. He showed how small changes in the large protein complexes that form viral capsids can have important consequences for stability, a property of critical importance for an effective immunogenic vaccine. Several movies demonstrated how capsid structures can adopt multiple conformations to allow both the protection and transport of their nucleic acid cargo and the subsequent release into the cell. An ideal system would be to employ viruses lacking nucleic acid. However, such empty particles were shown to lose their typical icosahedral symmetry, undergo an expansion of around 4% and become generally unstable. Structure-based design was used to construct stabilised picornavirus particles and preliminary trials in cattle demonstrate not only an increase in antibody production but also a 50% increase in protection from challenge with live virus. These studies hold great promise for the production of next-generation vaccines for both agriculture and human disease.

Overall the talks were very interesting and covered a wide array of supramolecular complexes, the significant challenges they present and the amount of useful information structural studies can yield. There was also extensive use of molecular graphics and movies, which helped the understanding of complex biological systems. There were many ideas and practical suggestions to take away from this meeting and I would recommend future meetings to anyone interested in structural biology.

Richard Martin, PhD Student, University of Portsmouth



(photography Rhiannon Lloyd)

CCG Autumn Meeting 16th November 2011

THE CCG Autumn Meeting entitled 'Dealing with Difficult Problems' was successfully held at the Research Complex at Harwell on the 16th of November 2011. The meeting was kindly sponsored by Agilent Technologies and the Research Complex at Harwell to whom we are very grateful. Thanks at this point should also go to **Mairi Haddow** for managing the registrations, and **Simon Coles** for organising an interesting program tackling various aspects of difficult structure determinations and experimental techniques. The day's talks began with **Loes Kroon-Batenburg** describing recent developments within EVAL-15 to improve integration by taking account of factors such as beam profile, crystal mosaicity and crystal shape; she gave particular focus to dealing with twinned structures and discussed planned future developments for more challenging data analyses. **Zoltán Gál** followed with examples of six of the more tricky data collections that he had encountered from visitors to their labs such as charge density data collections on compounds showing bromine-bromine interactions and high pressure studies of proteins! Following lunch and a chance to catch up with other delegates **Richard Cooper** took a look at the Hirshfeld test and provided insights into approaches to improve uncertainties on certain parameters by using

efficient strategies for the collection of additional data. The second speaker of the afternoon **Horst Puschmann** described their recent additions to the capabilities within the small molecule computational toolbox and gave a demonstration of the Olex2 software which provides a user-friendly interface to these programs enabling structure refinement and data analyses to be easily performed. After coffee **Helena Shepherd** discussed the properties of a number of spin crossover complexes she had studied; the results presented were obtained by combining data from crystallographic and other analytical techniques and gave novel insights into spin crossover behaviour. The final speaker of the day **Claire Wilson** gave a summary of the facilities available at the national crystallographic service and on I19 as well as discussing some of the more challenging, just crystalline, specimens that she had encountered. Overall thanks to the variety of talks and enthusiasm of the speakers this meeting provided attendees with an interesting and informative day of talks and hopefully new ideas for tackling difficult problems.

Hazel Sparkes
CCG Chair.

Speakers at the CCG Autumn Meeting from left to right: Horst Puschmann, Helena Shepherd, Zoltán Gál, Loes Kroon-Batenburg, Richard Cooper, Claire Wilson

BCA Joint XRF/XRD Meeting at the University of Leicester on May 23rd and 24th 2012

British Crystallographic Association
INDUSTRIAL GROUP
A UK Charity (284718) with an Educational remit

23 May 2012
XRF USER MEETING

CALL FOR PAPERS:
We are seeking offers of talks from XRF users at this meeting - please consider giving a talk and send details to any committee member. The format of the meeting will follow that of previous successful one day meetings.

Speakers include:
"XRF Fusion: Development and Application of Internal Standard Method for High Accuracy Analysis", **Frederic Davidts**, Socachim.

Your talk title could be here!

24 May 2012
XRD USER MEETING
We will be holding the XRD meeting on the 24th. Although we are still compiling the program we have decided to divide the day into two themes. Most of the morning will be taken up with discussions regarding good practice in XRD and phase identification; with or without the ICDD data base:

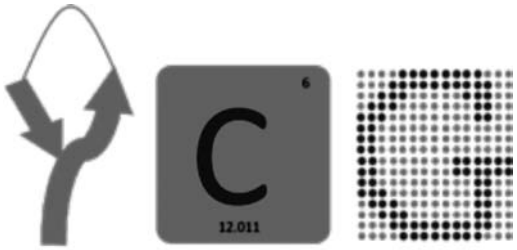
- Optimising your Diffractometer (**Judith Shackleton**).
- Phase ID with the Powder Diffraction File (**Dave Taylor**).
- Phase ID of Geological Materials (**Cheryl Haidon**).
- Discussions, question and answer session (led by **Dave Taylor**). Please come primed with your questions and the whole group will try and answer them....or at least find someone who can! Also, if you have discovered a really useful tip, please come along and tell everyone.
- We will also consider whether there is support for an ICDD Phase ID Workshop to be held at a future meeting.

The theme for the afternoon session will be "Earth Sciences" as well as "Crystallography in Industry". We have two confirmed speakers.
Sandie Dann (University of Loughborough, Department of Chemistry) will be speaking, and **Jennifer Graham** (University of Leicester, Department of Geology) will give a talk entitled "Using PXRD in Support of the Investigation of Lithofacies in Carboniferous Mudstones".

We are looking for more speakers to complete the afternoon program; please volunteer. Talks are not restricted to the theme of "Earth Sciences" We are looking for a speaker to discuss the effects of geology on the characteristics of whisky. We have held similar events discussing beer and wine at previous May meetings and hope to include a tasting session. Registration details will be available on our website soon.

CALL FOR PAPERS: We are seeking offers of talks from XRD users at this meeting - please consider giving a talk and send details to any committee member. The format of the meeting will follow that of previous successful one day meetings.

Young Crystallographers Satellite meeting 2012



THE Young Crystallographers Satellite meeting will take place in the traditional slot immediately preceding the BCA Spring meeting in Warwick on the 16th and 17th of April. There will be three sessions packed with oral presentations from Young Crystallographers as well as more established plenary speakers. There will also be an opportunity to present a flash presentation of your poster after the AGM on the Monday night.

The final session has previously been a careers session, and building on the success of this, we have dedicated this to science outreach this year. **Jessica Bland** from the Royal Society has agreed to speak about her work in public outreach in science, and this will be well worth attending. As always, there will be no registration fee for attending the Young Crystallographers Satellite (accommodation not included). There will be a poster session and a buffet dinner on the Monday evening. This is a great opportunity to present your work to your peers and is a fantastic way to meet people from different universities. There are a limited number of bursaries available for the meeting so please see the BCA website for further details.

This year there were a fantastic number of abstracts submitted for Young Crystallographers Oral Presentations. Unfortunately this will also mean that not everyone who applied will be able to speak, but I would like to take this opportunity to thank everyone who submitted an abstract for this meeting, and encourage you to try again in 2014. I hope this is a good sign of things to come.

Finally, if you are interested in becoming more involved with the YCG and would like to join the committee, then keep an eye on our website where we will be announcing any vacant positions.

I look forward to seeing you all in Warwick.

Duncan Sneddon

Café Scientifique

THE Young Crystallographers recently had the pleasure of inviting Prof. Chick Wilson to speak at a Cafe Scientifique in Reading. Held in association with the British Science Association in Reading, Cafe Scientifique is a place where, for the price of a cup of coffee or a glass of wine, anyone can come to explore the latest ideas in science and technology. A somewhat daunting task, but **Chick** was more than up for it. Armed with only two props, he enthralled the large crowd of more than 70 people with tales of pharmaceutical problems with polymorphs. The story of Cocoa Butter form V and VI particularly caught the imagination of many people, and the speaker and audience alike all enjoyed a nice square of the good stuff in the interest of science! The public were very eager to discuss the topic further, and the question session that followed the main event lasted for nearly an hour, with questions flying about liquid crystals, drug potency, and even the many forms of ice. A wonderful evening was had by all, and as the session chair quipped: 'it is nice to see that all the Young Crystallographers are sitting together neatly in rows!'

Claire Murray

Scientific Controversies and Crystallography

SCIENTISTS love to read an upbeat account like the discovery of X-ray diffraction and its rapid acceptance. We also love to read stories about embattled scientists like Galileo and Darwin who were assailed by non-scientists for unscientific reasons but ultimately prevailed. Far more painful are stories about scientists who put forward correct new ideas that were attacked and ridiculed by their own fellow scientists. Two such figures from the last century were **Alfred Wegener** and **Barry Marshall**. Their biographical details are well presented on Wikipedia. Incidentally, I used the English-language Wikipedia for my initial research; but when I attempted to follow it up on January 18, this source had closed down for the day. Reading the German-language www.wikipedia.de. Instead I found that significant factual information was available on one of the Wikipedias but not the other.

Wegener proposed the theory of continental drift, which ultimately led to plate tectonics. Initially he noted the shape complementarity of Europe, Africa and the Americas and suggested that they had once formed a supercontinent before drifting apart. Critics quite reasonably countered that the shape match could be fortuitous. Wegener provided a detailed analysis of rocks and fossils, showing that they were very similar across the joints in his proposed supercontinent. His blinkered opponents could only imagine the continents sailing through the viscous mantle like ships sailing through treacle, and they continued to ridicule Wegener. He went on to make his name in Arctic meteorology. In 1930 he led an expedition to establish an observing station to measure winter weather conditions in the middle of Greenland. Bad autumn conditions prevented the transport of sufficient supplies to the station. Having been funded by the German government at a time when some Germans were starving, Wegener felt a strong obligation to make the expedition a success. When winter had already started, he and a colleague took a dog-sled with the missing supplies to the station. On the way back, to lighten the load on the sledge when they only had a minimal number of dogs, Wegener proceeded on skis, but the exertion was too much for this 50-year-old smoker; and he died, presumably of a heart attack.

By the early 1980s most medical scientists believed that gastric and duodenal ulcers were a mature research field not requiring further investigation. It was an established dogma that bacteria could not survive in the strongly acidic contents of the stomach. Ulcers were attributed to excessive acid secretion induced by stress, spicy food and smoking, augmented by a hereditary predisposition. In fact, a few microscopists identified *Helicobacter pylori* in gastric washings from ulcer patients and animals at the end of the 19th century, but it was dismissed as a contaminant or a transient harmless commensal. More systematic studies by the pathologist and surgeon **Georg Ernst Konjetzny** from the 1920s to the 1940s found *H. pylori* in samples from many patients. However, unlike the courageous and principled **Max von Laue**, who shunned Nazi science, Konjetzny joined the Nazi party. Possibly because of his nasty political affiliation, his work was not followed up after the war. In Perth, Australia, in 1981 microbiologist **Barry Marshall** and pathologist **John Robin Warren** established an association between ulcers and the bacteria with impressive statistical validation. However, their results were not generally accepted, and one reason was that they had not yet satisfied all of Koch's Postulates. It was necessary to show that starting the infection in a healthy subject induced the disease. Marshall administered the bacteria to piglets, but they grew into inconveniently large healthy pigs with no sign of *H. pylori*. Marshall solved the problem by drinking a culture himself. Within a few days he developed severe gastritis, and a biopsy showed large numbers of *H. pylori* and pus cells. It took until 1989, but Marshall and Warren's methods of diagnosis and treatment were finally accepted, and they received a Nobel Prize in 2005. Marshall's Nobel Lecture, complete with a comic book illustration, is very entertaining.

By now you are probably wondering what all this has to do with crystallography. Geologists and medics may be prejudiced, but surely crystallography is so evidence-based and crystallographers are so open-minded that it could never happen to us. Well, it could and it did! Exactly 50 years ago **D. June Sutor** published a paper in *Nature* that presented a geometrical analysis of C-H...O interactions in crystals that was intended to confirm the presence of hydrogen bonding. However, the idea of C-H...O hydrogen bonding was condemned by some prominent crystallographers in the 1960s. For the next two decades only the bravest authors referred to "C-H...O hydrogen bonding". Others tiptoed around the subject with terms like "C-H...O interactions". I have submitted to *Crystallography Reviews* a review article about this controversy, including an analysis of the evidence available in the 1960s.

CCP4 at Warwick

THE annual Collaborative Computational Project in Macromolecular Crystallography (CCP4) Study Weekend was held at the University of Warwick on January 4-6, 2012. This is the first of three key crystallographic-focused meetings that will be held at this venue this year and next, soon to be followed by the annual British Crystallographic Association meeting, April 16-19 and then the European Crystallographic Association meeting, August 25-29, 2013. This meeting, entitled "Data Collection and Processing", covered the latest developments in these early steps of protein crystal structure determination. The scientific programme was organised by **Johan Turkenburg** (University of York, UK) and **Katherine McAuley** (Diamond Light Source, UK). Registered participants numbered 419 and drew scientists from a diverse range of academic and industrial institutions in the UK and from 15 other European countries as well as the United States, China, India, Brazil, Canada and Singapore.

The first session, "Introduction to Meeting Themes" opened with **Johan Turkenburg** and **Katherine MaCauley**, jointly welcoming the participants and reminding them of the important benefits that new macromolecular crystallographers extract out of the CCP4 study weekends, particularly for scientists new to the field of crystallography.

Zbigniew Dauter (National Cancer Institute, USA) then followed with his talk, "Effective Data Collection and Processing". He described numerous examples of common pitfalls and consequences of poor data acquisition, which occur in spite of good access to advanced hardware and sophisticated software. He explained how good data acquisition has the potential to yield benefits at latter stages of crystal structure determination. For example, the quality of refinement would certainly be improved by using as complete data as possible collected at the highest resolution possible. Thus, collection of high resolution data can be facilitated using a multi-pass strategy to minimise radiation damage. In contrast, acquisition of a high quality medium resolution data set (with no overloads!) benefits both molecular replacement structure solution of protein molecules as well as heavy atom sub-structure solution. Acquisition of high quality, accurate anomalous diffraction data can be maximised by using strategies aimed at minimising radiation damage that also focus upon collection of complete low resolution data. He commented that the type of detector one uses, in general, is largely insignificant as most modern detectors give comparable quality data sets; however, optimisation of collection parameters/ hardware is worth some attention. For example, the width of rotation width per frame should be chosen to minimise overlaps; fine phi-slicing enables the use of three-dimensional profile fitting; and the availability of a kappa goniometer allows optimisation of crystal orientation to avoid overlap and to record complete data sets. He also pointed out the importance of both understanding what data quality indicators mean and how to use them correctly.

James Holton (University of California at San Francisco, CA, and Lawrence Berkeley National Laboratory, Berkeley, CA, USA) then presented his talk "Signal vs Noise: Where They Come From and How to Tip the Balance in your Favour". Based on statistics from his beamline, he estimated that his facility has the capacity to collect up to 20 million data sets per year; but that the true number of collected datasets that prove useful in structure solution is orders of magnitude less, and ultimately yields about 100 PDB depositions per year. He then described a study he undertook aimed at trying to understand why the majority of datasets collected were not useful in structure solution, using a set of 2500 data sets. His work suggested that signal-to-noise levels significantly influence whether individual data sets were of value in a structure solution. He categorised sources of increased noise vs signal into three groups: i) photon-counting error proportional to the square root of the signal; ii) noise that is independent of the signal, e.g. read-out noise; and iii) fractional noise proportional to the signal. The third group has many contributors including but not limited to optimum exposure time, optimum size of the crystal, background reduction, beam flicker, shutter jitter, and detector calibration. Spot overlap was a significant problem, surpassed only by radiation damage. This last source of augmented noise would halve the lifetime of the sample after a dose of 10 MGy for diffraction up to 1.0 Å, 20 MGy for diffraction up to 2.0 Å and 30 MGy for diffraction up to 3.0 Å. Many recommendations were made to reduce radiation damage, emphasing the need to take time to establish dosage limits for specific samples as these can vary considerably.

The post-lunch session, "Fundamentals", opened with **Andrew Leslie** (Medical Research Council Laboratory of Molecular Biology, Cambridge, UK) who spoke about "Autoindexing: In Theory and In Practice." He described the theoretical basis of the Fast Fourier Transformation (FFT) used in autoindexing of a diffraction image. His slides were well-illustrated and he used an Ewald sphere simulation (mpeg) to illustrate the diffraction principle. The FFT method is implemented in MOSFLM, to find the reduced cell and assign the Bravais lattice and in certain cases the correct point and space groups. He also discussed various practical aspects involved in processing diffraction images.
James Pflugrath (Rigaku Americas, The Woodlands, TX, USA) introduced "d*TREK – A Device-Independent

Diffraction Image Processing Suite." The interface he developed includes both a graphical user interface and scripting for automated processing for use in high throughput applications. He described the methods incorporated to optimize data collection strategies. These include crystal ranking based on 10-11 rules after autoindexing.

Phil Evans (Medical Research Council Laboratory of Molecular Biology, Cambridge, UK) then presented his talk "How Good Are my Data and What is the Resolution?" He elaborated on the next step after integration: data reduction. This involves point group determination, putting the integrated intensities to a common scale and averaging symmetry-related reflections. These could be done by programs POINTLESS and SCALA, which will be replaced by a new scaling program, AIMLESS in the near future. He described the various statistics that provide the first important measures of data quality. Assessing the maximum resolution limit generated a lively discussion after his presentation.

Kay Diederichs (Universität Konstanz, Konstanz, Germany) ended this session with "Data Quality Measures that Are or Should be Used." He discussed theoretical and practical aspects to establish a direct quantitative relation between X-ray diffraction data and model quality. He elaborated on the definition and use of the various R-factors (together with (I)/sig(I) values) to decide high-resolution cutoff, which is a common type of disagreement between journal authors and their reviewers. He pointed out the not commonly realised fact that some of the scaling programs output unmerged and others merged (I)/sig(I) values, which cannot be directly compared with each other.

The final session of the first day, "Data collection techniques" covered challenges in diffraction at diverse sources, from electron microscopes to the X-FEL and the more familiar synchrotron. **Jan Abrahams** (Leiden University, Leiden, The Netherlands) in "Processing Electron Diffraction Data of 3D Nanocrystals," highlighted the common ground between these techniques. He opened his talk by posing the 'real' phase problem in crystallography: moving from solution to liquid. Electron diffraction offers a means of obtaining data from protein nano-crystals and new technology in the form of the medipix detector is making this possible with greatly reduced exposure times and hence absorbed doses.

Thomas White (Centre for Free-Electron Laser Science, DESY, Hamburg, Germany) followed with "Crystallographic Data Processing for Free-Electron Laser Sources." He explained that at the free electron laser, the question of tolerable dose can be ignored as each crystal is subjected to a very short single shot. The resulting huge volumes of data represent challenges in terms of indexing and integrating. A large fraction of reflections are partially recorded: the 'partialator' offers a means of scaling these and further improving the already impressive results obtained.

Andrew McCarthy (EMBL Grenoble, Grenoble, France) presented "The Use of a Mini-Kappa Goniometer Head in Macromolecular Crystallography Diffraction Experiments." He described how optimal data can be obtained from crystals through careful orientation of the crystal in a synchrotron environment. This can be achieved through use of kappa goniometry. Exploiting multiple axes of rotation through use of STAC software can lead to improved data enabling high energy S-SAD and successful structure solution from extremely weak anomalous data.

Gwyndaf Evans (Diamond Light Source, UK) end the session with "Micron Sized X-ray Beams and Their Application." He introduced the features of micron-sized beams and the application of these sources to not only small crystals but also well diffracting sub-regions of larger badly ordered samples. Key to the success of micro-crystallography is full exploitation of tools such as the diffraction grid scan and helical data collection. Careful use of these tools allows optimal data to be collected and was shown to aid structure solution from crystals <2 μm in size.

The first session on Friday morning "Software for data collection and processing" began with a talk by **Alexander Popov** (ESRF Grenoble, Grenoble, France) "Features and Development of BEST." BEST is a program for providing an optimum data collection strategy/plan. It uses RADDOSE for minimizing radiation damage, and implements this strategy in a number of ways including using multi-wedge data collection protocols, increasing exposure times during experiment, and carrying out helical scans. BEST is used routinely at the ESRF. Notably, radiation dose is currently not taken into consideration in Diamond Light Source data collection strategy scripts but after the presentation several users were prompted to ask whether this may be changed in the future.

Graeme Winter (Diamond Light Source, UK) followed with "You Cannot Get the Staff: an Electronic Alternative." He discussed of the xia2 system, available at Diamond Light Source. The system was conceived as an automated system for the automated processing and analysis of reasonable data (requiring little user intervention). It is an expert data processing pipeline (for indexing, integration, and scaling) that includes the use of MOSFLM, XDS, and SCALA. He also emphasized that it can be used for indexing from 3 images (0, 45, 90º), which can be very helpful for difficult cases.

Nicholas Sauter (Lawrence Berkeley National Laboratory, Berkeley, CA, USA) completed this session with "New Python-based methods for Data Processing." He discussed a new open-source package, Reciprocal Space Toolbox (rstbx), which will be of use for quick development of new crystallographic software. The rstbx package uses a combination of Python scripting and C++ to combine ease of use with adaptation with speed. He illustrated its use in the processing of data obtained from the relatively new LINAC Coherent Light Source (LCLS), the world first hard

free electron laser, located at the SLAC National Accelerator Laboratory in Stanford, CA, USA.

The next session "Practicals – Part I" began with a talk from **Tadeusz Skarzynski** (Agilent Technologies, UK) entitled "Collecting Data at Home: Evolution of Sources, Equipment and Applications." He emphasised the advantages of characterizing the diffraction qualities of crystals using a home source, both in terms of optimizing data collection parameters prior to collection at a synchrotron source, as well as in the rapid routine use of these systems for screening of ligand complexes. He illustrated his points with examples and emerging technologies, clearly showing that home sources are an important component of a crystallographer's tool box and their use is synergistic with data collection from higher energy sources such as synchrotrons.

Elspeth Gordon (ESRF Grenoble, Grenoble, France) then spoke about "How the ESRF Helps Industry and How They Help Us." She presented an excellent overview of the range of facilities and capabilities available to crystallographic users at the ESRF. She described how the services and support has evolved to be of particular use to industrial users who demand superior levels of automation and standardisation. She illustrated her points by describing their in-house developed sample SC3 changer, controlled by an intuitive graphical interface mxCuBE. The capabilities of remote access were apparent in the ISpyB database that enables users to monitor real-time experiments at a distance using a web interface. ESRF efforts to maintain services that attract an active industrial user base (20% of all users) are of key importance to the facility, and future developments are sure to benefit both industrial and academic crystallographic users.

The session concluded with **Armin Wagner** (Diamond Light Source, UK) with the amusingly titled "Fisherman's Friends – Practical Aspects on Sample Mounting." He presented technical developments of perhaps one of the most difficult areas to automate – crystal mounting – a step that many crystallographers know can result in the loss of precious samples if it is not done correctly. His talk described evolving techniques aimed at simplifying transfer of samples into holders with particular emphasis upon minimising solvent around the sample to improve signal-to-noise levels of data collected in the subsequent data collection experiments. The case for automation of this step was clearly made and most crystallographers would agree that implementation of such tools would be truly useful in improving successful sample maintenance under what can be a very stressful step in the crystallographic process.

The final session of the meeting, "Practicals – Part II" was opened by **Marcus Mueller** (Dectris Ltd, Switzerland) who presented "Optimal Data Collection Using Single Photon Counting Pixel Detectors." He described a comprehensive study on how to collect optimal data from these detectors. Such detectors have a short readout time allowing continuous data collection. Fine slicing thus adds no time penalty to the experiment while resulting in improved data.

Tobias Krojer (Structural Genomics Consortium, University of Oxford, Headington, UK) presented "Squeezing the Most from Every Crystal: It's the Details that Matter." He stressed the importance of recognising diffraction data collection as the last experiment: time and care taken at this point to account for crystal decay and use strategy programs makes all subsequent steps far easier. This was illustrated by the striking statistic that SGC Oxford collected 85 datasets last year resulting in 40 PDB depositions: a remarkable success rate.

David Stuart (University of Oxford) followed with "In Situ Data Collection – Blasts from the Past." He opened with a quote attributed to **Phil Jeffrey** "you should never assume that your handling of the crystal is inevitably benign." Room temperature crystals shot in the crystallisation drop often provide the gold standard for diffraction. Setups allowing such experiments are now available at synchrotrons worldwide, and room temperature MX can prove extremely valuable for both crystal screening and structure solution.

The meeting closed with the final talk by **Wayne Hendrickson** (Columbia University) "Robust Structural Analysis of Native Biological Macromolecules." He described the benefits of a multi-crystal approach for anomalous diffraction data collection. In the S-SAD experiment extremely weak differences must be accurately measured. The use of multiple crystals was shown to greatly improve the success of sulphur phasing. This together with future beamlines optimised for S-SAD data collection will make phasing from the intrinsic anomalous scatterers in a protein a routine process in the future.

Finally, the smooth and successful running of this year's CCP4 workshop was ensured by the dedicated and professional support provided by the UK Science and Technology Facilities Research Council (STFC) team of **Charles Ballard**, **Shirley Miller**, **Damian Jones**, **Wendy Cotterill**, **Karen McIntyre** and **Stuart Eyres** (photography) and the support of the UK-based sponsors: the STFC, the Biotechnology and Biological Sciences Research Council (BBSRC), the Medical Research Council (MRC) and Diamond Light Source.

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

ECM-27

MEETING Programme

Saturday 4th Opening of the satellite meeting on 'Methods of High-Pressure Single-Crystal X-ray Diffraction'

Sunday 5th Satellite meeting on 'Methods of High-Pressure Single-Crystal X-ray Diffraction' closes in the evening.

Monday 6th Workshop on Data Diffraction Deposition. Mounting of commercial exhibition. Opening with Laue Centennial Lecture from 18:00. Please be there – We will not be there for the bicentennial!

Tuesday 7th Scientific sessions starts 08:30. Posters.

Wednesday 8th Scientific sessions starts 08:30. Posters.

Thursday 9th Scientific sessions starts 08:30. Posters. Conference Banquet in the evening.

Friday 10th Scientific sessions starts 08:30. Posters. Scientific sessions close 18:00. Exhibition closes after lunch.

Saturday 11th Excursion day – per your own choice.

Keynote Speakers and Tentative Titles

- **Danny Shechtman**, Technion, Israel Institute of Technology, Haifa, Israel: *(Title pending)*
- **Michael Rossmann**, Purdue University, Purdue, USA: *EM X-ray interface*
- **Jacqueline Cherfils**, LEBS, CNRS, Gif sur Yvette, France: *The many roles of small GTPases*
- **Randy Read**, University of Cambridge, Cambridge, UK: *(Title pending)*
- **Henry Chapman**, DESY/University of Hamburg, Hamburg, Germany: *(Title pending)*
- **Jens Preben Morth**, University of Oslo, Oslo, Norway: *Membrane transporters*
- **Ross Angel**, University of Padova, Padova, Italy: *High Pressure Minerals and Materials*
- **Olivier Mentré**, UCCS, University of Lille, Villeneuve d'Ascq, France: *Solid-State Chemistry and Crystallography*
- **Björn Winkler**, University of Frankfurt, Frankfurt, Germany: *Computational Crystallography*
- **Mark Spackman**, University of Western Australia, Crawley, Australia: *(Title pending)*
- **Paul Midgley**, University of Cambridge, Cambridge, UK: *Towards Routine Structure Solution using Precession Electron Diffraction*
- **Paola Gilli**, University of Ferrara, Ferrara, Italy: *Towards the unification of intermolecular forces: The hydrogen bond as a charge-transfer interaction*
- **Simone Techert**, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany: *Time Resolved Crystallographic Processes for Molecular Systems*
- **Maryjane Tremayne**, University of Birmingham, Birmingham, UK: *Hot topic in powder diffraction*
- **Neil Champess**, University of Nottingham, Nottingham, UK: *Supramolecular Chemistry/Crystal Engineering*
- **Knut Urban**, Peter Grünberg Institute, Jülich, Germany: *Picometre electron microscopy*
- **Simon Parsons**, University of Edinburgh, Edinburgh, Scotland: *Absolute Structure Determination*

Registration is now open.

Type of Participant	After April 30th	Before May 1st
Full Participant	4600	3850
Full Participant & ECA member	4350	3600
Student*	2800	2250
Accompanying Person	2700	2700

*Up to age 35. Proof of status from supervisor is required. Fees are in NOK and include a light lunch and coffee breaks.

The Conference Venue – The Grieg Hall

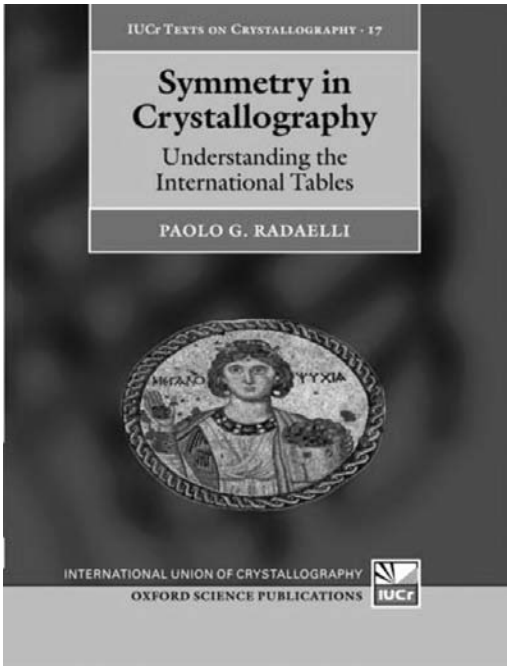
The Grieg Hall is the home of the Bergen Philharmonic Orchestra in particular and many of the city's cultural and musical events in general. It is also a modern and diversified conference and exhibition centre.

Go here for an official video presentation:
http://grieghallen.no/general_info/presentation/?l=en

Its location in the city centre makes it easily accessible by foot, public transport or private car. A spacious underground parking house is located directly underneath the venue.

Book Reviews

Symmetry in Crystallography – Understanding the International Tables



BY Paolo G Radaelli, published September 2011 by Oxford University Press for the International Union of Crystallography, xiv + 126 pp, price £49.95 hardback, ISBN 978-0-19-955065-4.

This slim book, weighing 500 grams, is a recent addition (*at Number 17*) to the collection of IUCr Texts in Crystallography. As the subtitle indicates, it is intended as an aid to understanding the International Tables for Crystallography (ITC). It aims especially at elucidating Volume A, a hefty tome of 3.35 kilograms; but also has relevance to parts of Volumes B and E. One has to be mathematically minded to appreciate fully this new book.

One is at first struck by the beautiful coloured picture on the cover, showing the fifth-century Megalopsychia mosaic which illustrates the symmetry of the surrounding frieze pattern. The book as a whole is well produced with plenty of diagrams and pictures, some showing patterns from ancient art as well as from the wonderful works of **Maurits Escher**. It suffers however from a number of minor typographical errors, such as 'Gaulois' for the famous French mathematician **Évariste Galois** (*page 6*); and '32' when the cubic point group 23 is meant (*page 80*). It is a pity that the index does not contain the names of people, such as Galois (1811-1832) and **Alex Gadolin** (1828-1892), whom I learnt (*from page 30*) had been a Finnish-born Russian artillery professor and who was the first to introduce the concept of crystal classes.

Part I is an introduction to symmetry groups, with chapters on symmetry around a fixed point, frieze patterns and frieze groups, and on plane 'wallpaper' groups. One realizes from the start (*page 1*) that one is in for an interesting study, as Noether's theorem, translational invariance of the Hamiltonian, Neumann's principle and Curie's asymmetry principle are all mentioned; but surprisingly they don't appear again in the book. The algebraic notation takes a bit of getting used to and in places the nomenclature does not appear to follow that of the ITC. I found myself trying to recall the algebra of my distant undergraduate days – and struggling! There are set problems to do, which are good; but it would have been most helpful for one's understanding to have had hints and answers supplied in an appendix. British readers will probably associate the three-legged symbol (triskelion) with the Isle of Man, so it is interesting to see it here representing Sicily (figure 1.7: depicting three-fold rotational symmetry without mirror planes). I found the diminutive reproduction of two vast pages of ITC Volume A (on the two-dimensional point groups) on to one small page of the book (figure 1.9) almost illegible to my ageing eyesight; and similarly for the reduction of a whole page from Volume E of ITC on to just part of a page here (figure 2.16). More explanation could have been given (in the text and in figures 3.2 and 3.3) to the proof of the important 'restriction theorem', which shows that five-fold rotational axes of symmetry, and those of order higher than six, cannot be combined with translational symmetry. I would have welcomed more help with the meaning of the rows and columns of the graphical multiplication table in two dimensions (figure 3.11). In contrast, the decision-making tree (figure 3.12), for identifying wallpaper patterns, is very clear and helpful.

Part II is on crystallographic coordinate systems and its four chapters cover coordinate transformations; symmetry

operators; distances and angles in real and reciprocal space; and an example of a phase transition in two dimensions. In the absence of a proof of the formula (equation 5.8) for the matrix representing a rotation about an axis of arbitrary orientation, it would have been helpful to have had a reference or two to the literature. It would be interesting to take a vote on whether crystallographers like to include a factor of 2ϖ in definitions of reciprocal vectors. Of course, one is at liberty to cross these factors out in this book. Throughout there appears to be a problem with the 'not equals' sign ($\neq$) which appears as /=. I don't like the heading "A dummies' guide to calculating reciprocal lattice parameters" – Anybody successfully reaching page 65 is clearly not a 'dummy'!

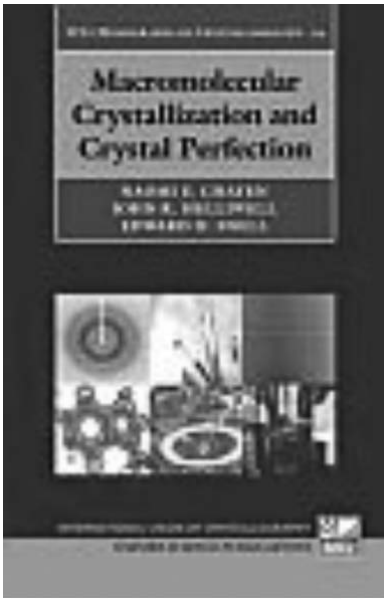
Halfway through the book we arrive at Part III on symmetry in three dimensions which has chapters on point groups in 3D; the fourteen 3D Bravais lattices; and 3D space-group symmetry. I would have liked to have seen more emphasis on three dimensions in this book, especially aimed at the newcomer who may have difficulty in imagining combinations of symmetry operations in 3D space. The caption for the diagram (figure 8.1), illustrating the six-fold roto-inversion operator (equivalent to 3/m), refers to a triangular prism, whereas a triangular bipyramid is meant. There is a spherical 'blob' missing from the illustration (figure 8.2) of 6/m; and the three symmetry axes of the cube shown in figure 8.3 should all pass through the centre. One has to wait until page 90 for the meanings of the letters (such as e, n and d) on page 81: they are various types of glide plane and would therefore be better placed later in the book than in the section on point groups.

The final Part IV is on reciprocal space and deals with symmetry and reflection conditions; the Wigner-Seitz constructions and Brillouin zones. Again, factors of 2ϖ turn up. I think that 'systematic absences' is the more common expression for 'centering extinctions'. A paragraph or two on diffraction and structure factors would have made this part more self-contained. It is interesting to see the Laue classes coming from a Fourier transform treatment. There are excellent geometric diagrams of Wigner-Seitz constructions, but the applications of these and of Brillouin zones are left unsaid; and the book comes to an abrupt halt with no concluding remarks.

I fear that this book is not for the absolute beginner: like a good crystal, it has its point defects. It is a fascinating compendium of ideas about crystal symmetry which, coming from a different perspective, may usefully be read alongside the Brief Teaching Edition of Volume A of the International Tables for Crystallography (edited by **Theo Hahn**, published by Kluwer for the IUCr, 2002).

Moreton Moore
Royal Holloway University of London

Macromolecular Crystallization and Crystal Perfection



IUCR Monographs on Crystallography 24 By Naomi E Chayen, John R Helliwell, and Edward H Snell published 2010 by Oxford University Press for the International Union of Crystallography, 240 pp, price £67.50 hardback, ISBN 978-0-19921325-2.

This, my third review of a recent crystallographic work, has caused me to wonder: how many do we need? Perhaps just one, but this is not what is commonly observed. What drives the authors to invest their time and energy in this way? In the case of the above title, and for most works of this type, the motives are clear; to provide a single source describing the latest developments in the technique whilst attempting the presentation of, often difficult, concepts with ever greater clarity; not forgetting a small financial reward. A good exercise to rehearse one's own understanding and ferret out any minor misconceptions. Modern science has, so I am told, entered the paradigm of model dependent reality where we must abandon ideas of a single truth/ theory and simply accept the model which best agrees with our experimental observations. Whilst we are not in the high realm of pure research here, we may still notice a zeitgeist in the use of differing approaches to the same set of phenomena. Students and cognoscenti alike will,

depending on their background and training, find some descriptions more palatable than others; and it is to the credit of our specialism that it has found its way into so many varied fields, employed by workers from diverse scientific backgrounds. So yes, it would seem that there is always room for another book.

At least some of you will have noticed the one of the authors is a Manchester scientist; so, considering this, and to preclude any notion of local patronage, (although I will just recall that our founding father, the then **Lawrence Bragg** succeeded Rutherford to the Langworthy chair of Physics at Manchester; a post he held from 1919-37. Also that the present incumbent, along with a colleague, was awarded the 2010 Nobel Prize in Physics) my review attempts to be as fairly critical, if not more so, than usual. And I know the said author would expect nothing less.

This work aims, as the title suggests, to provide a description of the crystallographic experiment in terms of that sine qua non of the whole business: the crystal. In this case it is a periodic array of some large biological molecule (a wonder in itself). An exquisitely appropriate choice as it is the intrinsic properties of this entity that give rise to the diffraction event and also to nearly every technical description of the recordable data. This volume is timely given the maturity of the technique, when the getting of a suitable crystal is just about the final barrier to truly routine 'structuring'. With this in mind the intelligent reader will be encouraged in efforts to obtain the finest crystal whilst understanding the limitations of poorer, or more available, ones. And also discover a much richer description of the crystal than our usual simple model. If you thought you knew what a crystal/X-ray interaction was, just wait till you read this!

Offered in 4 parts, there is a brief introduction where, on a few occasions, terms are introduced with some assumption of prior knowledge. Part II rehearses the major theme of crystallisation, providing an excellent survey of current methods. This is mainly but comprehensively anecdotal, reflecting the lack of a rigorous description of the process (only one equation appearing in some 24 pages). Apologists for the technique confess to constant defence of our lack of understanding here and the almost schizophrenic nature of hard diffraction physics on one hand and 'black art' crystallisation, thus far defying rational description, on the other.

In part III we return (happily) to the much better described 90-odd pages of hard diffraction theory and methodology. Here we have diffraction by a real-world crystal analysed in extraordinary detail and I am, once again, reminded of the huge effort that has gone into quantifying this phenomenon. To be read 'lest we forget' in this era of 'shoot and solve'. Pretty much every sort of experimental attempt to obtain data from, an often recalcitrant, sample is described from source to crystal to measurement. This makes the bulk of the text; then the authors conclude, in a brief six page part IV, with a tantalising glimpse of future possibilities for the technique.

This is not a book for the beginner: the information density is high making for a challenging read, but rather a very good rigorous guide once the basics have been digested and crystallographic terminology becomes familiar. References run to an impressive 42 pages; the common practice of chapter summaries is adopted. Supervisors: encourage your students. Students: surpass your masters.

Patrick K. Bryant
University of Manchester

December Puzzle Corner

I asked for whimsical names or humorous acronyms for crystallographic concepts or techniques. So far I have had no response beyond my own pessimistic MAD and SAD. Perhaps the lively and informative report by **Richard Martin** in this issue on the Biological Structures Group Winter Meeting, which included a talk by Helen Walden that mentioned the WD40 propeller, will lubricate further discussion.

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, c.h.schwalbe@hotmail.com . Assistance from the IUCr website and the Journal of Applied Crystallography is gratefully acknowledged.

11 - 15 March 2012
TMS 2012:
Linking Science and Technology for Global Solutions, including Neutron and X-ray Studies of Advanced Materials V Centennial,
Orlando, FL, USA.
http://www.tms.org/meetings/annual-12/AM12home.aspx

12 - 15 March 2012
Annual Meeting, German Crystallographic Society,
Munich, Germany.
http://www.iucr.org/news/notices/meetings/meeting_dgk_2012

19 - 23 March 2012
Annual ICDD Spring Meetings, Newtown Square,
PA, USA.
http://www.icdd.com/profile/march12.htm

23 March 2012
4th User Meeting at the FRM II,
Munich, Germany.
http://www.frm2.tum.de/en/aktuelles/events/user-meeting-2012/index.html

25 - 29 March 2012
Powder Diffraction and Rietveld Refinement School 2012,
Durham.
http://www.dur.ac.uk/john.evans/webpages/pcg_rietveld_school_2012.htm

25 - 30 March 2012
Winter School on Neutron Scattering in Soft Matter,
Björkliden, Sweden.
http://www.icddt.com/index.htm

26 - 27 March 2012
The Eleventh Ad Hoc Workshop on Jana2006,
Prague, Czech Republic.
http://www-xray.fzu.cz/jana/w011.html

26 - 27 March 2012
Intrinsically Disordered Proteins,
York, UK.
http://www.biochemistry.org/tabid/379/MeetingNo/SA128/view/Conference/default.aspx

26 - 27 March 2012
"Small Molecules in Interactions" International Symposium,
Ruhr-Universität Bochum,
Bochum, Germany.
http://www.ruhr-uni-bochum.de/smi/

30 March - 6 April 2012
International School of Nanophotonics and Photovoltaics,
Phuket, Thailand.
http://www.optolab.uniroma2.it/ISNP-2012/index.htm

9 - 13 April 2012
2012 MRS Spring Meeting and Exhibit Moscone West Convention Center,
San Francisco, CA, USA.
http://www.mrs.org/spring2012/

15 - 18 April 2012
NIUS2012.
Neutron Imaging User Symposium,
Bad Zurzach, Switzerland.
http://indico.psi.ch//event/neutron-imaging-user-symposium

16 - 19 April 2012
British Crystallographic Association Spring Meeting,
University of Warwick.
http://www.crystallography.org.uk/

19 - 20 April 2012
Science & Scientists @ ESS 2012,
Berlin, Germany.
http://esss.se/ess_conferences/

19 - 21 April 2012
Joint 5th Mineral Sciences in the Carpathians Conference (MSCC) and 3rd Central-European Mineralogical Conference (CEMC),
Miskolc, Hungary.
http://www.mscc-cemc.com/

23 - 27 April 2012
From Genes to Atomic Structures:
an Introduction to Synchrotron-Based Structural Biology,
Trieste, Italy.
http://cdsagenda5.ictp.trieste.it/full_display.php?ida=a11160

30 April - 4 May 2012
ICDD Clinic on X-ray Fluorescence Spectrometry,
Newtown Square, PA, USA.
http://www.icdd.com/education/xrf.htm

7 - 10 May 2012
MaMaSELF 2012:
Master in Materials Science. 4th Annual Status Meeting,
Rigi Kulm, Switzerland.
http://diffraction.web.psi.ch/mamaself-rigi-ch.htm

9 - 12 May 2012
European Cyclotron Progress Meeting ECPM XXXVIII,
Villigen, Switzerland.
http://www.psi.ch/ecpm2012

14 - 18 May 2012
E-MRS 2012 Spring Meeting, Congress Center,
Strasbourg, France.
http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=428&Itemid=1

15 - 18 May 2012
PPXRD-11.
11th Annual Pharmaceutical Powder X-ray Diffraction Symposium - XRD
Training for the Pharmaceutical Scientist, Fort Myers, FL, USA.
http://www.icdd.com/ppxrd/

17 - 19 May 2012
4th International Meeting on X-ray Techniques in the Investigations of the Objects of Cultural Heritage,
Krakow, Poland.
http://heritagescience.pl/workshop2012/

21 - 25 May 2012
ISC2012.
3rd Granada International School of Crystallization.
Drugs, Foods, Agrochemicals, Minerals, New Materials,
Granada, Spain.
http://www.iscgranada.org/

23 - 24 May 2012
BCA Industrial Group XRF and XRD Meetings,
University of Leicester
http://sites.google.com/site/bcaxrf/meetings/23-may-2012
http://sites.google.com/site/bcaindgrp/meetings/24-may-2012

27 May - 1 June 2012
Three Dimensional Electron Microscopy.
From Molecules to Systems - Visualizing Biological Complexity.
Gordon Research Conference,
Les Diablerets, Switzerland.
http://www.grc.org/programs.aspx?year=2012&program=threedim

31 May - 10 June 2012
Present and Future Methods for Biomolecular Crystallography,
Erice, Italy.
http://www.crystalerice.org/Erice2012/2012.htm

3 - 6 June 2012
23nd Conference on Crystal Growth and Epitaxy - West (2012 AACGE-west),
Fallen Leaf 3-8 June 2012Lake,
CA, USA.
http://www.crystalgrowth.us/accge_west23/

3 - 8 June 2012
Electronic Processes in Organic Materials.
Exploring the Fundamentals of Organic Electronics.
Gordon Research Conference,
Lucca, Italy.
http://www.grc.org/programs.aspx?year=2012&program=elecproc

3 - 8 June 2012
Multiphoton Processes.
Attoseconds, Intense Fields, and Ultrafast Imaging.
Gordon Research Conference.
South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=multiphot

4 - 8 June 2012
ICDD Clinic on X-ray Powder Diffraction.
Session I - Fundamentals of X-ray Powder Diffraction, Newtown Square,
PA, USA.
http://www.icdd.com/education/xrd.htm

7 - 14 June 2012
Bombannes 2012.
11th European School on Scattering Methods Applied to Soft Condensed Matter,
Gironde, France.
http://www.ill.eu/news-events/events/bombannes-2012/

9 - 10 June 2012
Plasmonics. Light-Matter Interaction at the Nanoscale.
Gordon Research Seminar,
Waterville, ME, USA.
http://www.grc.org/programs.aspx?year=2012&program=grs_plsmnc

10 - 15 June 2012
Plasmonics.
Light-Matter Interaction at the Nanoscale.
Gordon Research Conference, Waterville,
ME, USA.
http://www.grc.org/programs.aspx?year=2012&program=plasmonics

11 June 2012
10th International Workshop on Crystal Growth of Organic Materials,
University of Limerick,
Limerick Ireland.
www.cgom2012.com/

11 - 13 June 2012
Geo-Raman Xth Meeting,
Nancy, France.
http://georaman10.uhp-nancy.fr/georaman/scope.html

11 - 15 June 2012
ICDD Clinic on X-ray Powder Diffraction.
Session II - Advanced Methods in X-ray Powder Diffraction,
Newtown Square,
PA, USA.
http://www.icdd.com/education/xrd.htm

14 - 16 June 2012
Raman Spectroscopy Applied to Earth Sciences and Cultural Heritage.
International School,
Nancy, France.
http://georaman10.uhp-nancy.fr/internationalschool/scope.html

16 - 17 June 2012
Noble Metal Nanoparticles.
New Understanding in Synthesis, Characterization and Applications of Noble Metal Nanoparticles.
Gordon Research Seminar,
South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=grs_noble

17 - 20 June 2012
European Conference of Crystal Growth 2012,
University of Strathclyde,
Glasgow.
http://eccg4.org/

17 - 20 June 2012
Electron Crystallography School - Methods and Applications,
Stockholm, Sweden.
http://www.mmk.su.se/electron-crystallography

17 - 22 June 2012
Noble Metal Nanoparticles.
Gordon Research Conference,
South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=noblemetal

20 - 22 June 2012
International Symposium on X-ray and Electron Crystallography - from Materials Sciences to Structural Biology.
Celebration of Professor Sven Hovmöller's Scientific Career,
Stockholm, Sweden.
http://www.mmk.su.se/electron-crystallography

21-22 June 2012
Applied Mineralogy of Cement and Concrete.
MSA Short Course,
Trondheim, Norway.
http://www.icdc2012.com/

22 - 29 June 2012
Advanced Methods in Macromolecular Crystallization - V.
FEBS Practical Course,
Nove Hrady, Czech Republic.
http://www.febs.org/index.php?id=651

23 - 24 June 2012
Research at. High Pressure,
Gordon Research Seminar,
Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2012&program=grs_highp

23 - 24 June 2012
Correlated Electron Systems.
Current Issues in Correlated Electron Systems.
Gordon Research Seminar,
South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=grs_correl

24 - 29 June 2012
Research at High Pressure.
Gordon Research Conference,
Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2012&program=highpress

24 - 29 June 2012
Correlated Electron Systems.
Correlations and Topology in Electron Systems,
Gordon Research Conference,
South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=correlec

25 - 28 June 2012
IWPCPS-14 (International Workshop on Physical Characterization of Pharmaceutical Solids),
Barcelona, Spain.
http://www.iucr.org/news/notices/meetings/meeting_2011_252

2 - 6 July 2012
NSS-7.
7th International Workshop on Nano-scale Spectroscopy and Nanotechnology,
Zurich and Villigen, Switzerland.
http://indico.psi.ch//event/nss7

4 - 6 July 2012
3rd Workshop on Simultaneous Combination of Spectroscopies with X-ray Absorption, Scattering and Diffraction,
ETH Zurich, Switzerland.
http://www.psi.ch/csx2012

7 - 8 July 2012
Ion Channels.
Excitable Cells and Electrical Signaling.
Gordon Research Seminar,
South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=grs_ion

8 - 13 July 2012
Ion Channels.
Gordon Research Conference,
South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=ionchan

8 - 13 July 2012
UP2012.
XVII International Conference on Ultrafast Phenomena,
Lausanne, Switzerland.
http://www.up2012.org/

15 - 20 July 2012
35th Annual British Zeolite Association Meeting,
Chester, UK.
http://chemweb.bham.ac.uk/~hriljaja/bza2012/index.htm

15 - 20 July 2012
Sagamore XVII.
Great Potentials from Advanced Probes,
Kitayuzawa, Japan.
http://rsc.riken.jp/sagamore/home/

22 - 27 July 2012
15th International Conference on Experimental Mechanics,
Faculty of Engineering,
University of Porto,
Porto, Portugal.
http://paginas.fe.up.pt/clme/icem15/

28 - 29 July 2012
Radiation Chemistry.
Radiation Driven Processes in Physics, Chemistry,
Biology and Industry.
Gordon Research Seminar,
Andover, NH, USA.
http://www.grc.org/programs.aspx?year=2012&program=grs_rad

28 July - 1 August 2012
ACA Meeting 2012, Westin Waterfront Hotel,
Boston, MA, USA.
http://www.amercrystalassn.org/2012-meeting-homepage

29 July - 2 August 2012
Microscopy & Microanalysis
(M&M 2012),
Phoenix, AZ, USA.
http://www.microscopy.org/MandM/2012/

29 July - 3 August 2012
Radiation Chemistry.
Radiation Driven Processes in Physics, Chemistry,
Biology and Industry.
Gordon Research Conference, Andover, NH, USA.
http://www.grc.org/programs.aspx?year=2012&program=radchem

29 July - 3 August 2012
Stereochemistry,
Newport, RI, USA.
http://www.grc.org/programs.aspx?year=2012&program=stereochem

29 July - 3 August 2012
Scientific Methods in Cultural Heritage Research
Non-Destructive Imaging and Micro-Analysis in Cultural Heritage.
Gordon Research Conference, West Dover, VT, USA.
http://www.grc.org/programs.aspx?year=2012&program=heritage

6 - 10 August 2012
61st Annual Denver X-ray Conference,
Denver, CO, USA.
http://www.dxcicdd.com/

6 - 11 August 2012
27th Meeting of the European Crystallographic Association,
Bergen, Norway.
http://ecm27.ecanews.org/

12 - 17 August 2012
Defects in Semiconductors.
Gordon Research Conference, Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2012&program=defects

27 August - 1 September 2012
International Summer School on Crystal Growth and Photovoltaic Materials,
Brasov, Romania.
http://rocam.unibuc.ro/intschool/index.html

2 - 6 September 2012
First European Mineralogical Conference (EMC2012),
Frankfurt, Germany.
http://emc2012.uni-frankfurt.de/

2 - 6 September 2012
XXII Conference on Applied Crystallography (XXII CAC),
Targanice/Andrychów, Poland.
http://www.cac.us.edu.pl/

2 - 7 September 2012
Aperiodic 2012, Cairns,
Queensland Australia.
http://www.iucr.org/news/notices/meetings/meeting_aperiodic_2012

4 - 9 September 2012
22nd IUBMB and 37th FEBS Conference, Seville Conference and Exhibition Centre,
Seville, Spain.
http://www.iubmb-febs-2012.org/IUBMBFEBS2012/

15 - 20 September 2012
6th European Charge Density Meeting,
Štrbské Pleso, Slovakia.
http://ecdm6.stuba.sk/?page=home

16 - 21 September 2012
50th EHPRG Meeting,
Thessaloniki, Greece.
http://www.ehprg.org/meetings/

17 -20 September 2012
7th International Sample Environment Workshop,
Amora Hotel Jamison,
Sydney, Australia.
http://www.ansto.gov.au/research/bragg_institute/current_research/conferences_and_workshops/sample_environment_at_neutron_scattering_facilities

23 - 28 September 2012
ICCBM 14.
14th International Conference on the Crystallization of Biological Macromolecules,
Huntsville, AL, USA.
http://iccbm14.org/

1 - 3 October 2012
Basic Rietveld Refinement & Indexing Workshop,
Newtown Square, PA, USA
http://www.icdd.com/education/rietveld-workshop.htm

4 - 5 October 2012
Advanced Rietveld Refinement & Indexing Workshop,
Newtown Square, PA, USA.
http://www.icdd.com/education/rietveld-workshop.htm

14 - 18 October 2012
2012 AAPS Annual Meeting and Exposition,
Chicago, IL, USA.
http://www.aaps.org/annualmeeting/

16 - 18 October 2012
Handheld XRF Workshop,
Newtown Square, PA, USA.
http://www.icdd.com/education/handheld-xrf-workshop.htm

20 - 27 October 2012
BioCrys2012.
Fundamentals of Modern Methods of Biocrystallography,
Oeiras, Portugal.
http://www.febs.org/index.php?id=652

22 - 26 October 2012
Crystal structure prediction using the USPEX Code,
Lausanne, Switzerland.
http://www.cecam.org/workshop-0-635.html

28 - 31 October 2012.
EPDIC13.
13th European Powder Diffraction Conference,
Grenoble, France
http://epdic13.grenoble.cnrs.fr/

18 - 23 November 2012
International Small-Angle Scattering Conference (SAS2012),
Sydney, Australia.
http://www.sas2012.com/

26 - 30 November 2012
2012 MRS Fall Meeting and Exhibit,
Boston, MA, USA.
http://www.mrs.org/fall2012/

2 - 5 December 2012
AsCA 12/CRYSTAL 28,
Adelaide, Australia.
http://www.sapmea.asn.au/conventions/crystal2012/index.html

6 December 2012
Bragg Symposium:
Celebrating 100 years of Crystallography,
Adelaide, Australia.
http://www.sapmea.asn.au/conventions/crystal2012/bragg.html

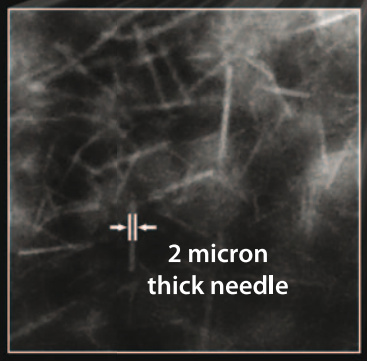
4 - 10 August 2013
ISSCG-15.
15th Summer School on Crystal Growth,
Gdansk, Poland.
http://science24.com/event/isscg15/

11-16 August 2013
ICCGE-17.
17th International Conference on Crystal Growth and Epitaxy,
Warsaw, Poland.
http://science24.com/event/iccge17/

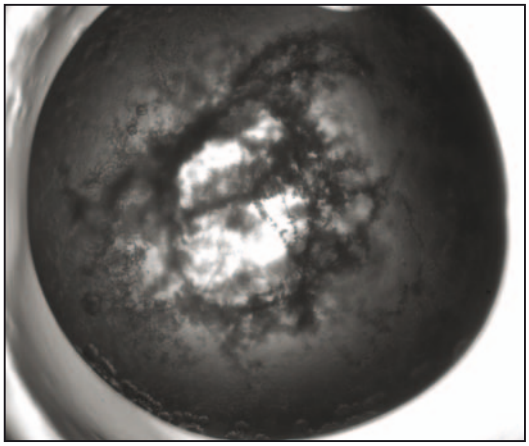
25-29 August 2013
28th European Crystallographic Meeting,
University of Warwick.
http://www.crystallography.org.uk/

5-12 August 2014
IUCr2014. 23rd Congress and General Assembly,
Montreal, Quebec, Canada.
http://www.iucr2014.org/

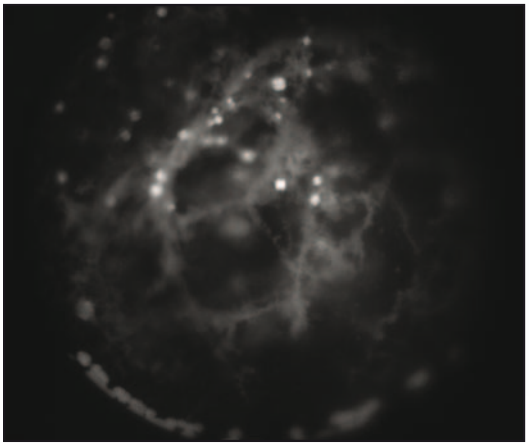
2 µm



Minstrel™ DT UV desktop imaging system



Visible image of microcrystals in precipitate



UV image of microcrystals in precipitate

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