Crystallography News

British Crystallographic Association

Issue No. 132 March 2015
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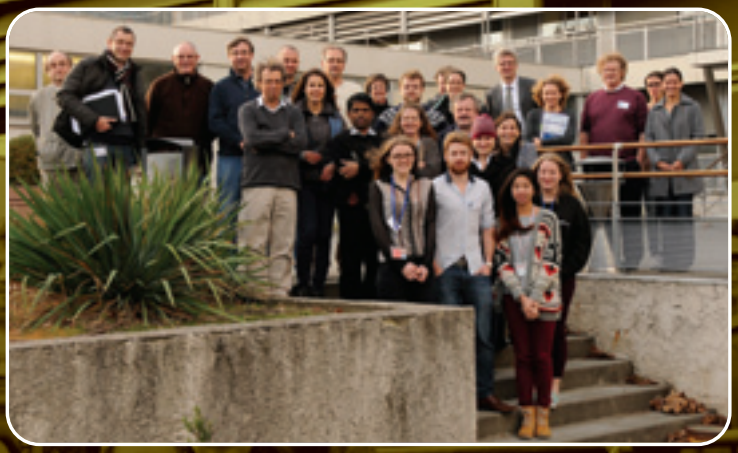
York, waiting to welcome you

…and delegates from recent CCG, BSG, IG meetings



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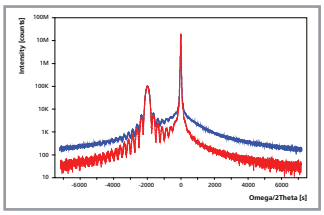
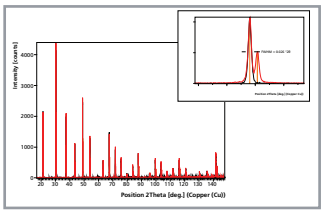
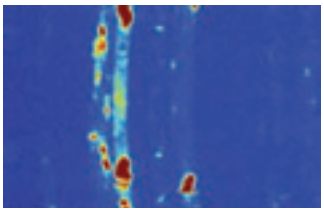
0D



1D



2D



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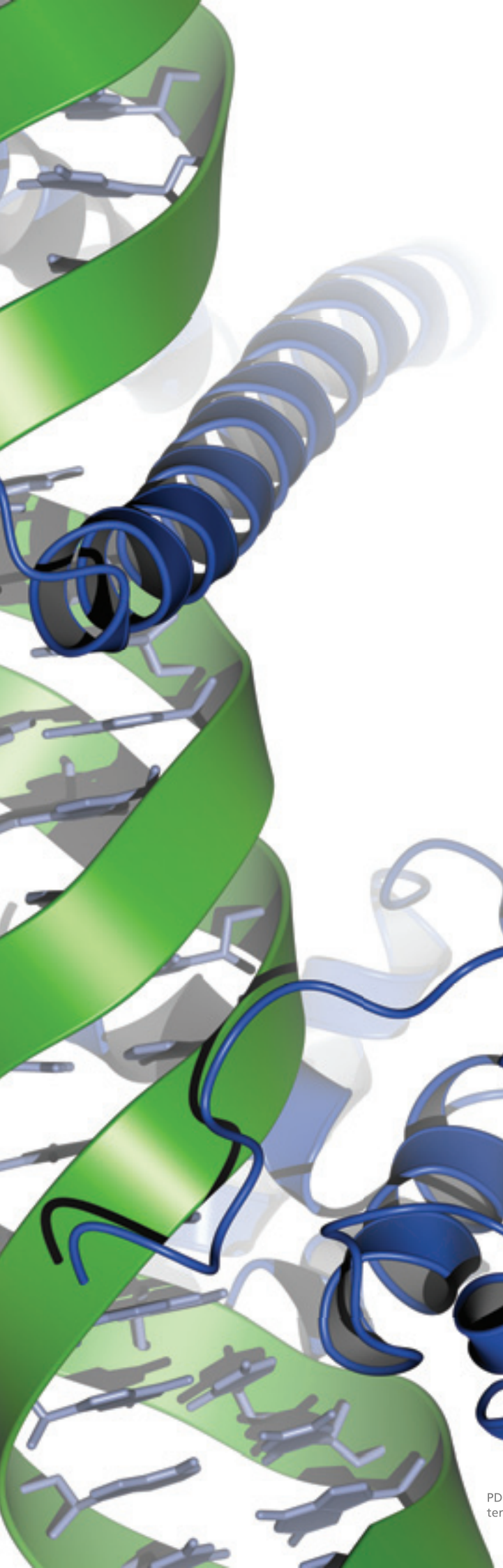

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PDB structure 1h8a: Crystal structure of ternary protein-DNA complex3

Science & Technology Facilities Council

Crystallography News March 2015

Contents

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by Bowmans, Leeds. 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 (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.
Please ensure that items for inclusion in the June 2015 issue are sent to the Editor to arrive before 25 April 2015.

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As required by the DATA PROTECTION ACT, the BCA is notifying members that we store your contact information on a computer database to simplify our administration.

These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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This month's cover:

*BSG, CCG, IG delegates; York awaiting **you***

From the President

WE are now firmly in 2015 which – as we surely all know by now – is one hundred years after the father and son team of William and Lawrence Bragg were awarded the Nobel Prize in Physics "for their services in the analysis of crystal structure by means of X-rays". Interestingly 2015 is also the centenary of the *announcement* of Max von Laue's 1914 Nobel Prize in Physics; the start of the First World War delaying the Nobel Prize Committee's 1914 decision[1]. Indeed the early history of crystallography is inevitably intertwined with WWI and the political aftermath. Lawrence Bragg received notification of their award while billeted near the front and is said to have 'celebrated' with comrades and the local curate with a bottle of Lachryma Christi ("tears of Christ")[2], a bittersweet celebration given that his brother had died in Gallipoli only weeks earlier. The Braggs didn't attend the Nobel Prize Ceremony in 1920 when all awards made during WWI were given[2], probably in part because of the general scientific boycott of Germany and its allies at the time[3]. And, although Lawrence Bragg regretted this decision and gave his Nobel lecture in 1922, William never delivered a Nobel lecture[4]. When we mark the tumultuous events of the First World War at this time, we might reflect a little on how it even had an impact on crystallography and international 'apolitical' science more generally.

Staying with crystallographic history – albeit from a very different angle – in my previous pre-Christmas column I asked, "who somewhat surprisingly wrote 'I do not want to label myself a crystallographer as against a physicist…' ?" The answer was Lawrence Bragg in a letter to Rutherford while he was considering returning to Cambridge in 1929 (see references in[5]. In part of that article I considered how visible crystallography was in Physics Departments and concluded that although crystallography was alive and vital within physics it was typically hidden behind other labels such as 'structural condensed matter physics' or 'nanoscale physics'. It felt a little as if physicists were embarrassed to be described as crystallographers (except of course for my colleague **Mike Glazer** and a number of other notable exceptions!), even though this was not so much the case within chemistry or biology. I hope that the centenaries that we have been celebrating, and the positive exposure that the subject has received, will perhaps also bring crystallography much more to the fore within physics departments. Let's use this final centenary year to consolidate the work that we did for the 2013 Bragg Centenary and the 2014 International Year of Crystallography. (In this context, you may be interested to know that the IUCr will publish 100 papers in their Open Access IUCrJ journal free of charge as part of the Bragg Nobel centenary and IYCr2014 Legacy – see journals.iucr.org/services/natchem.html.)

This issue of *Crystallography News* is with you just before we head off to our BCA Spring Meeting in York – see details in later pages – and I hope that I will be able to meet with many of you then. There is an excellent programme, York is a great venue and we have a full commercial exhibition. If you haven't yet booked to come then please do so! As usual we will also be having our Annual General Meeting at the Spring Meeting (see the announcement on page 10). In the meeting we will be electing a new President, a new Education and Outreach Co-ordinator and a new Ordinary Council Member – thank you **Sam Callear** and **Simon Parsons** for your hard work for us in the two latter roles, respectively. At the AGM we will also almost certainly have to make some decisions about ways to reduce our annual outgoings and to possibly increase our income. At a recent BCA Officers meeting (and my thanks to **Pamela Williams** for her excellent financial summary documents) we spent some time considering ways to ensure the Association breaks even year-by-year. Whilst we remain committed to education and outreach, student support and bursaries, we wish to live within our means.

Despite Carl's desire for me to adopt foul means to enable me to continue in this role for life – presumably because I have always got my copy to him in time – this is my final 'From the President' Crystallography News column. I can honestly say that I have enjoyed my time as BCA President, even the 'challenge' of writing something that hopefully people find interesting and informative four times a year and without referring to the weather too many times. I hope that you have enjoyed the areas that I have spent more time on, such as the various conferences – especially the ECM meeting in Warwick – and the diverse outreach work over the last three years and are happy with the transition from NNE to HG3 support. I also hope that you will forgive me for those aspects that I haven't prioritised so much! I believe that the BCA is in a good place; with more members and an increased enthusiasm for the subject within our Association and in the wider scientific community and, most importantly, reaching out to the general public. Thank you for working with me to make this possible.

I hope that you enjoy reading this issue of *Crystallography News.*

David Keen

Further reading:

[1] Liljas, A. *Acta Cryst.* (2013). A**69**, 10–15

[2] Hall, K. T. (2014). *The Man in the Monkeynut Coat.* (OUP, Oxford)

[3] Widmalm, *S. Minerva* (1995). **33**, 339–360

[4] Jenkin, J. (2008). *William and Lawrence Bragg, Father and Son.* (OUP, Oxford)

[5] Keen, D. A. (2014). *Phys. Scr.* **89** 128003; Open Access link from iopscience.iop.org/1402-4896/page/Crystallography-Virtual-Issue

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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**

From the Editor

SOMETIMES I fear that our March issue may seem unspectacular, at least in terms of places described, compared with previous reports on international or European meetings in exciting and desirable venues. However, some of the most recent autumn/winter meetings of the BCA Groups involved spectacular journeys, both physically and intellectually. I particularly commend to your attention the report by Jon Cooper on the Biological Structures Group meeting in the delightful surroundings of Grenoble. This trip outside the boundaries of the UK provided a perfect introduction *in situ* to the state-of-the-art facilities now available for structural biology, cutting-edge studies utilising them, plans for their future extension and procedures for accessing them. The Chemical Crystallography Group meeting report should also be of interest to every crystallographer since the meeting dealt with communication, to the general public *via* outreach activities, to students of related subjects, to our fellow scientists *via* traditional and the increasingly important open-access journals, and to posterity by saving the torrents of data we are now producing. For this reason we carry a summary by Natalie Johnson, accompanied by a more verbose account by me. That meeting took place in Burlington House, the stately home of the Royal Society of Chemistry shared with the Royal Academy of Arts among others. Our Industrial Group met in even more historic surroundings: the Royal Institution, the site of so many great scientific discoveries. The report on this meeting makes very clear the benefits of linking structural biology, structural informatics and aspects of crystallography that we usually think of as chemical, to industrial applications, particularly drugs and medicines. For its Autumn Meeting the Physical Crystallography Group / SCMP did not stray from its usual comfortable venue in Cosener's House; but together with the ISIS Crystallography Users Group, they enjoyed a stimulating intellectual tour of the ISIS facilities with special emphasis on the work of early career crystallographers.

Of course, March also provides the opportunity to look forward to upcoming meetings. Our own Spring Meeting in York will be starting before March is out. Alert readers who open their *Crystallography News* the moment it arrives and act upon the information it contains should just be able to catch the Early Bird registration discount if they haven't done so already, but even at full price this meeting will be well worth it. Featuring the usual cornucopia of interesting sessions with eminent speakers, it also offers record numbers of workshops that will acquaint participants with the newest and best software to make one's research progress efficiently. The high-speed brain activity that will be induced by the stimulating programme needs to be complemented with quiet contemplation; and the University of York campus with its winding waterways, diving ducks and drifts of daffodils is conducive to contemplation.

A summer of delights will follow. This year's American Crystallographic Association meeting will take place in the historic city of Philadelphia (the City of Brotherly Love) July 25-29. BCA members who attended the 2012 ACA meeting in Boston will almost certainly remember Faneuil Hall, the stately market house and assembly room known as "The Cradle of Liberty" because much of the opposition to the arbitrary manner of British rule started there. Visitors to Philadelphia will encounter Independence Hall, the building where vaguely formed discontent turned into decisive action and the Declaration of Independence was signed, enshrining rights to life, liberty and the pursuit of happiness. At an ACA meeting the Transactions Symposium is always a highlight, and in 2015 its topic will be "Crystallography for Sustainability", something that all of us must consider for the future. The ACA is particularly generous with poster prizes for undergraduates and postgraduates; up to a baker's dozen of such prizes will be awarded.

Approximately a month later the European Crystallographic Meeting will start in Rovinj, Croatia. Besides being the venue for a wide variety of interesting crystallographic presentations, Rovinj is located in an area of great natural beauty and is both a historic site and a seaside resort. For a small city with a population just over 14,000, which makes it easy to get around, it offers much to see and enjoy. Initially an Italian settlement developed on an island, becoming densely packed into the limited space as it thrived. Across a channel there were Croatian settlements on the mainland. In 1763 the channel was filled in, and subsequently the Italian and Croatian populations and cultures blended. As a fishing port, Rovinj has restaurants offering excellent seafood; and the Italian heritage guarantees excellent pizzas as well. With 16 keynote lectures and 48 microsymposia the ECM is certain to provide a selection of topics that appeal to every crystallographer.

The abstract deadlines for these two meetings are, respectively, March 31 and March 23. Thus there should be just enough time to get those abstracts written and submitted before the intellectual and social whirl of the BCA Spring Meeting!

Of course, the International Year of Crystallography has now finished. We are fortunate that we still have some connection with two International Years in 2015, those of Light and Soils. One developing application relevant to both Years is the analysis of biologically important trace elements in soils by X-ray fluorescence spectrometry. This mention of XRF should provide a reminder that our energetic Industrial Group has not one but two Group Meetings in a year, the meeting last November already described and an upcoming meeting on XRF that will take place on June 17 this year at the University of Leicester. At the time I write this, the programme is being assembled; keep checking **https://sites.google.com/site/bcaxrf/meetings/17-june-2015** to keep abreast of developments.

Carl Schwalbe

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- Eligibility of students and postdocs for an Arnold Beevers Bursary award
- A copy of Crystallography News every quarter
- Optional E-mail notifications of news items and meeting information
- Influence on the development of crystallography and the BCA

For current rates, and to join, please see **www.crystallography.org.uk/membership/**

Puzzle Corner

WITH the International Year of Crystallography still fresh in our minds, this and other "years" can be combined according to the operations shown below, giving the digits of a 4-digit number that should set your pulses racing.

Chemistry + Physics – Crystallography – Thanksgiving

Forests – Biodiversity + Planet Earth – Astronomy

Freshwater – Deserts + Mountains – Ocean

Soils – Family Farming + Quinoa – Potato

Answer to September Puzzle

From page 5 of the September issue:

First, assume that the star fields are sections of infinitely extended 2-dimensional patterns (an extreme example of "Wider still, and wider, shall thy bounds be set!), so can be described by one of the 17 plane groups.

5-pointed stars: 48 = pm; 49, 50, 51 = cm.

6-pointed stars (with the spacings adjusted so that the centres of the stars have a close-packed arrangement): 48 = pmm; 49, 50, 51 = p6mm.

This solution was contributed by Jim Trotter.

BCA Annual Spring Meeting
University of York, 30 March – 2 April, 2015

From the BCA 2015 Programme Committee

WE look forward to seeing you at the University of York for BCA 2015 very soon.

The **2015 BCA Named Lecturers** are:-

Dorothy Hodgkin Lecture:
Prof. Sir Tom Blundell FRS.
"Dorothy Hodgkin, Structural Biology and Drug Discovery"

Lonsdale Lecture:
Prof. Simon Parsons.
"High Pressure and the Molecular Crystalline State"

The **Plenary speakers** are:-

BSG:	***Prof. Gideon Davies FRS,*** University of York
CCG:	***Dr. Colin Groom,*** CCDC
IG:	***Dr. Peter Chupas,*** APS, Chicago
PCG:	***Prof. Anthony Cheetham FRS,*** University of Cambridge

Meeting website:
http://york2015.crystallography.org.uk/

Scientific Programme

Monday 30 March 2015 pm
and **Tuesday 31 March am**

Young Crystallographers Group Satellite Meeting

Plenary speakers:
Prof. Susan Lea
Prof. Chick Wilson

Parkin Lecture:
Dr Anna Warren (Diamond)

Teaching session *"Space groups – the final frontier"*
Prof. Bill Clegg (University of Newcastle) Part 1:
"A voyage into orbit"
Prof. Mike Glazer (Universities of Oxford & Warwick) Part 2:
"Into deep space"

Main Meeting
Tuesday March 31

12 noon to 12:50pm
Dorothy Hodgkin Lecture:
Prof. Sir Tom Blundell FRS.
"Dorothy Hodgkin, Structural Biology and Drug Discovery"

1:30pm to 2:20pm
CCG Plenary:
Colin Groom, CCDC.
"Fifty years of sharing crystal structures".
Chair: Simon Coles

2:30pm to 4:00pm
BSG: Drug design
Chair: Judit Debreczeni (Astra Zeneca)
Keynote: Chun-wa Chung (GSK) *Title to be confirmed*

Jon Read (Astra Zeneca) *"Cofactors and crystallization systems – targeting dehydrogenases"*

Claudine Bisson (University of Sheffield) *"Designing novel herbicides: unexpected equal potency of inhibitor enantiomers explained using high-resolution X-ray crystallography"*

CCG: Data Avalanche
Chair: Mark Warren (Diamond), *Co-chair:* László Fábián (University of East Anglia)

Keynote: Peter Wood (CCDC)
With the dramatic decrease in read out times of detectors the time to obtain a dataset has also dramatically reduced. An entire dataset can now be collected in a matter of milliseconds at synchrotrons and tens of minutes in-house. With this, the crystallographer has been bombarded with shed loads of data! How will we cope? Well, the "Data Avalanche" session will bring together experienced speakers who have come up with strategies to organise and compare all their processed data, and ways in which the vast number of resulting structures can be evaluated and summed up in manageable tables and graphs.

Simon Coles (University of Southampton) *"Data Avalanche! Search and Rescue using Systematics and Informatics"*

Rachael Skyner (University of St Andrews) *"Developing Predictive Models with Crystallographic Data"*

PCG: Beyond the Elastic Line – Resonant and Inelastic Diffraction
Chair: Mark Senn (University of Oxford)

Keynote: Steven Collins (Diamond) *"Resonant X-ray Diffraction and the elusive sign of the DM interaction in weak ferromagnets"*

This is an interdisciplinary session designed to bring crystallographers together with researchers who come from a background in resonant and inelastic scattering. The aim of the session is to explore the possibilities in crystallography beyond "conventional" charge scattering.

Matthias Gutmann (ISIS) *"Combining ab-initio phonons and diffraction to study thermal diffuse scattering"*

Chris Stock (University of Edinburgh) *"Helical and multipartlcle fluctuations in chiral magnets"*

4:30 to 6:00pm
BSG: Data acquisition
Chair: Elspeth Garman (University of Oxford).

Keynote: Gwyndaf Evans (Diamond) *"Exploring the limits of synchrotron radiation in macromolecular crystallography"*

Matthew Bowler (ESRF) *"Fully automatic data acquisition: MASSIF1 at the ESRF"*

Jonathan Brooks-Bartlett (University of Oxford) *"Progress in simulating the data collection process: modelling global radiation damage"*

CCG: Automation
Chair: Claire Wilson (Diamond/NCS), *Co-chair:* Pascal Parois (University of Oxford)

Keynote: Graeme Winter (Diamond) *"Development of Automated Data Analysis in Macromolecular Crystallography"*
Developments in areas such as detectors, sources and computing provide powerful drivers for automation in chemical crystallography. Automation also offers exciting opportunities to carry out new systematic scientific studies.

Richard Cooper (University of Oxford) *"Squeeze harder: Automated real-space modelling of disordered assemblies"*

Suzanna Ward (CCDC) *"Sharing 250 new structures every day"*

PCG: Challenges and Technical Advances in Powder Diffraction
Chair: Paul Saines (University of Oxford)

Keynote: Pascal Manuel (ISIS) *"Extreme Conditions and Magnetic Neutron Diffraction: how far can we push it?"*
Powder diffraction plays a crucial role in the characterisation of functional materials including studies in-situ and at extreme conditions; especially in the many cases where single crystals are unavailable. This session will examine recent developments in techniques and instrumentation alongside cutting edge results in this important field.

Claire Murray (Diamond Light Source) *"New Facility for Long Duration Experiments at Diamond Light Source"*

Yue Wu (University of Oxford) *"Observing MOF crystallization using in-situ diffraction"*

6:10pm to 7:00pm
BSG Plenary:
Prof. Gideon Davies FRS (University of York) *"Probing the reaction pathways of enzymes through crystallography"*

Chair: Prof. Eleanor J Dodson FRS

7:00pm
Buffet dinner, Exhibition and Posters.

Wednesday April 1

9:00am to 9:50am
PCG Plenary:
Prof. Anthony Cheetham FRS (University of Cambridge)
"Phase Transitions in Metal-Organic Frameworks"

Chair: Matt Tucker (ISIS/Diamond)

10:15am to 12:15pm
Student Prize Lectures

1:30pm to 3:00pm
BSG - CCG Joint Session: Ligand Chemistry
Chair: Ehmke Pohl (Durham University), *Co-chair:* Jason Cole (CCDC)

Keynote: Prof. Martin Noble (University of Newcastle)
"Chemical And Computational Tools For Drug Discovery: Targetting The Mdm2/X-P53 Interaction"
This session is focussed on the interface between chemical and macromolecular crystallography where structural information from the entire range of crystallography is used to analyse, understand and optimise small-molecular to protein interaction.

Isabel Usón (Barcelona) *"Macromolecular ab initio phasing with ARCIMBOLDO: Single workstation implementations"*

Jon Agirre (University of York) *"Deriving a chemical context from public data sources: a carbohydrate-centric case study"*

IG Symposium: Catalysis
Chair: Claire Murray (Diamond)

Keynote: Andrew Beale (UCL) *"Chemical imaging using X-ray diffraction computed tomography to tackle everyday problems in heterogeneous catalysis"*

PCG: Structural Insights into Ferroic Materials
Chair: Phil Lightfoot (University of St Andrews)

Keynote: Pam Thomas (University of Warwick) *"Structures and Properties of Lead-Free Piezoelectrics – Domains, Disorder and Disagreements"*
Materials that undergo phase transitions to ferroelectric, ferroelastic or (ferro)magnetically ordered states are technologically vital. This session will focus on the nature of these phase transitions, the symmetry breaking that occurs and the possibility of coupling these ferroic orders.

Mark Senn (University of Oxford) *"Hybrid multiferroics and novel negative thermal expansion mechanisms"*

Semën Gorfman (University of Siegen) *"Understanding high electromechanical activity in uniaxial ferroelectric by using single crystal time-resolved X-ray diffraction"*

3:30pm to 5:00pm
BSG: Data Mining – wealth & pitfalls
Chair: Kevin Cowtan (University of York).

Keynote: Dr. Robbie Joosten (Netherlands Cancer Institute)

CCG - PCG Joint Symposium: Complementary Calculations
Chair: Simon Parsons (University of Edinburgh)

Keynote: Keith Refson (STFC Rutherford Appleton Laboratory) *"Atomistic Dynamics from First-Principles Simulation"*
The use of computational methods has made great strides, both in structure determination, prediction of new structure types and their response to stimuli, providing insight and guidance to experimental studies.

Lauren Hatcher (University of Bath) *"Predicting Excitation Properties of Solid-State Linkage Isomers – A Synergistic Approach"*

Claire Hobday (University of Edinburgh) *"Combining high-pressure gas loading and GCMC simulations to elucidate 'breathing' mechanism of Zeolitic Imidazolate Frameworks"*

Education Session
Chair: Mike Glazer (Universities of Oxford & Warwick)

Keynote: Juliette Pradon (CCDC) *"Crystallographic education and research in the developing world: Experiences in the Democratic Republic of the Congo"*

Lucy Mapp (University of Southampton) *"Delivering instrument-centric practical classes to undergraduates"*

Lynne Thomas (University of Bath) *"Spreading the Word – Crystallography and the Public"*

5:10pm to 6:00pm
Lonsdale Lecture: Prof. Simon Parsons *"High Pressure and the Molecular Crystalline State"*

6:00pm to 7:00pm
BCA AGM

7:30pm for 8:00pm
BCA Conference dinner

Thursday April 2

9:00am to 9:50am
IG Plenary: Dr. Peter Chupas (APS, Chicago) *"Hard X-ray Studies of Materials for Energy Storage and Conversion"*

10:15am to 11:45am
BSG: Simultaneous use of EM and MX data
Chair: Garib Murshudov (LMB, Cambridge)

Keynote: Alan Brown (University of Cambridge) *"Cryo-EM at near atomic resolution - recent developments in model building, refinement and validation"*

Arun Pandurangan (Birkbeck College, University of London) *"Simultaneous fitting of multiple subunits into low-resolution cryo electron microscopy maps of macromolecular assemblies"*

Martyn Winn (STFC) *"Collaborative Computational Project for Electron cryo-Microscopy"*

CCG: Problem Data
Chair: Stephen Moggach (University of Edinburgh),
Co-chair: Jamie Gould (University of Liverpool)

Keynote: Andrew Goodwin (University of Oxford)
Recent advances in crystallographic software and hardware have resulted in significant advances within many areas of crystallographic research. These include time resolved studies, experiments involving different sample environments and the extraction of detailed information from between the Bragg reflections.

K. E. Christensen (University of Oxford) *"Towards Understanding Modulation in Molecular Materials"*

J. R. Price (Australian Synchrotron) *"Cryo control and detector high angle corrections, Chemical Crystallography at the Australian Synchrotron MX Beamlines"*

IG - PCG Joint Session: Amorphous Materials, Nanomaterials and Liquids (Part 1)
Chairs: Christoph Salzmann (University College London) and Spoorthi Dharmayat (LGC Group)

Keynote: Sam Callear (ISIS) *"No Bragg Peaks? No Problem! – Amorphous and Nanomaterials Research at ISIS"*
Lacking long-range order, liquids, nanomaterials and amorphous materials are notoriously difficult to characterise structurally. From a technological and scientific point of view they are, however, immensely important classes of materials. This double session will highlight some of the recent advances in this area ranging from structural characterisations to the applications of these materials.

Nicholas Funnell (University of Oxford) *"Reverse Monte Carlo modelling of low-dimensional materials"*

Additional speaker to be confirmed.

12:00noon to 1:30pm
BSG: Low-resolution refinement
Chair: Keith Wilson (University of York)
Keynote: **Steven Johnson** (University of Oxford) *"Through the Distorted Looking Glass: tales of low resolution refinement"*

CCG: Would you publish this?
Chair: Bill Clegg (University of Newcastle), Co-chair: Gary Nichol (University of Edinburgh)

Keynote: **Larry Falvello** (University of Zaragoza) *"Why Would You Publish That, and How?"*
This session will have an unusual format. After an opening talk by Prof. Larry Falvello from the points of view of a crystallographer, author, and editor, anyone present can briefly describe one or more structural results that raise the session title question for the audience to discuss, with the aim of constructive rather than negative criticism. We particularly encourage submissions from Young Crystallographers. Problems might include charge imbalance or other chemical issues, low resolution or data completeness, tricky disorder, highly restrained models, residual electron density and other artefacts, etc. A formal abstract is not required, but please contact the session organisers in advance of the meeting (as soon as possible!) if you wish to contribute; we will request 1–3 slides for concatenation into a single session presentation.

IG - PCG Joint Session: Amorphous Materials, Nanomaterials and Liquids (Part 2)
Chairs: Christoph Salzmann (University College London) and Spoorthi Dharmayat (LGC Group)

Keynote: **Fiona C. Meldrum** (University of Leeds) "*Structure and Crystallization of Amorphous Calcium Carbonate"*

Sylvia McLain (University of Oxford) *"The essential role of water in the structure of biomolecules in solution"*

Neal Skipper (UCL) *"Neutron diffraction studies of aromatic interactions in liquids"*

BCA 2015 Spring Meeting: Workshop Programme

Tuesday 31 March				
14:30-15:15	R1	**Agilent**	Fraser White Dan Baker	CrysAlisPro 38: Data quality, fast experimentation, AutoChem 2.1 & StructureExplorer
15:15-16:00	R1	**Bruker**	Martin Adams	APEX2 Software Suite – The must-have solution for crystallography
			COFFEE BREAK	
16:30-17:15	R1	**Rigaku**	Joe Ferrara	HKL-3000R: Data collection and processing for Rigaku instruments
17:15-18:00	R1	**STOE**	Jens Richter	STOE software for data collection and reduction
Wednesday 1 April				
10:15-11:00	R1	**PANalytical**	Paul O'Meara	HighScore Plus and what it can do for you
10:15-12:00	R1	**CCP4I2**	Liz Potterton Jon Agirre	Structure Solution via a flexible interface with informative feedback and robust archiving
10:15-12:15	R2	**PDBe**	Sameer Velankar John Berrisford	Making the most of PDB and EMDB data
			LUNCH BREAK	
13:30-14:15	R1	**CRYSTALS**	Richard Cooper Pacal Parois	Modeling and refining disorder
14:15-15:00	R1	**Olex2**	Horst Puschmann Oleg Dolomanov	Getting Started with Olex2
13:30-15:00	R2	**ISODISTORT**	Branton Campbell	Introduction to ISODISTORT and the exploration of symmetry-lowering phase transitions
			COFFEE BREAK	
15:30-16:15	R1	**XPac**	Thomas Gelbrich Graham Tizzard	XPac
16:15-17:00	R1	**CCDC**	Pete Wood Suzanna Ward	The CSD: From Deposition to Analysis
Thursday 2 April				
10:15-11:45	R1	**CCP4mg**	Stuart McNicholas	Visualizing macromolecular structures with CCP4MG.
12:00-13:30	R1	**CCP4 Data Processing**	Phil Evans Johan Turkenburg	CCP4 Data processing

R1/ R2 denote the two rooms that are available for these workshop sessions throughout the BCA.

AGM 2015

THE 2015 Annual General Meeting of the British Crystallographic Association will be at the University of York at 18:00 on Wednesday 1 April 2015.

Elections
Elections for several positions on Council will be held at the AGM: the President (**David Keen** completes a 3-year term); one ordinary member (**Simon Parsons** completes a 3-year term); and the Education and Outreach Coordinator is stepping down at the AGM.

Nominations for any of these vacancies may be made by any two members and should be accompanied by the written consent of the candidate to serve if elected. Nominations must be received by the Secretary (secretary@crystallography.org.uk) not less than 4 days before the AGM (i.e. by March 26 2015).

Draft Agenda

1) Approval of Agenda
2) Apologies for Absence
3) Minutes of last AGM
4) President's Report
5) Secretary's Report
6) HG3 Report
7) Report of the Treasurer to include Presentation of the Accounts for 2014 and the Examining Accountant's Report
8) Acceptance of the Accounts
9) Appointment of Examining Accountant for 2015
10) Elections to Council
11) Honorary Members
12) Membership, annual subscriptions and subventions
13) Any other business

Draft minutes of the BCA Annual General Meeting 2014

James France Building,
Loughborough University,
18:00, 9 April 2014

1. Approval of Agenda

Proposed by Amber Thompson and seconded by Pamela Williams

2. Apologies for Absence

Received from Alex Griffin, Andrea Thorn, Elizabeth Shotton

3. Minutes of the last AGM

Mike Glazer proposed and Georgina Rosair seconded the approval of the minutes.

4. President's report

The President thanked Lee Brammer, HG3 and their teams for the excellent current Spring Meeting. The next meeting will be held in York from 30 March to 2 April 2015. John Helliwell is the programme chair for the 2015 meeting and everyone was encouraged to note the dates and to attend next year.

The President drew attention to the fact that the BCA website has been revamped and there has been increased traffic to the website in the last year. He thanked Scott McKellar and Richard Cooper for their work on this. He also encouraged people to follow the BCA @BritCryst twitter feed.

Much has been done and more is planned for public engagement during the Bragg Centenary year and the IYCr and events specifically mentioned were the Big Bang Fair in Birmingham and the exhibition which has run for several months at the Oxford Museum of the History of Science. There is also the Royal Institution's Crystallography collection on the Ri channel. The Education and Outreach Coordinators have produced a new resource website learn.crystallography.org.uk collating information to help learn about or teach crystallography and they would welcome more people adding content to this. There is also a twitter feed @whatsinacrystal which is very valuable. They need 4 more followers to reach 200. Anna Warren, Claire Murray and Lynne Thomas were thanked and presented with gifts for doing a fantastic job as the Education and Outreach coordinators.

Membership of the BCA continues to increase and Nicola Peel and her team at HG3 were thanked for their tenacity in chasing members to renew.

The President gave thanks to the BCA officers, the members of the BCA council particularly Richard Cooper and Scott Mckellar the webmasters, Carl Schwalbe, the CN editor and Nicola Peel and HG3. All members of the BCA members thanked for their continued support of the Association.

5. Secretary's report

There was nothing to report and no questions.

6. HG3 report

Nicola Peel gave the report from HG3. She reported that the total membership is now 696, increased from 581 last year; 361 standard, 151 student, 24 Honorary, 24 life, 44 retired, 21 overseas, 3 unemployed and 68 corporate members. The membership of the groups was reported as 252 for Biological Structures, 229 Chemical Crystallography, 48 Industrial, 73 Physical Crystallography, 21 Young Crystallographers, 24 with no affiliation and 49

unknown. Nicola also highlighted the importance of members indicating their main interest group in order to receive emails sent to the groups. This can be done by logging in and updating their details.

363 copies of Crystallography News were posted out to members and members are encouraged to take the pdf copy but the wishes of the advertisers need to be considered in this drive as the revenue is very important, £4150 per issue from 6 advertisers.

There had been 132 full and 21 day registrations for the current Spring meeting, with 15 exhibitor stands and 27 exhibitor staff present which brought in a total sponsorship and exhibition revenue of £11460. The BCA now has 10 corporate members. This year an exhibitors passport was introduced to encourage delegates to visit the exhibitors. John Helliwell asked a question about the numbers of corporate members and Nicola clarified that each Corporate member is entitled to up to 10 individual members which leads to 68 individuals listed as corporate from the 10 corporate members.

7. Treasurer's report

Printed copies of a summary of the accounts were circulated in the meeting and the Treasurer indicated that the full accounts are available via email or online through the charity commission website. She also clarified that the accounts are given for a calendar year. Overall the BCA total funds have increased to £257,784 boosted by £21,000, the BCA's 50% share of the surplus from ECM28. The investments held by the BCA also generate some income. The income and outgoings were affected by there being no Spring meeting in 2013 but it affects both income and outgoings, including reduced governance costs. The Treasurer pointed out that the BCA funds continue to allow the award of bursaries and sponsorship of outreach and IYCr2014 events. Thanks were given to HG3, council members, SIG treasurers, Charles Stanley Bank and The Young Company accountants.

Mike Glazer asked where the YCG funds came from and whether they should be increased. Anna Warren clarified that the money they held came from grant income they have raised for outreach events. The Treasurer made clear that the BCA income would be used to bolster these funds, the Arnold Beevers Bursary fund and other educational spending, she also clarified that the spending for the general outreach events comes from the BCA rather than the YCG.

8. Acceptance of the accounts

This was proposed by Mike Glazer and seconded by Anthony Philips and approved.

9. Approval of the Examining Accountants for 2014

The appointment of the Young Company, with an increased fee of £4800 compared to last year at £4500, was proposed by Dave Taylor and seconded by Amber Thomson and approved.

10. Elections to BCA Council

The following positions on council were due for election:

Treasurer as Pamela Williams had completed her first term

Pamela Williams was nominated by David Keen and seconded by Richard Cooper

Education and Outreach Coordinator which was an elected position for the first time

Sam Callear was nominated by Nick Funnell, seconded by Richard Cooper

Ordinary Council Member as Amber Thompson completed her term

Amber Thompson was nominated by Kirsten Christensen, seconded by Richard Cooper.

In all cases the nominations were unopposed.

11. Honorary Members

The President clarified that Honorary members of the BCA are chosen for their contributions both to crystallography and to the BCA. They may be proposed by any member by sending a recommendation to the President who, usually after consultation makes the decision on any new Honorary members. An Honorary member retains their membership for life and their number is limited at any one time. Members were encouraged to consider any nominations for new Honorary members for 2015.

12. A.O.B.

There was no other business.

The meeting closed at 18:30.

BCA-BSG / CGC / IG Group Meetings 2014

BCA-BSG Winter Meeting

Research Infrastructures in Structural Biology

THE 2014 Biological Structures Group winter meeting which ran from 15-17 December was, for the first time, held outside the UK, this being the International Year of Crystallography which marks a number of very important crystallographic centenaries. The meeting was very kindly hosted by the European Photon and Neutron (EPN) campus in Grenoble where the organisers: **G. Leonard**, **E. Mitchell** and **T. Forsyth**, put on a spectacular scientific programme. On arrival at the EPN site, it was pleasantly clear to this attendee that the mild weather was more akin to that of a BCA spring meeting than a winter one, if not milder! The first session of the meeting was on Research Infrastructures, was chaired by **Vilmos Fulop** (Warwick) and began with a welcome and presentation by **Harald Reichert**, the ESRF Director of Research for Physical Sciences, who described how support for the ESRF stems from the science-drivers in its respective member countries, of which there are 21, along with 8 associate members. Approximately 30% of the users and proposals are biological. The 30+ beamlines constructed at this facility are maintained by a 100 mega-Euro operating budget which funded an upgrade programme that commenced in 2009 with the objectives of improving the facilities for structural biology and soft matter, analysis of extreme conditions, time-resolved studies, nanotechnology and X-ray imaging. Phase 2 of the upgrade, which includes 'deep refurbishment' will involve building a new storage ring to provide a 2-orders of magnitude increase in intensity and allow serial crystallography to be undertaken at this facility. Harald concluded his presentation by describing a number of case studies including low-dose *in vivo* tomography for high resolution imaging of cells involved in the neurobiology of ageing. Phase nano-tomography has allowed amazing images of bone cells to be obtained along with studies of the haemozoin deposits in the malaria parasite. The next lecture was given by **Helmut Schober**, the ILL Director of Science, who introduced attendees to the biological applications of neutrons, such as their ability to 'see' hydrogen atoms and water-structure with improved detail as well as their strengths in probing slow dynamics. Some fabulous recent examples of high-resolution neutron diffraction studies of pyrophosphatase, fatty-acid binding protein and HIV protease were given along with a recent fascinating study of cytochrome c peroxidase in which cryo-neutron diffraction yielded previously unobtainable data on the catalytic mechanism. Some very interesting neutron solution scattering studies of SXL, an RNA-binding protein involved in alternative splicing, and fibrillarin, another protein involved in RNA processing, were then described. Finally, Helmut presented some spin-echo studies of alcohol dehydrogenase and monoclonal antibodies to analyse their physical properties such as inter-domain motion and viscosity.

After much-needed coffee, the next session began with a presentation on recent developments in single-particle electron cryo-microscopy by **Christiane Berger-Schaffitzel** from EMBL Grenoble and Bristol. As emphasised by the speaker, 2014 has seen numerous high-profile EM structures published on systems of outstanding interest. Christiane described how the proteins to be studied are dropped onto holey carbon films and flash-cooled in liquid ethane to allow imaging in the electron beam. The technique relies heavily on averaging the images of the particles and the signal-to-noise ratio increases as the square-root of the number of particles averaged. The recent advent of direct electron detectors with their enhanced sensitivity allows for a high frame-rate and has facilitated studies of beam-induced movements in samples. The application of maximum-likelihood statistics is allowing further improvements in classification and sorting of the particle images. Christiane concluded with a summary of the on-going discussion on how best to validate and deposit EM structural results. The next speaker, **Pamela Williams** from Astex Pharmaceutical, Cambridge, UK, gave an intriguing account of how protein crystallography has been utilised for high-throughput fragment screening in parallel with biophysical, spectroscopic and other techniques. Pamela emphasised the roles played by sample changers, new detectors, remote access to synchrotrons and automated data processing. Whilst Astex have traditionally speeded-up the screening process by use of fragment mixtures, technical advances mean that the speed of data collection is such that 'cocktailing' may no longer be necessary in the near future. Indeed with the advent of XFEL and developments in *in situ* data collection and compound handling, the future looks particularly bright for crystallography as a drug-screening technique. Pamela described studies of hepatitis C helicase to discover inhibitors that bind between the protease and helicase domains of the precursor protein. Studies of bacterial DNA ligase, a good target for new antibiotics due to a difference in its cofactor requirement from the human host enzyme, were then described. This lecture was followed by a presentation from **David Scott**, Nottingham, who described the use of neutrons to study intrinsically disordered proteins and their interactions with DNA. David began describing studies of KorB, a transcriptional regulator involved in

chromosome partitioning which has intrinsically disordered dimerisation- and DNA-binding domains. David described how the Guinier and Kratky plots are well-known tools for solution scatterers and how the normalised Kratky plot can reveal the presence of significant disorder in the sample. Contrast matching studies with perdeuterated protein were undertaken to look at the structure of the KorA-KorB-DNA complex as well as the interaction of single-strand binding protein with DNA. Attendees were then treated with a guided tour of the facility of their choice (ILL, D-LAB or ESRF) and the evening was rounded-off with a cheese and wine reception.

The next day began early with a session on Future Opportunities for UK Structural Biology in Grenoble and was chaired by **Kate Brown** (chair of the STFC Life Sciences and Soft Materials Advisory Panel). The first presentation was by **Florent Bernaudat** who outlined the Grenoble Partnership for Structural Biology (PSB) – a consortium involving the ILL, ESRF, IBS and CNRS, all of whom funded the construction of the on-site Carl-Ivar Branden laboratory which opened in 2006. Amongst many other things, the laboratory specialises in screening for optimised expression constructs along with post-graduate and post-doctoral training, provides around 23 biophysical platforms including high-throughput crystallisation and has on-site high-field NMR. All facilities have a peer-reviewed scheme for external access. Next up, **Gordon Leonard** from ESRF introduced the 2020 upgrade plan for this facility which has the aim of reducing the divergence of the source to allow data collection from micro-crystals and the use of serial data collection techniques. Gordon gave the example of ID29 which currently has a beam-size of 60 x 30 µm at the crystal. Following the source upgrade, this will be reduced to 8 x 2 µm and should construction of a longer beamline be approved, a further reduction of the beam-size at the sample to 0.5 x 0.1 µm will be possible and will allow analysis of exceptionally small crystals – indeed, crystals which many of us are very expert at growing in great abundance, although, of course, they defy most of the current techniques for data collection. Gordon explained how fully automated data collection from 'sludges' of such micro-crystals mounted in loops and processed by techniques that are currently being developed for XFEL serial crystallography are likely to make major breakthroughs in structural biology. Fast-readout detectors (such as the Eiger 4M) will reduce exposure times perhaps to as low as 0.1 sec for a complete data collection. Gordon explained that these developments may allow us to go back to room-temperature data collection as a routine technique, although it was clear that many of the attendees would not remember such times! In addition, time-resolved studies using photolysis of caged-compounds will be far more feasible than at present. These developments may allow studies of *in vivo*-grown crystals of recombinant proteins and possibly even whole-tissue work. Extending the capabilities of the synchrotron to the nano-crystal range will also exploit the potential for direct phase measurement stemming from the increased coherence of the new source. Gordon pointed out an excellent, light-touch review of these phasing concepts from 2014 by J. Miao and J. A. Rodriguez (*Phasing tiny crystals.* IUCrJ 1, 3-4) which is recommended. Next-up, **Trevor Forsyth** from ILL spoke on the neutron facilities and the planned 2020 upgrade work. Trevor described the LADI-III instrument which is the centre-piece for neutron protein crystallography at ILL and exploits the many benefits of using a quasi-Laue beam and perdeuterated samples to allow work on crystals as small as 0.1 mm3. Important recent studies include that of HIV protease with a bound drug. This instrument is complemented by the monochromatic D19 thermal diffractometer which also provides an excellent facility for protein data collection and has been used recently for revealing the water structure of rubredoxin in unprecedented detail. Trevor outlined the ILL facilities for neutron solution scattering work (D11, D22 and D33) and reflectometry (Figaro) - both techniques benefit from perdeuterated samples and the use of phase-contrast techniques, as well as reverse labelling in which the component of interest in a complex is left hydrogenated for incoherent scattering. Time-of-flight spectroscopy, back-scattering and spin-echo studies have all allowed the dynamics of proteins to be studied and thus powerfully complement other structural techniques such as X-ray, NMR and EM. **Andrew Harrison**, CEO Diamond Light Source, then outlined the basis for the UK's participation in large-scale facilities and summarised the findings of the recent government capital consultation exercise. This highlighted that the UK essentially 'wants' to achieve a high level of scientific excellence in its use of these facilities for answering the grand-challenges facing society as well as providing a service to industry including the development of advanced materials and agri-science. The survey highlighted the importance of the reliability of the source as well as the need for next generation detectors and optics. Andrew mentioned that whilst a DLS upgrade is planned for some time in the next decade, one of the major recent investments is in the construction of the National Electron Microscopy facility which will allocate 30 - 50 % of instrument-time to peer-reviewed user applications. Andrew mentioned that the UK has a developing interest in the Hamburg XFEL and a Diamond FELS is under consideration, although a Europe-wide landscape-document on large-scale facilities is clearly needed to gauge the strength of this case. Next, **Colin Miles** from the UK BBSRC explained his role as chair of the RCUK large facilities steering group and how the UK funding model is essentially structured with the HM Treasury at its pinnacle, underpinned by the Department of Business, Innovation and Skills. This supports the research councils with a budget of around £3 billion per annum, of which the BBSRC is allocated around £450 million. Colin described how the biology community had responded well in the UK science requirements survey and how improvements in data-analysis and support for EM, XFEL other high-resolution microscopy techniques had been requested by the user-base. This was followed by a (forgive the term) 'lively' round-table discussion. Subjects covered were the perceived 'gaps' in the UK facilities and the need for personnel on the ground to support instrumentation. Indeed it was astutely observed that the increase in automation at these facilities has not decreased the need for people to support them, support for personnel being a key facet of the ESRF funding model. Other sagacious and insightful observations included a comment that the ILL also rightly favours a model of high technical and physical science support of the instrumentation and how the perdeuteration facility (D-LAB) was indeed brought into existence by UK funding.

Following the coffee break, the session on Combining X-rays and Neutrons in Structural Biology was chaired by **Jean Susini** (ESRF). **Arwen Pearson**, Hamburg, gave an introduction to studies of dynamics and catalysis in the crystal, covering intermediate-trapping methodologies, the use of active site mutants with reduced turnover and slow substrates as well as pump-probe experiments in which the sample is excited multiple times and diffraction data are accumulated in short, synchronised X-ray exposures at fixed

time-points in the reaction cycle. Indeed, an archetypal study of this nature on carbon monoxide binding to myoglobin was undertaken at a well-known local facility. Arwen explained that with XFEL timescales as low as 10^{-15} sec will be accessible and at the ESRF, following the 2020 upgrade programme, timescales of 10^{-12} - 10^{-9} sec will be observable. Arwen then went on to explain the manifold applications and advantages of the Hadamard transform to fully exploit the redundancy of measurements and to minimise the experimental error in obtaining time-dependent structure factors. Finally, Arwen outlined fascinating studies of thaumatin in which a time-dependent study of the structural consequences of radiation damage was undertaken. Next-up, **Cecilia Casadei** from Leicester and ILL described how very recent work on Laue and monochromatic cryo-neutron diffraction studies of perdeuterated cytochrome c peroxidase at high resolution had shed new light on the mechanism of catalysis. Soaking the crystals in the substrate hydrogen peroxide shows that the enzyme forms an iron (IV) oxo-ferryl intermediate with the distal histidine (residue 52) being protonated in the complex. **Julia Richardson** from Edinburgh then described structure-function studies of integrases, which are involved in DNA transposition events, including structure analysis of the protein Mos1 complexed with DNA. The talk began with a colourful demonstration of how transposable elements can give rise to very striking patterning in maize kernels and Julia pointed out that around 45% of our own genome is indeed transposable. The talk covered how genetic transposition events are mediated by enzymes known as integrases which themselves are very attractive targets for antiviral and anticancer drug discovery. Structural studies of Mos1 showed that the inverted repeats in the DNA (features which are critical for this class of enzyme) bind in parallel with each other in the complex. SANS studies with phase contrast using perdeuterated protein shows that the complex forms a long thin dimer which is held together end-to-end by the DNA-binding motifs. The final talk in the morning session was given by **Selma Maric** from the Karolinska Institute who described application of phospholipid nanodiscs as a very promising tool for studying the structure and function of integral membrane proteins. The disks which are around 10 nm in diameter can be assembled around the protein of interest using a membrane scaffold protein and appropriate detergents. It is, of course, possible to incorporate deuterium into the lipids and into the protein itself, by expression in *E. coli*, for phase contrast studies.

Following lunch, the afternoon session on Structural Biology on the EPN campus was chaired by **Jon Cooper** and commenced with a presentation by **Stephen Cusack** (EMBL, Genoble) who spoke on a novel drug-target from the influenza virus. Stephen began by explaining how influenza is a segmented, negative-strand orthomyxovirus which uses ribonucleoproteins to package its 8 mini-chromosomes. Indeed it is the swapping of these chromosomes between different strains of the virus which causes new and serious epidemics or even global pandemics to occur. Replication of the virus involves, amongst many things, the copying the parent negative-strand RNA into positive sense cRNA which can be transcribed to give mRNA encoding the viral proteins. These reactions are catalysed by a heterotrimeric RNA polymerase which possesses PB2 cap-binding domains that allow it to recognise the 5‘ and 3‘ ends of the vRNA. Stephen reported how the successful crystallisation of the enzyme from a strain of virus affecting bats allowed the structure to be solved, by a combination of molecular replacement and MAD phasing using a platinum derivative. The structure includes 16-18 bp of RNA showing how it interacts with the cap-binding domains and how the 3‘ end of the RNA sits in the active site. The enzyme possesses an interesting loop structure which allows it to perform un-primed initiation. Following this, **Andrea Dessen** from IBS spoke about a new class of drug-target from bacteria namely the α2-macroglobulins which are well-known as non-specific serine proteinase inhibitors, normally present in large amounts in the plasma. Andrea described the structure of the bacterial cell wall and explained how the enzymes involved in its biosynthesis are well-known targets for antibiotics. Andrea explained how the bacterial α2M's, like their better-studied mammalian counterparts, contain a thioester-forming domain which is responsible for inactivation of the serine protease target. Crystallisation of the salmonella α2M protein required surface entropy reducing (SER) mutations to be engineered in the gene, which were suggested by the SER-server (developed by **Zygmunt Derewenda** and **David Eisenberg**). Intriguingly one of the suggested mutations introduced a novel crystal contact which allowed the structure of this periplasmic protein to be determined, showing the organisation of its multiple macroglobulin domains and the position of its ‘bait’ region. This acts as a target for the host proteases that this molecule ‘preys’ on as a part of the bacteria's self-defence system. The final speaker in this session was **Catarina Silva** from CEA, Grenoble, who gave an interesting talk on MADS transcription factors from plants which affect germination and flower formation.These proteins possess DNA-binding and oligomerisation domains. Structure analysis required the application of high-throughput construct-screening techniques to achieve soluble expression. So far, a fusion of the DNA-binding domain with one of the oligomerisation domains has been amenable to NMR and a construct containing the remaining two oligomerisation domains has been crystallised and analysed by Se-Met MAD. The structure shows that the protein monomers adopt a very long helix-turn-helix structure and form very striking cross-shaped tetramers with their DNA-binding motifs some 200 Å apart. Atomic-force microscopy has been used to study how this protein binds to DNA and has shown that it is able to cross-bridge different parts of the DNA molecule together forming an intriguing network. This session was followed by a coffee break and then an opportunity for poster presenters to give a 2 minute overview of their results which yielded many interesting insights into the range of research going on in-and-around the Grenoble campus. Following this, attendees were treated to the conference banquet at one of the fabulous restaurants close to the Notre Dame Musee where wine flowed inexorably, many stories were told and the food was truly fantastic. Although the BSG chair, site-directors and organisers gave some great speeches, the author's memory of their content (and the return journey) is rather vague.

Wednesday morning began early with a session chaired by **Mark Roe** (Sussex) who oversaw the ensuing presentations on Emerging Techniques in Structural Biology. First-up was **Antoine Florent** from IBS who described the facililties at ESRF for low-temperature, *in crystallo* UV, visible and IR spectroscopy. Antoine emphasised the applicability of these studies to redox proteins, as well as those playing key roles in photoactive and photosynthetic processes along with those having intrinsic or exogenous fluorophores, with the caveat that the user first must check that the reductive effect of the incident X-ray beam does not affect the system under study. Antoine described a detailed case study of superoxide reductase in which work was undertaken to determine the

structure of its peroxy-intermediate by soaking the crystals with hydrogen peroxide and analysing the resulting spectra and maps. Another study of urate oxidase gave fabulous insights into how the substrate binds as a peroxo-intermediate although increasing the X-ray dose was shown to cause the bond to the oxygen to break. Next, **Gemma Newby** from ESRF described the time-resolved X-ray scattering beamline ID09b which allows pump-probe experiments (cycles of laser activation followed by X-ray exposure) to be undertaken. The beamline incorporates a high-speed beam-chopper and a milli-second shutter which allow picosecond pulses of X-rays. An infra-red laser can be used to induce rapid temperature jumps in the sample and the associated conformational change in the protein target can be followed by SAXS. Systems studied include amyloid fibre precursors, haemoglobin, ubiquitin and lysozyme with the objective of analysing unfolding pathways. **Liz Duke** from Diamond then gave a very interesting description of soft X-ray microscopy which is being developed as a tool for ultra-structural studies of subcellular structure. Individual cells can be imaged in fabulous detail by freezing in liquid ethane without any of the staining, drying and sectioning procedures which are common-place in the EM community. Gold particles are used as fiducials for the image analysis. A study of autophagy demonstrated the outstanding potential of this technique. **Manfred Burghammer** then gave a description of plans for serial microdiffraction studies at the ESRF with an account of facilities available on the microfocus ID13 beamline and how the new Eiger detector will allow data collection at 750 Hz, or up to 3kHz if lower-resolution sampling of the images is acceptable. Manfred described how serial studies are performed using the cubic lipid phase or sludges of microcrystals injected into, or held in, the beam and the data processing suite (CrystFEL), which was developed originally for XFEL studies, has been utilised successfully. Data reduction requires the diffraction from something like 10,000 crystals to be indexed and combined.

Following much-needed coffee, the final session (chaired by **Florent Bernaudat**) began with a presentation by **Matthew Bowler** from ESRF who outlined the plans for fully automated macromolecular crystallography, as implemented in the MASSIF beamlines. These essentially aim to automate all of the processes involved in data collection, including the centring of the crystal in the X-ray beam. This is done by scanning through the loop and analysing the diffraction images produced at each point using an interesting piece of software, DOZOR by Sacha Popov which detects protein-like diffraction in the images. The best part of the crystal for data collection is then chosen as that giving diffraction with the

Conference photo

Jon Cooper

lowest Wilson B-factor! The current capacity of the MASSIF system is something like 150 - 400 samples per day. Following on, **Ulrich Zander** from ESRF spoke further about local plans for serial crystallography beamlines, emphasising that data collection by this technique involves processing a series of still images from randomly oriented microcrystals that can be mounted in conventional loops. The resulting datasets need to be ranked by hierachical cluster analysis before merging to give the final dataset. Ulrich illustrated his presentation with some proof-of-concept studies involving *T. brucei* cathepsin B, proteinase K and bacteriorhodopsin. The cathepsin B study at PETRA III is particularly interesting since the microcrystals of this recombinant enzyme were grown *in vivo* using baculovirus-infected insect cells. Last, but not least, **Estelle Moussou** from ILL/Keele spoke on recent neutron studies undertaken using the monochromatic D19 beamline with a 2D position-sensitive detector including DNA fibre diffraction and detailed analyses of the water structure of rubredoxin. Studies of xylose isomerase demonstrated that one of the active site magnesium ions is replaced by a hydronium ion in certain conditions.

The meeting was formally concluded by the BSG chairman, **Vilmos Fulop**, who presented the poster prize to **Alycia Yee** (ILL/Keele). Vilmos went on to thank the local organisers (**Gordon Leonard**, **Trevor Forsyth** and **Ed Mitchell**) on behalf of the BSG committee for putting together such a spectacular programme on behalf of the BCA. The BSG sincerely thank the meeting hosts and sponsors, the local administrative team (**D. Davison**, **F. Mengoni** and **L. Tellier**) and the ever-present and tirelessly enthusiastic conference photographer (**Serge Claisse**) whose excellent work is, I hope, amply illustrated here.

Jon Cooper, UCL

Photographs from the BCA-BSG Winter Meeting

Selected Speakers ▼

H. Schober, T. Forsyth, C. Miles, H Reichert

S. Maric

C. Miles, H. Reichert

C. Berger-Schaffitzel

M. Burghammer

A. Harrison, H. Schober, T. Forsyth

A. Dessen

C. Casadei

E. Moussou

Scenes from the cheese and wine evening ▼

Speakers and BSG committee members looking suave, sophisticated and not always very well-shaven

Conference dinner ▼

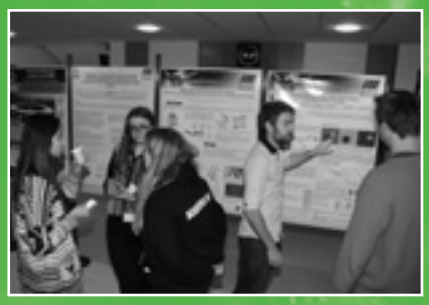




Tour of the beamlines

Poster prize winner – **A. Yee** ▶

Poster sessions ▼






Lively discussion fuelled by coffee and patisserie

CGC Autumn Meeting

THE 2014 CCG autumn meeting, in partnership with the RSC and kindly sponsored by Agilent Technologies, took place on the 19th of November at the RSC Chemistry Centre at Burlington House in London. Three sessions of talks encompassed the theme of 'Communicating Crystallography' from educational, publishing and data presentation points of view.

The first session, 'Crystallography in Education', chaired by Dr. **Simon Coles**, provided a guided tour through various aspects of teaching crystallography. Dr. **Anna Warren**, Diamond Light Source, began by giving a review of 'The Structure of Stuff is Sweet', a series of outreach activities that have been used to engage and educate the public about the importance of crystallography. Those in attendance were given the opportunity to try out one such tasty activity – making a model of a unit cell out of marshmallows and cocktail sticks.

Dr. **Peter Hoare**, University of Newcastle, spoke about the development of A-level and undergraduate resources which utilize the free CSD teaching database. These have been successfully used in schools in the North East of England (and beyond), and consist of a series of video tutorials, powerpoint presentations, theory and worksheets that have been written by year 12 Nuffield bursary and MChem students over the past 4 years, on a variety of topics.

Professor **Chick Wilson**, University of Bath, described a hands-on approach of teaching crystallographic techniques to undergraduate and first year PhD students, which, over a number of weeks, immerses students in the entire process, from the growth of previously unsolved crystals to the final refinement of diffraction data.

'Publishing and Crystallography', chaired by, comprised 3 talks by presenters from the RSC. Dr. **Guy Jones** gave a useful overview of the publishing process in high impact journals, as well as reviewing the submission process for crystallographic data. He also discussed the idea of greater access to scientific articles through open access journals, giving insight into the future of scientific publishing.

Dr. **Serin Dabb** gave a description of the EPRSC funded National Chemical Database Service, which acts as a host for other chemistry databases and tools, providing free access to members of UK academic institutions. She also outlined the RSC's vision of providing a data repository for UK chemical research data.

David Sait presented an engaging talk on how 'Education in Chemistry' magazine uses social media to increase its visibility and audience. He provided many useful tips on how best to use different social media platforms to communicate academic research.

The final session, 'Disseminating Structures', was chaired by **Lynne Thomas**. **Brian McMahon** gave the final talk of the day, providing an interesting summary of the different types of CIF formats to present structural data. He also posed the concern of structural information being lost to the wider community with the deindexation of ActaE and subsequent reduction in structural data being published.

The session ended with a panel discussion around the theme of 'Data, databases and deposition', in which many thought-provoking points were raised. There was much debate on the possibility of a repository to share publicly funded crystallography research data: including what data would be most useful to share, the need for guidelines to streamline judgement when deciding what is important data and the consideration of how valuable the data would be versus the effort required to record it in a useful manner.

All in all an enjoyable and informative day was had by everyone. This was a great introduction to the crystallographic community. Roll on the spring meeting.

Natalie Johnson
Newcastle University
(1st year PhD)

Simon Coles

Anna Warren

Peter Hoare

Chick Wilson

Guy Jones

Serin Dabb

THE Chemical Crystallography Group held its Autumn Meeting, entitled "Communicating Crystallography", jointly with the Royal Society of Chemistry (RSC). The venue was Burlington House, a stately Palladian mansion which was expanded and given over to science and art in Victorian times and now includes the home of the RSC. Sessions were held in the elegant library. Topics included: outreach to students and the general public; communication of results in journals, databases and social media; curation of data. The insights expressed here have relevance well beyond the confines of chemical crystallography.

Anna Warren reminded us that, with nearly 30 Nobel Prizes awarded to crystallographers, we can be rightly proud of our subject and should communicate that pride. She described recent activities intended to increase public awareness of crystallography, inspire schoolchildren about science, and promote the International Year of Crystallography and the Bragg centenary. A central feature is "The Structure of Stuff Is Sweet", which the audience partially re-created by making unit cells out of marshmallows and toothpicks.

Next, **Peter Hoare** addressed the specific needs for structural information of chemistry teaching at A-level and in early years of university. The Cambridge Structural Database is a genuine research resource which has a teaching subset that is universally available free of charge. Peter has extracted a double helping of educational value by commissioning high school year 12 summer students and MChem project students, mentored by post-grads and post-docs, to produce worksheets for exercises illustrating important concepts such as VSEPR. More information can be obtained from www.ncl.ac.uk/chemistry/outreach/ccdc .

Chick Wilson extended undergraduate teaching of crystallography to include hands-on research experience. In its present form "Frontiers of Crystallography" comprises 10-12 sessions in a 10-week period. Starting with the design, synthesis and characterisation of the target compound, students proceed to crystal structure determination. Compared with conventional practical classes with their sometimes unhealthy emphasis on "getting the right answer", the atmosphere is relaxed and informal, but students work with intense enthusiasm. They are expected to write up their results in the style of a paper in *Chemical Communications or CrystEngComm*.

This information provided a perfect bridge to the afternoon session, which continued after a tasty buffet lunch designed to suit all palates and waistlines. **Guy Jones**, the deputy editor of *Dalton Transactions* and *CrystEngComm*, gave us valuable tips about "Publishing chemical crystallography in high impact journals". He outlined the steps from submission of a manuscript to its appearance in a journal published by the RSC, and the role of editors in this process. He reminded us that the RSC uses CrossCheck to screen for plagiarism, both the inexcusable theft of others' work and more insidious self-plagiarism such as the re-use of one's own introduction. Finally, he discussed the trend for journals to move from subscription to open access, which can be "gold" (author pays, immediately available) or "green" (available only by subscription initially but also via a non-commercial repository after an embargo period expires).

Serin Dabb told us how the RSC, having won the contract to host the National Chemical Database Service between 2013 and 2017, provides best-in-class databases and a repository for research results. With the aim to be more than just a "big disk" or "data dump", after automated validation of data, results are made findable. The repository will also have embargoed and private areas. Learning resources are provided in the form of workshop material, flyers and fact sheets, videos and webinar series.

Supplementing the traditional means of scientific communication, social media are providing an increasingly important informal channel. **David Sait** produces tweets and blog posts for the RSC journal *Education in Chemistry*. Social media are useful in three ways: suggesting leads for articles, extending our reach and encouraging our audience to provide feedback. Successful use of social media depends on choosing a suitable platform (e.g. LinkedIn, Twitter or Facebook) and tailoring content to its requirements. Timing is also important. If you want to reach chemistry teachers, they are likely to be online around 4:05 PM, shortly after class has finished.

From the viewpoint of the International Union of Crystallography, **Brian McMahon** reminded us that chemical crystallography, along with macromolecular crystallography, has very highly developed systems for quality control. Starting with the core CIF dictionary in 1991, extensions have been adopted or are being drafted to include: images, electron density, incommensurate structures, magnetic structures, twinning, constraints and restraints. The integrated workflow eliminates transcription errors, provides consistent lossless data capture and makes all data searchable and reusable. For instance, *Acta Cryst., Section E* now publishes the CheckCIF validation

David Sait

Brian McMahon

John Helliwell

result and the structure factors so that the entire community can carry out improved re-refinement, possibly using newly developed techniques. In October 2014 *Acta Cryst., Section D* had a special section on Diffraction Data Deposition. A recurring theme at CODATA meetings has been the need to give due recognition to scientists who collect data sets.

After a tea break that was particularly welcome to those of us who had had to get up before the crack of dawn to attend the meeting, the day's proceedings were summarised and further developed in a panel discussion featuring **John Helliwell**, **Ian Bruno**, **Serin Dabb** and **Simon Coles**. In particular, John boosted our egos by reminding us that, aside from facilities like the Square Km Array radio telescope, we are among the world's most prolific generators of data; and Ian agreed that it would be highly desirable to archive all such data, but, being critically dependent on depositors' goodwill, it is at present a "big enough ask" to request but not demand structure factors. Simon noted that whilst we generate a vast amount of data we are only actually publishing a fraction of it and therefore databases are not as full as they could be – perhaps a solution is to not be wholly reliant on journal publishing and begin to think about ways in which we might "publish" data ourselves. Serin closed the panellists' presentations by demonstrating the complexity and diversity of the information we should be making available and talking about some of the barriers to making broader chemistry data available. A lively discussion ensued, with questions ranging from "what is metadata" to the deeper "what is worth sharing" or "what is the value vs the effort when sharing".

John Helliwell has posted a report on the Diffraction Data Deposition Working Group forum (**http://forums.iucr.org/viewtopic.php?f=21&t=355&hilit=CCG**) that highlights and comments on some of the topics discussed in the panel session.

Carl Schwalbe

IG Autumn Meeting

THE 2014 Industrial Group Autumn Meeting was held at the Royal Institution in London's Mayfair on the 12th November 2014. The day consisted of eight talks from speakers specialising in different areas of crystallography and crystallisation science and was attended by a number of industrialists, academics and students.

Lecture Session 1

Chair **Brett Cooper**, Paion UK Ltd

The day's lectures were kicked off with an introduction to the Royal Institution by **Frank James**. Frank took us back in time to 1799 when the building was purchased for a substantial amount of £4850. The talk took us through Davy's discovery of laughing gas, Faraday's work on magnetism, James Dewar's work on cryogenics and the Bragg's work on X-rays for structure determination (for which they were awarded the Nobel Prize in 1915).

The second lecture of the day entitled *'Structural studies at the salt-cocrystal interface'* was delivered by **Chris Frampton** from Brunel University. Chris began by explaining that the differing regulatory pathways between salts and co-crystals could save the pharmaceutical industry $19.5 million, simply through the transfer of one hydrogen atom. He then went on to show

examples of co-crystals for the modification of physical properties, focussing on the enhancement of dissolution profile of a pharmaceutical and the decrease in solubility of a common agrochemical. Chris then explored the ambiguous world of intermediates and the possibility of using DFT calculations to calculate the proton position from a powder pattern.
The third talk of was given by **Luca Russo** of GlaxoSmithKline and explored the use of *'Crystallography in support of pharmaceutical product development: The story of a channel solvate'*. In his talk, Luca showed how crystallography was able to provide an explanation for the high water absorption of a succinate API. He also showed that molecular modelling allowed for an insight into the actual arrangement of the water molecules within the channels.

The final talk of the morning session was delivered by **Michael Probert** from Newcastle University, entitled *'High pressure-the polymorph playground'*. His talk began with an advertisement of the current exhibition 'Illuminating Atoms' at the Royal Albert Hall, highlighting the growing publicity the area of crystallography is receiving in this international year of crystallography. Michael's talk then went on to explore the high pressure studies undertaken on a variety of monofluorotoluenes, 2-fluorophenylacetylene (2FPA) and the well renowned polymorphic material ROY. The work on 2FPA explored the effect of rate of application of pressure on the polymorph produced. The talk culminated in an interesting result from the high pressure studies of ROY; the ability to remove crystals from the diamond anvil cell for analysis. Michael finished with some words of wisdom; if you use the correct (best) tools for the job and know how to use them you often get truly unexpected results.

Lecture Session 2

Chair **Qendresa Osmani**, GlaxoSmithKline

The afternoon session started with a wonderful 3D talk *'ABC of GPCR Structural Biology'* delivered by **Andy Doré** of Heptares Therapeutics. G-Protein coupled receptors (GPCRs) are important drug targets accounting for 40% of drugs on the market which are unstable once removed from the cell membrane environment. The work presented looked at stabilising and trapping GPCR's, resulting in a more stable receptor that is more amenable to crystallisation. The fascinating work has now been published in *Nature*.

Delegates look at structures in 3D during Andy Dore's talk

Jeremy Cockcoft of UCL then gave a talk entitled *'Quick quick slow: Fast but long PXRD experiments'*. This talk focussed on modifications to the powder beamline I11 at Diamond Light Source to enable it to perform Long Duration Experiments (LDEs). This would allow the high intensities of the beamline to still be exploited but the sample could then be left and measured weeks or months later without moving the sample. To facilitate this improvement, a second hutch and second data analysis suite has been developed, with the first users in October of this year.

Jitka Waterman and Alex Dias of Diamond with the model structure of lysozyme in the Ri Museum

The third talk of the session was from **Ghazala Sadiq** of the CCDC entitled *'Solid Form Control and Design through Structural Informatics'*. The area of structural informatics is used to try and predict how a new molecule may crystallise or behave based on previous crystal structures; a tool which would be highly beneficial to many crystal engineers. It was shown that had this tool been around a decade ago, instances such as Ritonavir may not have happened as this tool clearly shows that Form I displays an unlikely set of hydrogen bonds and is therefore unlikely to be the stable form. The tool can therefore be applied to other polymorphic APIs to ensure that the most stable form is being produced.

The day's lecture programme was completed by **Kate Wittering** from the University of Bath who showed how *'X-ray diffraction is a fundamental tool in the development and understanding of continuous multi-component crystallisation'* in relation to the co-crystal of urea barbituric acid (UBA). As part of the EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation (CMAC), Kate explored the industrial benefits of continuous manufacturing and how she had applied three different crystallisation platforms to obtain a co-crystal that displays enhanced solubility compared to the parent API.

The day concluded with tea and cake in the museum of the Royal Institution, allowing delegates to look around and see how science has advanced over the centuries. Fun was had by all trying to keep up with the interactive periodic table song.

Lauren Agnew, University of Bath

CCP4 Study Weekend – University of Nottingham

THE annual Collaborative Computational Project in Macromolecular Crystallography (CCP4) Study Weekend was held at the East Midlands Conference Centre at the University of Nottingham on January 7-9, 2015. This year's meeting, entitled "Advances in Experimental Phasing", provided a comprehensive overview of phasing techniques including a historical review of the field, current and emerging methodologies and future challenges. The scientific programme was organised by Thomas Schneider (DESY, Germany) and Airlie McCoy (University of Cambridge, UK). Registered participants numbered 372 and drew scientists from a diverse range of academic and industrial institutions in the UK and other European countries as well as China, India, Singapore and the United States.

Neil Isaacs (Glasgow University, UK) opened the first session of the main meeting with a historical view of developments in phasing crystallographic data. The first structure to be determined by the Braggs, in 1914, did not need phases to be calculated, as it was deduced from considerations of diffraction, symmetry and atomic scattering power. A year later W.H. Bragg, shown in *Figure 1*, famously stated in his Bakerian lecture about X-rays and crystal structure, "If we know the nature of the periodic variation of the density of the medium, we can analyse it by Fourier's method into a series of harmonic terms." The small compounds whose structure was determined could still be phased by siting atoms on special positions in high symmetry space groups. But as the structure complexity increased and lower symmetry encountered, analytical expressions of Fourier terms, including phases, appeared in the 1920s. Patterson, 1934, used distance vector maps to overcome the imaginary phase contribution; and Harker, 1936, used Patterson maps to locate atoms or molecules in a unit cell. Lonsdale, 1936, published the first tables containing simplified structure factor and electron density formulae for all 230 space groups. Robertson, 1937, was able to phase data for phthalocyanine *(Figure 2)* by comparing maps with and without Ni, opening the way for routine phasing of centrosymmetric space groups.

Developments followed rapidly as Cox & Jeffrey deduced phases by comparing glucosamine hydrobromide/hydrochloride, producing the first isomorphous replacement exercise. Harker & Kasper, 1947, developed the inequalities and unitary structure factors; Hauptman, Karle and Sayre, 1951/1952, developed direct methods of phasing, followed by the tangent formula in 1956; Bijvoet, 1951, phased strychnine by SO_4/SeO_4 diffraction comparison, identifying the hand in this chiral molecule by comparing models in mirror images; Perutz, 1951, phased the first electron density map of a protein, myoglobin, using a Hg derivative; Harker, 1956, phased with 2 derivatives and extended the exercise to enantiomorph decision and non-isomorphism limit; Blow, Crick, Rossmann, 1960s, developed molecular replacement.

In the 1970s, computing and data acquisition infrastructures were slowly developing, acccompanied by establishment in 1979, of the Collaborative Computational Project 4, CCP4, by the Computer Board of the UK Science Research Council. Meanwhile, phasing methods continued to be developed: Hendrickson & Teeter, 1981, phased crambin with the anomalous signal from S; Wang, 1985, introduced solvent flattening; Hendrickson, Smith & Sheriff phased directly with the anomalous signal; Hendrickson, 1990, phased ribonuclease H with SeMet. These modern methods of still form the foundation of many approaches to solving the "phase problem" today.

The second presentation was made by **Janet Smith** (University of Michigan, USA), who discussed current strategies for phasing with weak signals from anomalous

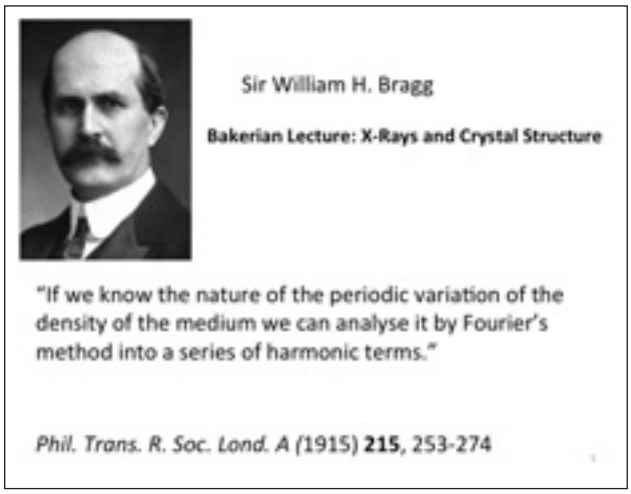


Fig. 1 – W.H. Bragg

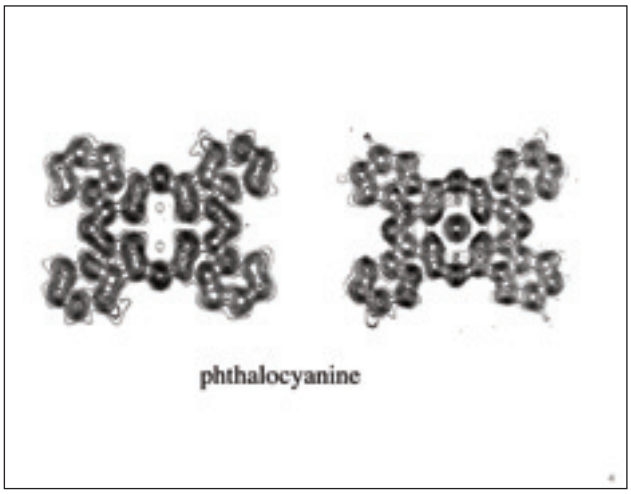


Fig. 2 – Electron density of phthalocyanine

scattering atoms in protein, such as sulfur and phosphorus. Data sets with anomalous scatters have become commonplace, thanks to cryoprotection and tunability of synchrotron radiation sources. The rapid expansion of multiwavelength anomalous diffraction techniques in the 1990s, gave way to single wavelength methods in more recent years. The size of the anomalous signal is dependent on the atomic species of the anomalous scatterer. However, the inability or disinclination to make SeMet or other heavy atom derivatives, led to careful recording of data sets to exploit the anomalous signal from the native sulfur atoms in a protein. The example of non-structural flavivirus proteins, with no equivalent in the structural database to provide a molecular replacement model, was used to explore the requirements for successful phasing with the sulfur anomalous signal. Apart from using relatively longer wavelengths, data acquisition strategies to reduce error in measurements were used, e.g. inverse beam geometry, fine phi slicing, and crystal alignment to ensure near concurrent recording of equivalent reflections. Up to 100 crystals were tested, resulting in 28 usable data sets. After the determination of the S subset, phase extension and map interpretation gave a good solution, and the phases extended up to 2.6 Å resolution. The sulfur substructure could be solved at 5.2 Å but not at 4.5 Å resolution, possibly due to the natural dip in the signal around the water ring, or maybe due to the accumulation of error. Ultra high multiplicity of the anomalous data was also necessary, where 50-fold redundancy could not produce a solution while 100-fold did. Phase calculation for the full data set from sulfur substructure was successful with 33-fold redundancy, but not with 17-fold. Phase refinement and extension, combined with 2-fold NCS averaging, completed the phase set. A quality indicator was used which combined the correlation coefficients of various parts of the data set as $CC_{comb} = CC_{all} + CC_{weak} > 45\%$.

The second session was composed of four case study presentations primarily illustrating how derivatives are used in phasing. **Liz Carpenter** (Structural Genomics Consortium, University of Oxford, UK) opened the session with a detailed and highly informative talk about the use of heavy atoms in phasing. She gave comprehensive descriptions of heavy atom preparation, crystal soaking, and data collection methods. In some cases, obtaining a derivative for phasing is the only feasible way of obtaining phases, particularly for very challenging problems such as structure determination of membrane proteins. She illustrated this point with recent examples from her group including the use of a mercury derivative (along with seleno-methionine) to phase ABCB10, an ATP transporter; and the use of an intrinsic and extrinsic anomalous scatterers to phase crystals of the nuclear membrane zinc metalloprotease ZMPSTE24.

In the second talk by **Veronica Cane Dickson** (Memorial Sloan Kettering Cancer Center, NY, USA), described the methods used to phase the crystal structure of Bestrophin, a eukaryotic calcium-activated chloride channel. She explained how crystals of Bestrophin suffered from common problems associated with membrane proteins including severe anisotropy, moderate resolution, crystal twinning and poor uptake of heavy atoms. Improvement in crystal quality was obtained by creating a Fab-protein complex of the pentameric form of Bestrophin. However, since molecular replacement methods failed, SAD phasing of the structure of the complex was eventually obtained using tantalum bromide clusters.

Richard Bunker (Friedrich Miescher Institute for Biomedical Research, Basel, Switzerland) next described a “heroic” effort

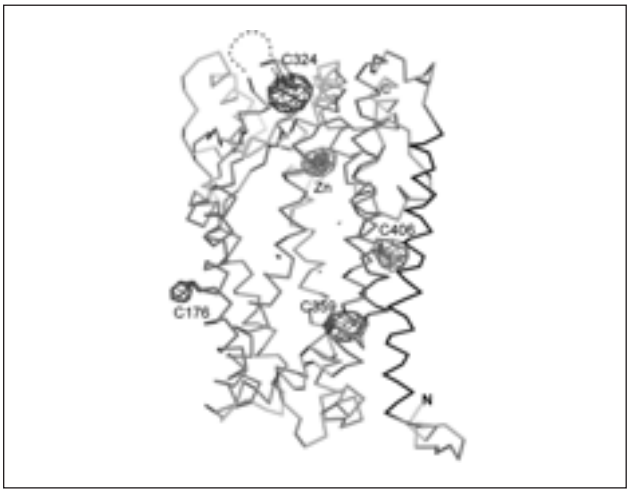


Fig. 3 – **ZMPSTE24 with the anomalous peak for the native zinc atom and the three mercury anomalous peaks associated with the three Cysteines. Adapted from Quigley et al., Science. 2013 339:1604-7. The image was prepared by Ashley Pike and Liz Carpenter, SGC, Oxford.**

of a 4 Å-structure determination of the COP9 signalosome (CSN). CSN is a major regulator of intracellular protein degradation, composed of eight proteins assembled in a 350 kDa complex. Phasing of the structure was initially complicated by rotational pseudo-symmetry, twinning, non-isomorphism and lack of experimental phase information beyond 8 Å resolution. Again, the use of cluster heavy atom compounds proved to be critical for obtaining phases in a multiple isomorphous replacement with anomalous scattering (MIRAS) strategy. Selenomethionone-containing proteins, differentially substituted into the complex and multi-crystal averaging then enabled individual polypetides to be assigned within the complex, facilitating the complete model to be built and refined.

The final talk of this session was presented by **Bernie Kelly** (University of Cambridge, UK) focused on how selenomethionine substitutions has been used to assign sequence in low resolution structures. He provided a comprehensive overview of how one can introduce, if necessary, point mutations into a sequence that permit higher levels of incorporation of selenomethionine compared to using a native protein sequence that may contain few substitution sites. He described methods for crystallization and explained how the presence of selenomethonine can be enabling for sequence assignment, particularly in low resolution structures. He presented a case study involving the determination of the crystal structure of the AP2 adaptor complex, where log-liklihood gradient maps were used to successfully locate selenium sites. He also emphasised how consistent indexing and merging multiple datasets were key to the successful structure determination of AP2.

The session after tea on Thursday was on Phase Determination methods. The first talk was ‘The Phase Problem: an introduction’ by **Paula Salgado** (Newcastle University, UK). She introduced the phase problem, Argand diagrams and Harker circles for the students in the audience and proceeded to explain how SIR/MIR can be understood in terms of these. She then went on to show that while AS is theoretically similar to MIR, MAD techniques are better than MIR, due to it having smaller errors (as long as there is no radiation damage). She finished with a good example of in-house S-SAD phasing.

The second talk was given by **Tom Terwilliger** (Los Alamos National Laboratory, Los Alamos, USA) entitled 'X-Ray structure determination using weak anomalous data'. He showed how a weak anomalous signal often led to hard substructure determination, poor phasing from the substructure model and hard model building and refinement. He introduced an equation to calculate $<S_{ano}>$, and from past solved datasets showed that if $<S_{ano}>$ was >10 then the structure could be solved easily, if lower then it would be hard. He also showed how $<S_{ano}>$ could be estimated prior to the experiment to guide the data collection with respect to I/σI and true multiplicity.

Randy Read (University of Cambridge, UK) presented the third talk on 'Accounting for intensity errors in SAD phasing'. He started by showing that while the French and Wilson distribution designed to calculate F's from I's works well for strong intensities, it may not work well at the very weak intensities that we now use routinely since the introduction of the $CC_{1/2}$ has extended data limits. He has formulated a new Rice function that estimates the errors in weak data much more accurately and incorporated this into an intensity based likelihood function that can be used for refinement and map calculation.

The last talk in the session was given by **Garib Murshudov** (MRC Laboratory of Molecular Biology, Cambridge, UK) on 'Using experimental phases in refinement'. He presented data showing that in problem cases the extra information contained in the dataset used to phase the structure may help. He showed that Refmac has a SAD refinement function that allows it to use all the data (F+, F-), which may give an advantage in difficult cases and also that these phases are useful in density modification steps. He further extended the use of the phases to show how they can be of help in the fitting of atomic models into high resolution EM maps in a maximum likelihood manner.

The first session on Saturday morning was focused on radiation damage and began with **Robin Owen** (Diamond Light Source, UK) providing an excellent talk on the radiation damage and how it can affect phasing with derivatives. Although radiation damage can be apparent in many cases, it may not always be immediately obvious. However, it is almost always present, causing site-specific damage (e.g., modifications to side chains) on short time scales compared to global damage, the latter of which is more easily monitored. Such damage clearly alters intensities. For derivatives, monitoring of intensity changes from X-ray damage and derivatization can be compared and used in the development of improved data collection strategies.

Max Nanao (ESRF, Grenoble. France) followed with a talk describing a methodology that takes advantage of radiation damage to specific atomic groups within crystal structures in a phasing methodology called "RIP" – radiation induced damage phasing. In this case the "derivative" dataset is the data from the crystal prior to radiation damage and the native dataset is the crystal after radiation damage. The success of the method requires 'novel' data collection strategies that can include a controlled "burn" of the crystal, with data collected prior to and after the burn has been applied. The speaker illustrated the success of the methods with a number of examples, pointing out that this method favored high resolution data sets with radiation damage directed to sulfur-containing atomic groups.

Gerard Bricogne (Global Phasing Ltd., Cambridge, UK) presented a set of protocols aimed at enhancing the quality of data collected for phasing, based around original methods used for MAD data collection. In his "Back to the Future" approach, he showed how these interleaved protocols for data collection and processing can be modernized for use with state-of-the-art facilities available on modern synchrotron sources. These integrated workflows enable even novice users to obtain high quality data, thin wedges of data with high-S/N dispersive differences. The success of this approach has involved close interactions between Global Phasing and a number of other groups based at SOLEIL, SLS, Diamond, and the MXCube collaboration.

The final speaker of this session was **Gwyndaf Evans** (Diamond Light Source, UK) who presented recent developments in data analysis that could impact on the future composition and application of multicrystal data sets. The re-emergence of using data sets collected from more than one crystal has arisen from difficulties of producing large single crystals suitable for collection of a complete data set and the expanding number of facilities equipped with microbeams. He introduced DIALS, Diffraction Integration for Advanced Light Sources, which is software that utilizes techniques of parallel processing using multiple CPU and GPU machines, facilitating not just speed, but highly accurate analysis based on a comprehensive physical model. He also described BLEND, a CCP4 program for the management of multiple data sets. Such programs aim to take advantage of the higher redundancies afforded by multiple data sets that translate into better-quality structure factors, with positive effects for phasing, model building and refinement, as well as enhanced anomalous signals for phasing.

The theme of following session was on beamlines and phasing. The opening speaker, **Michele Cianci** (EMBL c/o DESY, Germany), told us about some of the challenges of long-wavelength (2.7Å) data collection at beamline P13 at PETRA III. Despite optimisation of the beamline for operation at such wavelengths and the use of a helium cone in front of the detector, challenges remain. At low energies particular care must be taken to choose loops well matched to the crystals, and in the case described twinning provided an additional obstacle.

Andy Thompson (SOLEIL, France) described phasing successes at PROXIMA 1, demonstrating the importance of true redundancy through collection of sequential datasets with multiple kappa offsets. It was also shown that anomalous information can be used as markers to identify ligand, methionine or cysteine positions when building into maps of limited resolution.

Daniele De Sanctis (ESRF, France) gave details of beamlines and software available for phasing at the ESRF MX beamlines. Clear examples of good practice such as good sample mounting, cryo-protection and exploitation of strategy programs and protocols such as inverse beam data collection were shown to greatly improve the chances of a successful experiment.

Vincent Olieric (SLS at Paul Scherrer Institute, Swizerland) highlighted that of >6000 SAD structures in the PDB, only ~100 derive from native-SAD phasing. Experiments at the SLS, exploiting instrumentation such as the PRIGo goniometer, demonstrated that a low-dose, high redundancy approach can result in successful native-SAD even for large (> 260 kDA; 130 site) complexes.

Fig. 4 – **Armin Wagner in front of the P12M detector of the I23 long-wavelength MX beamline.**

Armin Wagner gave a glimpse into the near future of long-wavelength MX at DLS *(Figure 4)*. A beamline optimised for data collection at 3 – 8 keV in vacuum will become available for use later this year. First results from the beamline showed excellent data with promise of more when some of the final challenges of sample loading are overcome.

The meeting concluded with a final session devoted to evolving methods and was opened by **Bjorn Panyella Pedersen** (Aarhus University, Denmark), who elaborated on their n-dimensional search using a wide spectrum of molecular replacement parameters, such as clustering different conformers. The result is used to identify heavy atom positions from anomalous difference Fourier maps for further phasing of membrane protein structures.

Sang-Kil Son (CFEL, DESY, Germany) described the new opportunities and challenges of high-intensity phasing methods using X-Ray Free-Electron Laser (XFEL). Under those conditions many ab initio phasing methods would fail, since the atomic scattering factors have to be reformulated due to the electronic damage during ionization. He presented new phasing methods such as high-intensity Multi-wavelength Anomalous Dispersion (MAD) and Radiation damage Induced Phasing (RIP).

Monarin Uervirojnangkoorn (Stanford University, CA, USA) presented the phase ambiguity arising from SIR and SAD experiments. To overcome this problem she developed a new program within PHENIX called SISA. The method is based on identifying optimized phases for a small number of strong reflections prior to density-modification processes. This leads to improved electron density maps for more successful model building runs.

Julien Jorda (UCLA, CA, USA) presented his ideas about low-resolution ab initio phasing. This involves a genetic algorithm framework that evolves to a number of initial reflections with random phases. Iterative steps involving mutation, recombination and selection over many generations – in a genetic fashion – could approach the final solution. This development is in a very early stage.

Finally, this year's CCP4 workshop ran smoothly and successfully due to the dedicated and professional support provided by the UK Science and Technology Facilities Research Council (STFC) team comprised of **Karen McIntyre**, **Gail Peddle**, **Damian Jones**, **Laura Johnston**, and **Stuart Eyres** and **Laura Bennett** (photography, AV). In addition, this meeting benefited greatly from 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 current members of the Biological Structures Group Committee and edited by Katy Brown (BSG Vice-chairman).

Figures 1 and 2 supplied by Neil Isaacs

Diamond MX User Meeting

MARTIN Walsh began the meeting with an overview of the MX village and soft condensed matter beamlines at the Diamond Light Source, highlighting the wide range of facilities currently available for life sciences. The successful combination of automation, sample transport and short shifts has seen the proportion of remote experiments grow to over 50%. Further investment in remote access, including the development of the BART high capacity system (23 pucks, 368 samples) and the end-station upgrade programme to Pilatus P6M detectors will further support remote access. Martin covered new development highlights including the commissioning of compound refractive lenses (CRLs) to allow variable beam focussing with a selection of beam-size and energies, starting with I04 and then to be rolled out for MX beamlines. The new VMXi to replace I02 is scheduled for autumn 2016 with VMXm to follow in autumn 2017, while B24, a cryo full-field transmission microscope, will come online this summer to enhance biological imaging capabilities. Circular dichroism on B23 is now running a high-throughput sample environment (96 and 384 well plates). The electron microscopy facility is well underway after securing funding to the tune of £15.6M over 5 years and will house four state-of-the-art Titan microscopes, with two dedicated to life sciences. The facility will open in Autumn of this year but rapid access to a FEI Polara microscope with a Gatan quantum K2 direct electron detector is available through the rapid access route at Diamond (see Diamond home page or follow this link: (http://www.diamond.ac.uk/Science/Integrated-facilities/Electron-Microscopy/Polara.html).

Beamline I24, the micro-focus MX facility, has undergone a complete endstation rebuild to provide two independent goniometers: a high precision vertical goniometer (design spec 500 nm SOC) dedicated to standard cryo-crystal mounts and data collection and a horizontal goniometer dedicated to in situ plate screening and data collection. **Danny Axford** explained how the upgrade work incorporated repolishing of the beamline's microfocus mirrors leading to increased flux and smaller beamsizes down to 2.5 (v) x 5.0 (h) µm. A new optical system will provide unprecedented imaging for very small crystals at a resolution of 1µm, together with the ability for laser excitation.

Frank von Delft brought us up-to-date with an overview of developments on fragment-screening at beamline I04. Finding high-affinity ligands has been a long-standing problem and the approach here is to take advantage of recent advances in fast data collection, with an emphasis on provision of completely unattended use. Frank explained how large libraries can be screened using the latest automated technologies including high throughput soaking with efficiencies of up to 800 crystals being prepared in 30 minutes and the use of a new High Pin Density System (HPDS).

Beamline I23 is one of the most technically challenging endeavours in the Phase III programme for long-wavelength MX. **Ramona Duman** explained the design and commissioning of the new in-vacuum sample mounting, data collection and tomography setup. The stunning P12M curved detector in combination with an EM-style sample mounting system will allow users to solve structures utilising the weak anomalous signal from the intrinsic sulphur and phosphorus atoms of proteins and nucleic acids respectively in the 1.5 – 4 Å range. The first sulphur-SAD protein structure has already been solved and first users are expected in October. It is anticipated that there will be a workshop on the use of the beamline in September.

Graeme Winter described developments in software pipelines that now have to cope with up to 500 large files per second when all the MX Pilatus detectors are running. Diamond has invested extensively in computer resources to support this data stream and the average dataset now takes just two minutes to process. The implementation of the latest CC1/2 metrics for improved automated resolution cut-offs was seen as a particularly useful resource for MX users. The Fast Experimental Phasing (Fast EP) pipeline will shortly be implementing automated chain tracing.

Katsuaki Inoue provided an overview of a typical SAXS workflow using both I22 and B21 beamlines and support laboratories. A new software pipeline now allows a throughput of around 20 samples per hour and improved automation has increased efficiency and reduced sample volumes. A new detector system is due for installation this summer allowing camera lengths to vary between 1.5 – 8.5 m. Data processing is now available using a single integrated package, ScÅtter (downloadable from **http://bioisis.net/welcome**) which is being developed by the new Principal beamline scientist for B21 (Rob Rambo), and the online HPLC/MALS setup has been commissioned.

Kamel El Omari concluded the talks with a recent example of sulphur-SAD in action on I04. The limits of the technique were explored using the Hepatitis C glycoprotein E1 that contained no methionines, had no successful soluble mutants available, and proved refractory to soaking experiments. Although phases were only collected to a resolution of 6Å, the combination of very low detector background and improved signal-to-noise using the mini-kappa significantly improved the data. Multi-crystal processing resulted in a successful outcome.

The session was concluded with a question and answer session hosted by the Diamond MX User Representatives, **David Lawson** and **John McGeehan**. Some of the points raised and discussed included the use of Diamond computer resources for post-visit reprocessing of data, communication tools to aid remote access and the importance of providing feedback on the utility of webpages to aid continual improvement. Users are encouraged to contact the DUC with any feedback.

John McGeehan, University of Portsmouth

Call for nominations: 2015 Max Perutz Prize

THE European Crystallographic Association is pleased to announce the Eighth Max Perutz Prize, that will be awarded in recognition of meritorious achievements in any branch of crystallography to an individual scientist clearly affiliated with the ECA.

Nominators may be ECA Individual Members, or any person from a national member of ECA, or any Corporate Affiliated Members. The nominator must ensure a signed acceptance of the nomination by the nominee.

The nominator must indicate briefly why the candidate is nominated and may include matters such as publication record and impact of their research in the scientific community. However, the uniqueness of their pioneering contributions and the usefulness of the nominee's work will be of prime consideration to the selection committee.

The nominee shall not hold a current position on the ECA Executive Committee or be member of the current Max Perutz Prize Committee and must be a listed member of the World Directory of Crystallography. The winner receives the award at the official opening of the following ECM and presents a lecture at this occasion.

- More information can be found at http://www.ecanews.org/ecaprize.php
- Nominations are now open and will close on **March 8th 2015.**
- Nominations must be sent to the ECA Vice President at the address: vice.president@ecanews.org

Georgina Rosair
Heriot Watt University

Frank H. Allen 1944-2014

FRANK Allen died at the age of 70 on 10 November 2014. He leaves his wife Sandy, sons Andy and Stuart, and granddaughters Isabel and Eleanor. Frank and Sandy's eldest son, Ashley, was tragically killed in a road accident in 1988.

Frank was born in Reading and raised in Pangbourne, a village on the River Thames. He gained a First in chemistry and a PhD in crystallography at Imperial College, London, the latter under the supervision of Don Rogers. His first structures were of terpenoid derivatives, done the hard way with intensity measurement by eye (Sandy helped). He moved to Vancouver in 1968 to take up a NRC post-doctoral fellowship in Jim Trotter's group. One of the structures he and Jim solved was that of the notorious drug thalidomide. To everyone's great good fortune, Olga Kennard recruited Frank in 1970 to work for the fledgling Cambridge Crystallographic Data Centre. He remained there for the rest of his life, becoming Scientific Director and then Executive Director before retiring in 2008 to take on the role of Emeritus Research Fellow.

Searching the Cambridge Structural Database for 'F. H. Allen' yields 69 hits, but Frank drifted away from the diffractometer during his early years at Cambridge and turned to the computer. At a time when 'data' was not as fashionable as it is now, he worked with Sam Motherwell and others to write the programs that turned the CSD from a data library into a scientific instrument. It is easy to forget how innovative that software was. The CCDC was one of the pioneers of techniques such as chemical-name searching, two-dimensional and three-dimensional substructure searching, and structure- and substructure-sketching. Frank was also one of the first to use the CSD as a research tool in its own right, beginning with a study of the geometries of cyclopropane derivatives. He was one of the lead authors (Guy Orpen being the other) of two massive compilations of average bond lengths, which have now attracted some ten thousand citations. At the other extreme, his tongue-in-cheek letter on 'Retino-rectal connexions' has never been cited – until now: Allen, F. H. & Isaacs, N. W. (1971), *Nature,* **234**, 426.

Frank was a sportsman. He played cricket for his county at school level and opened the bowling for a strong University Chemical Laboratory team. A desire to play cricket was one of his stated reasons for wanting a return home from Canada! He was a mainstay of Sawston hockey club, his CCDC colleague John Rodgers being a teammate there for a time. He sustained frequent injuries, including a broken nose, as is always a possibility when several men in close proximity to one another wave heavy sticks and propel hard spheres at high speed. In addition to these physical injuries, Frank had a lifetime of mental trauma as a long-suffering fan of Reading FC.

While Olga Kennard was shrewd and determined in attracting grants to support the ongoing maintenance of the CSD, it was always a concern that the next grant application might fail, leaving the CCDC in crisis. In the mid-1980s, as industrial interest in the CSD grew, the possibility emerged that the centre might become self-financing, supported by user subscriptions. The die was cast in 1987: the CCDC became an independent, not-for-profit company with its own new building. Frank was by then Principal Scientist in charge of R&D. He was convinced that CCDC's funding policy was the right one. It attracted some criticism because the CSD was not 'free' like the Protein Data Bank (in other words, it was not directly funded by taxpayers). But he argued that the CCDC model gave more stability and made it easier to draw up and execute long-term plans. He remained of this view to the end of his life, by which time the CCDC was in its fiftieth year.

Frank was the vigorous editor of *Acta Crystallographica Section B* from 1993 to 2002, highly valued by his co-editors for the astute advice he gave on difficult cases. He was also on the editorial boards of several other journals. Even more important to crystallographic publishing was his work with Syd Hall and David Brown on the crystallographic information file. Its dictionary-based format, well ahead of its time, allows exchange of crystallographic information in a standard, extensible and information-rich manner. Frank took responsibility for selecting and defining the 423 data items in the initial CIF dictionary, critical work that exploited his careerlong interest in the management of crystallographic data. It is no overstatement that maintenance of the CSD would have become impossible without the CIF or something very like it.

An equable man, Frank could nevertheless get annoyed: for example, with the editors of two journals who refused to accept CSD-based research because 'reprocessing existing data isn't novel'. (Jack Dunitz pointed out that, on that basis, Mendeleev would not have got the Periodic Table published.) Annoyed, too, with those who thought the CSD could be maintained by a part-time post-doc and some clever software. The CCDC had very clever software – Frank wrote some of it – but he knew from experience that a great deal of manual effort was required to maintain a comprehensive database of high accuracy. From its beginning, Olga and DavidWatson had set high standards for the CSD. Frank shared and promulgated this view, knowing that it was essential if the database were to be suitable for top-quality research.

As Frank grew older and less able to terrorize opening batsmen and hockey goalkeepers, he took to more sedentary pastimes. He was very active in village life and served on the Governing Body of Impington Village College for many years, as its Chair from 1995 to 2001. With Sandy, he became quite expert at ornithology.

He won the RSC prize for Structural Chemistry in 1994 and the ACS Herman Skolnik Award in 2003, probably the highest accolade that can be awarded to a chemical information scientist. He was a Visiting Professor of Structural Chemistry at the University of Bristol, was on the International Advisory Board of the PDB (RCSB), a member of many commissions and committees of the IUCr, on the Council of the European Crystallographic Association, and Vice President of the British Crystallographic Association from 1997 to 2001. He was on the Board of Lhasa Limited, another not-for-profit scientific institution. He gave countless invited lectures and played his part as a conference organiser, including codirecting (with Judith Howard) the 1998 Erice School of Crystallography. Frank was warm hearted, relaxed, totally reliable, sometimes emotional, always caring. He was naturally and unconsciously egalitarian. He would laugh with a visiting Nobel laureate and then walk over to the chemistry lab for lunch and make the same jokes to the young man at the sandwich bar. He treated everyone the same because it never occurred to him to do otherwise. Most of all, he loved to talk to his students, some based at the CCDC, others in the labs of longterm collaborators such as Judith Howard and Paul Raithby. He was passionate about research, producing a steady output of influential papers – over 200 in total – on a range of subjects: intermolecular interactions, structure correlation, conformational analysis, data-mining techniques, molecular recognition and the application of the CSD to chemical education. He wrote several highly cited reviews of the CSD, including one in a 2002 joint *Acta B/Acta D* special issue on databases that he put together with Jenny Glusker.

Frank, tunelessly whistling, coffee mug and notebook in hand, would wander into the CCDC seminar room where several people and an empty seat waited to start a meeting. He habitually met deadlines and was normally punctual, but always managed to be a little late for these meetings. Occasionally, this would elicit a moan from his grumpiest colleague. Frank would nod apologetically but both he and his admonisher knew that nothing would change. Now something has and there will be an empty seat at the CCDC for ever.

Robin Taylor
Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, England

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Donald Anthony (Tony) Broad

DONALD Anthony Gifford Broad who everyone knew as Tony was born on 3 August 1921 in London, his family lived in a number of places including Cirencester but finally in Ruislip. He had a younger brother, Peter. He lived for a lot of his childhood with his Aunt Hilda. She was a headmistress and very influential during his school and college days and Tony lived with her for months on end.

Tony went to Technical College and his scientific and practical gifts began to become apparent. He could operate any wood or metal working machine, produce items made out of any material and mend anything.

After leaving school, he joined EMI in1938 with the help from his Uncle Jack who ran the Harrods Music Department. His boss and scientific mentor was Otto Klemperer (cousin of Otto Klemperer the conductor), and his knowledge of all things technical continued to grow.

Tony spent the war years working on the Cathode Ray Tube design for radar and television. He gained his HND at night school at that time and was also a member of the Home Guard. Tony spent his late teens and early twenties in London throughout the war.

Following the war, Tony met his wife Mavis and married her in 1947 after a six month whirlwind romance. Together they had 3 children Gillian, then twins Hilary and Stephen. Sadly, Stephen was drowned when he was 7. He joined the Cavendish Laboratory, Cambridge in 1949. In Cambridge he worked with many eminent scientists including Sir Lawrence Bragg, Max Perutz, John Kendrew and many postgrads who were doing research and became well known later (including Crick and Watson). He was in charge of the in-house making of items needed in the laboratory. His most important work was the design and construction of the rotating anode tube which allowed for much higher volumes of X-rays for the X-ray crystallographers and attracted many gifted scientists to come to work at the Lab. He is mentioned in a number of Nobel Prize submissions, in books and on the internet. He also made the first small model of DNA used for demonstration at conferences by Crick and Watson. Their original model was made from balls to represent the atoms, joined with wire, and was much too floppy to move. Tony suggested making metal plates which showed the atoms in the correct places, then attaching those via a rod in the middle to make a stable model. In addition, he did a lot of work designing the new building the MRC moved to in the early 60s. He also designed his own house and had it built in Cambridge.

He left Cambridge in 1961 and went to work at the Atomic Energy Research Establishment at Harwell. Finding work there much more bureaucratic and less satisfying, he left after about three years. Together with some friends, he set up his own company. They made a number of things over the years including some of the first power supplies for hole-in-the-wall cash machines and weather stations and soil moisture probes for the Institute of Hydrology. He sold the firm in 1989.

What makes Tony's life even more remarkable is that he lived from a teenager with the condition narcolepsy. By great willpower he dealt with it and did not allow it to prevent him from developing and using the skills that he needed for his working life.

Hilary Wallace

Georgina Ferry wrote this paragraph about the significance of Tony Broad's rotating anode design in her acclaimed biography of **Max Perutz**:

'A year later the Unit [Medical Research Council Research Unit on Molecular Structure of Biological Systems] added to its small staff an electrical engineer, Tony Broad. With the well-staffed and equipped Cavendish workshop close by, it might seem odd for the Unit to feel the need for its own engineer, but this was a far-sighted and extremely astute appointment that was to have huge benefits in the years to come. Broad was hired to design and build a new kind of X-ray tube called a "rotating anode" tube. X-ray tubes generate a lot of heat, along with the X-rays: if not turned off in time, their anodes can burn out. Now, in the late 1940s, tubes were produced in which the anode rotated, so that no single part of it became hot enough to incur damage. These tubes were capable of producing X-ray beams twenty times as strong as conventional tubes, making it possible to work with smaller crystals and to obtain sharper diffraction images. Broad's designs were extremely successful, eventually being produced commercially (they are still in use today): more importantly, they meant that from the early 1950s Max's unit was using the best X-ray equipment in the world.'

From *Max Perutz and the Secret of Life* by Georgina Ferry (2007), p. 131, Chatto & Windus

Colin Robertson, who was a senior engineer at Elliots in the 1960s, contributed the following evaluation:

'Tony Broad did not invent the rotating anode but he did enable the principle to be applied successfully to the quite different and growing requirements for higher powered X-ray generation in crystallography. In my opinion the main value of Tony's work lay in the engineering design of the bearing and sealing arrangements that allowed the rotating anode drum to be driven and water-cooled reliably from outside the continuously evacuated enclosure of the tube itself. This resulted in a tube capable of providing much higher outputs for very long continuous periods that crystallographers needed for the advanced work they were doing. The tube is "demountable". It can be dismantled and its parts can be replaced or exchanged as required, for example to use anodes with various target materials having different characteristic radiation properties. The design was covered by UK Patent No.854,363.'

New CCDC Web Interface and **750,000th Entry**

WE are pleased to announce the launch of our new public web interface for viewing and retrieving structures from the Cambridge Structural Database (CSD). This interface provides a rich user experience for viewing over 750,000 CSD entries found through our Get Structures service or linked to from within journal articles and external web sites and databases.

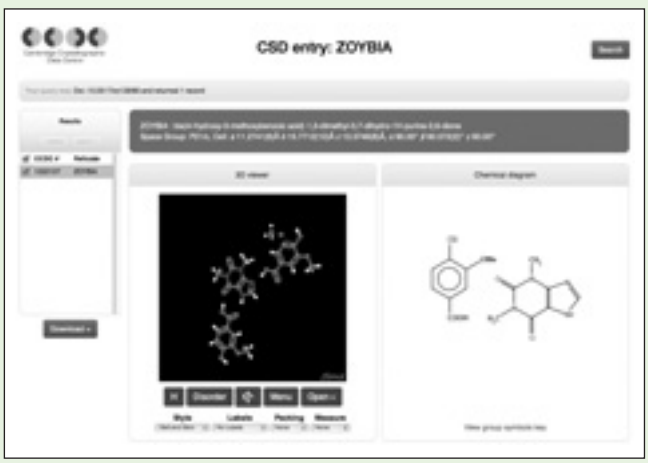
The service offers interactive 3D visualisation of structures with chemical interpretations generated by our expert editors, displayed using the splendid JSmol visualiser. This 3D visualisation allows easy identification and interactive exploration of structures. The interface also provides easy download of the deposited data in CIF format and of course allows all deposited structure factor data to be retrieved.

Read more at:

http://www.ccdc.cam.ac.uk/Community/Blog/pages/BlogPost.aspx?bpid=44

To view our 750,000th structure and search for all the other structures in the CSD using this exciting new interface go to:

http://dx.doi.org/10.5517/cc139l66



Suzanna Ward
Manager - Cambridge Structural Database

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.

1 March – 1 April 2015
HERCULES 2015 – European School, Grenoble, France.
http://hercules-school.eu/

2-6 March 2015
7th ILL Annual FullProf School, Grenoble, France.
www.ill.eu/FPSchool2015/

8-12 March 2015
Pittsburgh Conference (PITTCON 2015), New Orleans, LA, USA.
www.pittcon.org

9-13 March 2015
Clays and Clay Minerals, Karlsruhe, Germany.
www.dttg.ethz.ch/workshop%202015%20Karlsruhe.pdf

9-13 March 2015
Hybrid Materials 2015, Sitges (near Barcelona), Spain.
www.hybridmaterialsconference.com/

10-13 March 2015
IMAGINENANO2015: Incorporating Graphene2015 and PPM2015, and NanoSpain 2015 (Chemistry, Bio&Med, SP + Toxicology), Bilbao, Spain.
www.imaginenano.com/GENERAL/index.php

12-15 March 2015
The Eighth Workshop on Structural Analysis of Aperiodic Crystals, Bayreuth, Germany.
http://aperiodic.uni-bayreuth.de/workshop_2015/

15-18 March 2015
WCPCW. XXII West Coast Protein Crystallography Workshop, Monterey, CA, USA.
www.wcpcw2015.info/

16-19 March 2015
23rd Annual Conference of the German Crystallographic Society, Göttingen, Germany.
www.dgk-conference.de/organizational-matters/goettingen/

21-29 March 2015
XV Intensive Teaching School in X-ray Structure Analysis, Durham.
http://community.dur.ac.uk/durham.x-ray-school/

22-26 March 2015
249th ACS National Meeting, Denver, CO, USA.
www.acs.org/content/acs/en/meetings/spring-2015.html

29 March – 2 April 2015
Microscopy of Semiconducting Materials (MSM-XIX), Cambridge.
http://msm2015.iopconfs.org/home

30-31 March 2015
Magnetism 2015, Leeds.
http://magnetism2015.iopconfs.org/home

30 March – 1 April 2015
Nucleation - a Transition State to the Directed Assembly of Materials. Faraday Discussion, Leeds.
www.rsc.org/ConferencesAndEvents/RSCConferences/FD/Nucleation-FD2015/index.asp

30 March – 2 April 2015
BCA Spring Meeting, York.
www.crystallography.org.uk

30 March – 2 April 2015
Interdisciplinary Surface Science Conference (ISSC-20), Birmingham.
http://issc-20.iopconfs.org/home

6-10 April 2015
2015 MRS Spring Meeting & Exhibit, San Francisco, CA, USA.
www.mrs.org/spring2015/

9-11 April 2015
1st CSSB International Symposium "Systems in Infection Biology - From Molecules to Organisms, Hamburg, Germany.
www.cssb-symposium2015.de/

9-12 April 2015
Membrane Protein Structures 2015 Meeting (MPS 2015) and one-day workshop on Membrane Protein Technologies, Argonne National Laboratory, Lemont, IL, USA.
http://aps.anl.gov/mps2015

13-15 April 2015
Corrosion Chemistry. Faraday Discussion. London.
www.rsc.org/ConferencesAndEvents/RSCConferences/FD/Corrosion-FD2015/index.asp

13-16 April 2015
Advanced School in Soft Condensed Matter 'Solutions in the Spring', Loughborough.
http://scmspring2015.iopconfs.org/313476

13-17 April 2015
Structural Systems Biology – From Molecules to Organisms, DESY Campus, Hamburg, Germany.
https://indico.desy.de/conferenceDisplay.py?ovw=True&confId=11462

16 April 2015
Crystallisation & Polymorphism for Discovery Chemists, Cambridge.
https://www.soci.org/Events/Display-Event?EventCode=YCP445

19-24 April 2015
56th Experimental Nuclear Magnetic Resonance Conference, Pacific Grove, CA, USA.
www.enc-conference.org/

20-22 April 2015
Nanoparticle Synthesis and Assembly. Faraday Discussion. Chicago, IL, USA.
http://www.rsc.org/ConferencesAndEvents/RSCConferences/FD/Nanoparticle-FD2015/index.asp

22-24 April 2015
Crystallography for the next generation: the legacy of IYCr
www.iycr2014.org/legacy/conference

27 April – 1 May 2015
ICDD Clinics on practical X-ray fluorescence, Newtown Square, PA, USA.
www.icdd.com/education/xrf.htm

3-8 May 2015
RapiData 2015. Data Collection & Structure Solving. A Practical Course in Macromolecular X-ray Diffraction Measurement, SSRL, Stanford, CA, USA.
http://smb.slac.stanford.edu/

10-13 May 2015
International conference: Multi-Pole Approach to Structural Science, Warsaw, Poland.
http://multipole-meetings.org/

11-15 May 2015
2015 E-MRS Spring Conference & Exhibit, Lille, France.
www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=800&Itemid=1

11-15 May 2015
PolyChar 23. 23rd World Forum on Advanced Materials, Lincoln, NE, USA.
http://polychar23.unl.edu/

18-22 May 2015
EMBO Practical Course. Small angle neutron and X-ray scattering from proteins in solution, Grenoble, France.
http://events.embo.org/15-saxs/

18-22 May 2015
Practical X-ray course on methods in protein crystallography: data collection, data processing, and phasing, Oulu, Finland.
www.oulu.fi/biocenter/instruct-nac/courses

20-22 May 2015
Fourth International Symposium Frontiers in Polymer Science, Riva del Garda, Italy.
www.frontiersinpolymerscience.com/index.html

24-29 May 2015
ISBC. 5th International School on Biological Crystallization, Granada, Spain.
www.isbcgranada.org

25-28 May 2015
To.Sca.Lake: Total Scattering Analysis of Nanoscaled Materials, Como, Italy.
www.toscalake.com

1-5 June 2015
6th Workshop on Neutron Scattering Applications in Structural Biology, Oak Ridge, TN, USA.
https://public.ornl.gov/neutrons/conf/gcnb2015

5-14 June 2015
Engineering Crystallography: from Molecule to Crystal to Functional Form. 48th Erice Course, Erice, Italy.
www.crystalerice.org/Erice2015/2015.htm

7-11 June 2015
ICSG 2015. International Conference on Structural Genomics 2015, Weizmann Institute, Rehovot, Israel.
www.weizmann.ac.il/conferences/ICSG2015

7-12 June 2015
Computational Aspects - Biomolecular NMR: Exploring the Frontiers of NMR, Computations and Complementary Biophysical Methods. Gordon Research Conference, Lucca, Italy.
www.grc.org/programs.aspx?id=14571

7-12 June 2015
Sagamore XVIII. Conference on Charge, Spin and Momentum Densities, Santa Margherita di Pula (CA), Sardinia, Italy.
www.sagamorexviii.org/

7-13 June 2015
ISSC15. Second International Summer School of Crystallography 2015, DESY, Hamburg, Germany.
http://conferences.cfel.de/issc15

7-20 June 2015
The Zürich School of Crystallography: bring your own crystals, Zürich, Switzerland.
www.chem.uzh.ch/linden/zsc/

8-12 June 2015
ICDD X-ray Diffraction Clinics: Session II - Advanced Methods in X-ray Powder Diffraction, New Orleans, LA, USA.
www.icdd.com/education/xrd.htm

8-12 June 2015
Summer School on Methods and Applications of Neutron Spectroscopy, NIST, Gaithersburg, MD, USA.
www.ncnr.nist.gov/summerschool/ss15/index.html

9-12 June 2015
2nd NovAliX Conference: Biophysics in Drug Discovery 2015, Strasbourg, France.
www.ldorganisation.com/v2/produits.php?langue=english&cle_menus=1238915905&cle_data=1360153412

14-18 June 2015
DSE2015. 100 Years of the Debye Scattering Equation, Cavalese, Trentino, Italy.
www.dse2015.org/

14-19 June 2015
20th International Conference on Solid State Ionics, Keystone, CO, USA.
www.mrs.org/ssi-20/

15-17 June 2015
BioStruct-X Industrial Workshop, EMBL, Hamburg, Germany.
www.embl-hamburg.de/training/events/2015/BSX15-01/

16-23 June 2015
APS Data collection workshop and CCP4 school: From data collection to structure refinement and beyond, Argonne National Laboratory, Lemont, IL, USA.
www.ccp4.ac.uk/schools/APS-2015/index.php

16-25 June 2015
ISIS Neutron training course, Abingdon.
www.isis.stfc.ac.uk/learning/neutron-training-course/isis-neutron-training-course9135.html

17 June 2015
BCA Industrial Group – XRF meeting, University of Leicester.
https://sites.google.com/site/bcaxrf/meetings/17-june-2015

22-24 June 2015
Mesoscopic & Condensed Matter Physics, Boston, MA, USA.
http://condensedmatterphysics.conferenceseries.com/

24-26 June 2015
57th Electronic Materials Conference, Columbus, OH, USA.
www.mrs.org/57th-emc/

28 June – 2 July 2015
ZMPC 2015. International Symposium on Zeolites and MicroPorous Crystals, Sapporo, Japan.
www.zmpc.org/

28 June – 3 July 2015
Crystal Growth & Assembly. Gordon Research Conference. Biddeford, ME, USA.
www.grc.org/programs.aspx?id=12673

29 June – 3 July 2015
AFM2015. International Conference on Advances in Functional Materials, Long Island, NY, USA.
http://functionalmaterials.org/afm-2015/

29 June – 8 July 2015
EMBO Practical Course on High Throughput methods for protein production and crystallization, Marseille, France.
http://events.embo.org/15-htp-protein/

30 June – 3 July 2015
2nd International Conference on Nanomagnetism and Spintronics (RTNSA) & 7th International Workshop on Magnetic Wires (IWMW), Ordizia, Spain.
www.ehu.es/en/web/rtnsa-iwmw2015/home

6-10 July 2015
SRI2015. 12th International Conference on Synchrotron Radiation Instrumentation, New York, NY, USA.
www.bnl.gov/sri2015/

12-17 July 2015
22nd International Conference on the Chemistry of the Organic Solid State (ICCOSS XXII), Niigata, Japan.
www.iccoss2015.org

18-22 July 2015
ESBA2015. 10th European Biophysics Congress, Dresden, Germany.
www.ebsa2015.com

20-23 July 2015
12th International Conference on Materials Chemistry (MC12), York.
www.rsc.org/ConferencesAndEvents/RSCConferences/MC12/index.asp

25-29 July 2015
ACA2015. American Crystallographic Association Annual Meeting, Philadelphia, PA, USA.
www.amercrystalassn.org/

2-7 August 2015
20th American Conference on Crystal Growth and Epitaxy (ACCGE-20), Big Sky, MT, USA.
www.crystalgrowth.org/ACCGE-20---OMVPE-17-Conference.html

3-7 August 2015
64th Annual Denver X-ray Conference (DXC2015), Westminster, CO, USA.
www.dxcicdd.com/

6-14 August 2015
IUPAC-2015: 48th General Assembly and 45th World Chemistry Congress, Busan, Korea.
www.iupac2015.org

16-20 August 2015
250th ACS National Meeting, Boston, MA, USA.
www.acs.org/content/acs/en/meetings/nationalmeetings/meetings.html

20-22 August 2015
Advanced Software Development for Crystallographers, Duga Uvala, Croatia.
http://sig9.ecanews.org/rovinj.html

23-28 August 2015
ECM29. The 29th European Crystallographic Meeting, Rovinj, Croatia.
http://ecm29.ecanews.org/

24-27 August 2015
Structural Biology on the Move, Copenhagen, Denmark.
www.benzon-foundation.dk

24 August – 4 September 2015
European School on Magnetism (ESM), Cluj-Napoca, Romania.
http://magnetism.eu/esm/2015/index.html

30 August – 4 September 2015
VI European Conference on Neutron Scattering, Zaragoza, Spain.
http://ecns2015.unizar.es/index.php/home

30 August – 4 September 2015
Aperiodic 2015, Prague, Czech Republic.
http://crysa.fzu.cz/aperiodic2015/

6-10 September 2015
European Conference on Molecular Magnetism (ECMM2015), Zaragoza, Spain.
http://ecmm2015.unizar.es/

7-10 September 2015
VI International Conference of Synchrotron Radiation in Polymer Science, Madrid, Spain.
http://srps6.com/

9-11 September 2015
Fifth European Conference on Crystal Growth, Bologna, Italy.
http://www.eccg5.eu/

13-18 September 2015
SAS2015. 16th International conference on Small-Angle Scattering
www.helmholtz-berlin.de/events/sas/

14-18 September 2015
23rd International Congress on X-ray Optics and Microanalysis (ICXOM23), BNL, Upton, NY, USA.
www.bnl.gov/icxom23/

14-25 September 2015
13th School on Synchrotron Radiation, Grado,Italy.
www.synchrotron-radiation.it

15-18 September 2015
2015 E-MRS Fall Conference & Exhibit, Warsaw, Poland.
www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=13&Itemid=1651

20-24 September 2015
XXIII Conference on Applied Crystallography, Krynica Górska, Poland.
www.cac.us.edu.pl/

28-30 September 2015
Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.
www.icdd.com/education/rietveld-workshop.htm

28 September – 2 October 2015
ICESS-15. International Conference on Electron Spectroscopy and Structure, Stony Brook, NY, USA.
www.stonybrook.edu/commcms/icess/index.html

1-2 October 2015
Basic & Advanced Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.
www.icdd.com/education/rietveld-workshop.htm

12-16 October 2015
8th International Conference on Electromagnetic Processing of Materials, Cannes, France.
http://epm2015.sciencesconf.org/

29 November – 4 December 2015
Materials Research Society 2015 Fall Meeting, Boston, MA, USA.
www.mrs.org/fall2015/

5-8 December 2015
AsCA2015. The 13th Conference of the Asian Crystallographic Association, Science City, Kolkata, India.
http://www.asca2015.org/

6-10 December 2015
4th Nano Today Conference (Nano Today 2015), Dubai, United Arab Emirates.
www.nanotoday-conference.com/

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