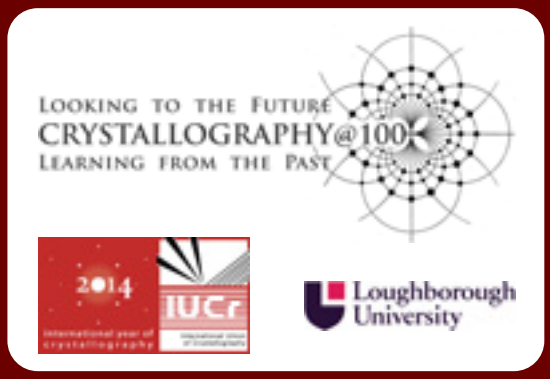
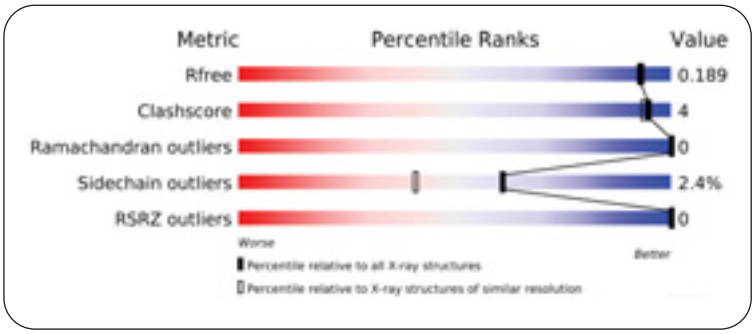
Crystallography News

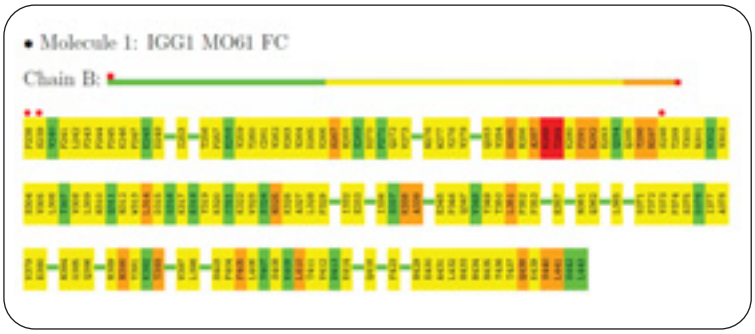
British Crystallographic Association

Issue No. 129 June 2014
ISSN 1467-2790



INSIDE: Validation reports available for all X-ray structures in the PDB (see page 30)





Spring Meeting & PDB Highlights

Spring Meeting reports p6
Prize winners p25
Education & Outreach p28
PDB Validation reports p30
XRF Meeting 2014 p33

APPLY SMART SENSITIVITY CONTROL

Confidence means a detector that automatically optimizes its sensitivity for every sample you investigate. Agilent's new Eos S2, Atlas S2, and Titan S2 CCD detectors employ groundbreaking Smart Sensitivity Control, which maximizes data quality by intelligently tuning detector sensitivity to match the strength of the data observed.

Combined with up to 2x faster readout times and instantly switching hardware binning, the S2 range redefines expectations for X-ray diffraction detector performance.

Learn how to apply Agilent S2 detectors and Smart Sensitivity Control to your research at **www.agilent.com/chem/S2CCD**.

The Measure of Confidence

ACADEMIC & INSTITUTIONAL RESEARCH

Agilent is a Proud Global Partner of the International Year of Crystallography

Agilent supports a variety of **IYCr2014** activities for advancing crystallography worldwide. Learn more at **www.agilent.com/chem/iycr2014**.

Agilent Technologies

The New D8 VENTURE With METALJET X-ray Source

The introduction of the revolutionary liquid-metal-jet X-ray source marks an impressive breakthrough in high performance home lab X-ray source technology. With an X-ray beam brighter than any other home X-ray source, the D8 VENTURE with METALJET and PHOTON 100 CMOS detector enables you to collect better data faster on smaller, more weakly diffracting crystals.

The D8 VENTURE with METALJET is easy to use and has lower maintenance requirements than traditional high-performance systems. It is the ideal solution for increasing the productivity of your structural biology lab.

www.bruker.com

Crystallography

Innovation with Integrity

BETTER MEASUREMENTS.
BETTER CONFIDENCE.
BETTER WORLD.

BioSAXS-2000

Expert SAXS results at home

The new BioSAXS-2000 provides more than double the flux on SAXS samples, resulting in faster experiments. With user-friendly intuitive tools, you can achieve expert SAXS results at home:

- **Automatic Analysis Pipeline quickly evaluates sample quality**
- **Automatic Sample Changer provides unattended sample loading and data collection**
- **Automated hardware and software tools ensure high precision, reproducible SAXS experiments**

Rigaku

Rigaku Corporation and its Global Subsidiaries
website: www.Rigaku.com | email: info@Rigaku.com

Crystallography News June 2014

Contents

From the President 2

BCA Council 2014 3

From the Editor 4

BCA Spring Meeting Reports 6

Prize Winners 25

Summary Financial Statements for year ended 31 December 2013 26

Education & Outreach Update 28

Validation reports available for all X-ray structures in the PDB 30

2014 Ludo Frevel Crystallographic Scholarship 31

News from the Groups 32

XRF Meeting 2014 33

Puzzle Corner 34

Meetings of Interest 35

BCA Administrative Office,
First Floor
Hornbeam House
Hornbeam Business Park
Harrogate HG2 8QT
Tel: +44 (0)1423 855 990
Fax: +44 (0)1423 855 999
e-mail: bca@hg3.co.uk

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 September 2014 issue are sent to the Editor to arrive before 25 July 2014.

Carl Schwalbe
15 St Augustine Drive
Droitwich
Worcs WR9 8QR
Tel: 01905 775257
e-mail: carlschwalbe@hotmail.com

Printed by Bowmans
Westland Square, Westland Road, Leeds, LS11 5SS
Tel: 0113 272 0088
Web: www.bowmans77.co.uk

This month's cover:

Spring Meeting scenes; PDB validation graphs

From the President

I confess that I don't often take much notice of the annual announcement of new Fellows of the Royal Society (see royalsociety.org/news/2014/new-fellows), but this year I was delighted to hear that my colleague at ISIS, Alan Soper has been elected to their fellowship. Alan is a pioneer of the total scattering technique – largely investigating liquids and solutions – and has been a great help to me as I try to apply similar methods to crystalline powders. It is also fantastic to see other crystallographers in the list of new Fellows: chemist Paul Attfield from Edinburgh (who spoke at ECM28 last year); materials scientist Paul Midgley from Cambridge (who spoke at a recent BCA Spring meeting on electron diffraction); the structural biologists Peter Colman (Australia) and Sheena Radford (Leeds); and the protein crystallographer Randy Read (Cambridge) who gave the Max Perutz prize lecture at the ECM28 Opening Ceremony. More than 10% of the new fellows this year can be broadly categorised as crystallographers – is this a record?

I have also been reading an interesting article on how the BCA came into being on 6th April 1982 (see Blow and Wallwork *Notes Rec. R. Soc. Lond.* **58** (2004) 177; rsnr.royalsocietypublishing.org/content/58/2/177.full.pdf). Probably many of you are already aware of this BCA 'prehistory', but for those of us who are not it is a fascinating description of how crystallography groups from different societies manoeuvred themselves into a single crystallographic association that could represent the whole UK community internationally.

The Inaugural Meeting of the BCA was held in Durham and began our series of Spring Meetings, the latest of which was held in April in Loughborough. I'd like to thank **Lee Brammer** and his team on the Programme Committee and **Nicola Peel** and her team at HG3 for putting on a well-run meeting with an excellent scientific programme. The highlight for me, if I had to choose just one, would probably be the session of Prize Lectures given by 'young' researchers. It was great to hear the diversity of subject matter that crystallography encompasses and the enthusiasm of the presenters. Thank you to those who have sent us helpful feedback on the meeting; we are mindful that the meeting was not as well-attended as we have come to expect and we need to ensure that our next meeting attracts larger numbers of delegates. This is a challenge that we must rise to for BCA Spring Meeting 2015 in York (30th March to 2nd April 2015). Please support the programme committee, chaired by **John Helliwell**, as they meet later in June to discuss and determine the structure and themes for the 2015 meeting. It is vitally important for the ongoing success of these meetings that all the Groups (and thanks to Blow and Wallwork above I now have a clearer understanding of how the BCA came from the CCG and PCG Groups, not vice-versa) play leading roles in their organisation.

The next big meeting on the horizon is of course the 23rd IUCr Congress and General Assembly in Montreal in August. I hope that many of you are able to go and I am confident that there will be a good representation of talks and posters from our BCA community. I'm looking forward to an exciting meeting. I also expect that several of you, like me, will be taking advantage of the trans-Atlantic travel and spending some time on holiday before or after the meeting. I'd be interested in hearing suggestions – *Crystallography News* readers travel tips(!) – on what to do on holiday in Canada, or alternatively what exciting things you did while in Canada. Perhaps the best examples could appear in the next edition of *CN* alongside the reports on the meeting?

The BCA Annual General Meeting took place during the Spring Meeting in Loughborough. There are no great changes to report; **Pamela Williams** was re-elected as Treasurer and **Amber Thompson** as an Ordinary Council Member. **Sam Callear** was elected as the BCA Education and Outreach Co-ordinator and will be working with the previous three EOCs on events happening throughout the rest of IYCr2014. Thank you to all who are continuing to support the running of the BCA through the work of BCA Council and Group Committees and to those who have recently completed their term of office and have passed on the baton to others.

Education and outreach and other public engagement activities are continuing apace with events such as the Big Bang Fair in the NEC in Birmingham back in March and the Cheltenham Science Festival this June. The Big Bang Fair stand was again a great success – thank you again to those who planned, co-ordinated, volunteered and supported the event financially and logistically. My day was great fun, although I was not the best at producing beautiful lysozyme crystals from tiny (invisible to me) drops of solution and showing them to hordes of expectant school kids down a microscope; I decided that I needed a trip to the optician. I also now know how many boxes are needed to ship £500 of marshmallows and other sweets – they fill the boot of an estate car. The events happening in the UK as part of IYCr2014 are too many to mention here, please see learn.crystallography.org.uk/crystallography-events for further information. Incidentally the @Whatsinacrystal twitter site (twitter.com/Whatsinacrystal) is an excellent place to discover what is topical in our field, if you are on Twitter please add to their over 200 followers! The BCA president has even been known to very occasionally tweet (@BritCryst_Pres).

I guess if I am starting to write about Twitter then it is probably time to stop writing, but before I do I want to point out that for IYCr2014 Physica Scripta has commissioned a virtual series of 'comments' articles from as many past Aminoff prize winners as possible (see www.kva.se/en/Prizes/Gregori-Aminoff-Prize/Laureates). Some of these articles have already appeared and many will be published later this year. These articles promise to be a fascinating insight into the lives and work of the many great crystallographers who have been awarded this prestigious crystallography prize by the Royal Swedish Academy of Sciences.

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

David Keen

BCA Council 2014

COUNCIL OFFICERS

President (2015)
Prof David Keen
ISIS Facility, Rutherford Appleton Laboratory, Harwell Oxford, Didcot Oxfordshire, OX11 0QX
Tel: 01235 446556
david.keen@stfc.ac.uk

Vice President (2016)
Dr Richard Cooper
Department of Chemistry, University of Oxford, 12 Mansfield Road, Oxford, OX1 3TA
Tel: 07525 687431
richard.cooper@chem.ox.ac.uk

Secretary (2016)
Dr Claire Wilson
National Crystallography Service
Diamond Light Source
Diamond House, Didcot
Oxfordshire OX11 0DE
Tel: 01235 778250
claire.wilson@diamond.ac.uk

Treasurer (2017)
Dr Pamela Williams
Astex Pharmaceuticals
436 Cambridge Science Park, Milton Road, Cambridge, CB4 0QA
Tel: 01223 226232
pamela.williams@astx.com

ORDINARY MEMBERS

Prof Simon Parsons (2015)
Room 90, King's Buildings, University of Edinburgh, West Mains Road, Edinburgh, EH9 3JJ
Tel: 0131 650 5804
s.parsons@ed.ac.uk

Dr Andrea Thorn (2016)
MRC Laboratory of Molecular Biology
Francis Crick Avenue
Cambridge Biomedical Campus
Cambridge CB2 0QH
Tel: 01223 267828
andrea.thorn@web.de

Dr Amber L Thompson (2017)
Department of Chemistry, University of Oxford, 12 Mansfield Road, Oxford OX1 3TA
Tel: 01865 285018
amber.thompson@chem.ox.ac.uk

GROUP REPRESENTATIVES

Biological Structures
Dr John McGeehan
Biophysics Laboratories, School of Biological Sciences, University of Portsmouth, Portsmouth, PO1 2DY
Tel: 02392 842042
john.mcgeehan@port.ac.uk

Chemical Crystallography
Dr. Pascal Parois
Chemical crystallography, Department of Chemistry, University of Oxford
pascal.parois@chem.ox.ac.uk

Industrial
Dr Elizabeth Shotton
Diamond Light Source
Diamond House, Didcot
Oxfordshire, OX11 0DE
Tel: 01235-778797
elizabeth.shotton@diamond.ac.uk

Physical Crystallography
Dr. Paul Saines
Department of Chemistry, University of Oxford, South Parks Road, Oxford OX1 3QR
Tel: 01865 272698
paul.saines@chem.ox.ac.uk

Young Crystallographers
Dr. Scott McKellar
School of Chemistry
The University of Edinburgh
West Mains Road,
Edinburgh, EH9 3JJ
Tel: 0131 650 4804
smckella@staffmail.ed.ac.uk

GROUP CHAIRS

Biological Structures
Prof Vilmos Fulop
School of Life Sciences, University of Warwick, Coventry, CV4 7AL
Tel: 024 7657 2628
vilmos@globin.bio.warwick.ac.uk

Chemical Crystallography
Dr Simon Coles
Chemistry, Faculty of Natural and Environmental Sciences, University of Southampton
Southampton, SO17 1BJ.
Tel: 023 8059 6721
S.J.Coles@soton.ac.uk

Industrial
Dr Cheryl Doherty
Principal Scientist at Pfizer IPC009
Ramsgate Road, Sandwich, Kent, CT13 9NJ
Tel: 01304 616161
cheryl.doherty@pfizer.com

Physical Crystallography
Dr Ivana Radosavljevic Evans
Department of Chemistry, Durham University, Durham, DH1 3LE, UK
Tel: 0191 334 2594
ivana.radosavljevic@durham.ac.uk

Young Crystallographers
Dr. Scott McKellar
School of Chemistry
The University of Edinburgh
West Mains Road,
Edinburgh, EH9 3JJ
Tel: 0131 650 4804
smckella@staffmail.ed.ac.uk

CO-OPTED MEMBERS

Bursary Co-ordinator
Dr Alexandra Griffin (2015)
Rigaku Life Science, Unit B6, Chaucer Business Park, Watery Lane, Kemsing, Sevenoaks, Kent TN15 6QY
alex.griffin@rigaku.com

Education & Outreach
Dr Sam Callear (2017)
ISIS Facility, Rutherford Appleton Laboratory, Harwell Oxford, Didcot Oxfordshire, OX11 0QX
Tel. 01235 445162
Sam.Callear@stfc.ac.uk

EX-OFFICIO MEMBERS

Editor
"Crystallography News"
Prof Carl H Schwalbe
15 St. Augustine Drive, Droitwich, Worc, WR9 8QR
Tel: 01905 775257
carlschwalbe@hotmail.com

Webmaster
Dr. Scott McKellar
School of Chemistry
The University of Edinburgh
West Mains Road,
Edinburgh, EH9 3JJ
Tel: 0131 650 4804
smckella@staffmail.ed.ac.uk

(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

OUR first Big Event of 2014 was the BCA Spring Meeting which took place in Loughborough from 7-10 April. These dates left very little time to prepare reports on proceedings, but our bursary recipients and many session chairs rose to the occasion magnificently. Therefore much of the meeting is covered in this issue, and the remainder will come in September. In accordance with the theme of the meeting, great events in the development of crystallography were described along with recent advances in the state of the art. A recurring theme of the latter coverage was the progress of X-ray free-electron lasers from the bright idea of a few visionaries to working facilities producing spectacular results. As usual, the presentations by Young Crystallographers that I witnessed were of excellent quality and delivered with great enthusiasm. Sometimes in moments of gloom I think that "diffract then destroy" applies not just to samples irradiated with free-electron lasers but also to the budding careers of some crystallographers, as universities restrict their recruitment and Big Pharma seems to be contracting into ever fewer companies. Two well-chosen sessions addressed this problem: a debate on "Are Crystallographers Still Necessary?", and a symposium on "Getting a job".

While the excitement of this year's Spring Meeting is fresh in our minds, we should take note of the dates for next year: Monday 30 March – Thursday 2 April. The venue will be the University of York, where I have happy memories of previous meetings. I anticipate that this environment will simultaneously stimulate the intellect and soothe the senses. The University campus features extensive tranquil watercourses with ducks happily quacking and daffodils lining the banks. The exhibition spaces and lecture theatres are close together; but for visitors who wander further afield, a lot of the walkways are covered to provide protection from the intense Yorkshire sunshine and the occasional April showers.

Our friends in the American Crystallographic Association have successfully launched their new journal "Structural Dynamics". An open access and online-only journal, it is now accepting short communications, topical reviews and regular papers. It will highlight research articles on structural determination and dynamics of systems, enabled by the emerging new instruments (e.g. XFELs, electron sources, etc.) and new experimental and theoretical methodologies. The first articles can be viewed at http://scitation.aip.org/content/aca/journal/sdy/browse .

I know that the idea of designating an International Year of Crystallography has been around for a few years, but not many crystallographers were aware of the bureaucracy involved in designating such a year. It seemed that 2012 would have been suitable, to celebrate the 100th anniversary of the discovery of X-ray diffraction by Laue, Friedrich and Knipping, or 2013, to celebrate the anniversary of the Braggs' first structure determinations. But why 2014? The comments by **Philip Ball** on the "Chemistry World opinions" website last October were typical: "If there was ever an ideal time for the **International Year of Crystallography**, you'd have thought it would be 2013. 100 years ago **William Bragg** and his son **Lawrence** first showed that the pattern of x-rays reflected from a crystal encodes the spatial coordinates of its constituent atoms. And 60 years ago the fruits of this discovery were used by **James Watson** and **Francis Crick** to deduce the molecular structure of DNA… But who know how these decisions work?" I think it is true that clearing the bureaucratic hurdles took longer than most of us expected, but it is my contention that 2014 is exactly right for the *International* Year because the academic year September 1913 to August 1914 was the first truly *international* year of crystallography. Whereas the significant progress in 1911-1912 was made in Germany, and most of it in 1912-1913 was in Britain, many nations contributed in 1913-1914. Sadly, much of the progress and the international respect and goodwill that accompanied it were snuffed out after the outbreak of war. Major contributions from important countries during this year have been concisely summarised via timelines on a poster that I presented at the recent BCA meeting. If you missed my poster, don't worry: it will be going up again at the IUCr Congress in Montreal this August, so just ask your grant provider for a travel grant. If that is too expensive, you still needn't worry. Unlike all the other posters I have ever presented, my contribution is in the presentation, not the content, which has been cribbed from two excellent sources. The book *Early Days of X-ray Crystallography* by **André Authier** with its careful descriptions of the science and its lively biographical details costs only £45, and the "we-were-there" accounts compiled by **Peter Paul Ewald** half a century ago are completely free at http://www.iucr.org/publ/50yearsofxraydiffraction/full-text . Illustrating the early pioneers' remarkable combination of blazing originality and dogged determination, both are well worth reading.

This topic leads me to a related matter. In compiling my poster, I found that in 1912-1915 many papers had similar titles, something like "Reflection of X-rays". To identify the unique points in a particular paper, it was necessary to read it in full. On-line, this was commendably easy in the cases of *Proceedings of the Royal Society*, *Proceedings of the Tokyo Mathematico – Physical Society*, and *Comptes Rendus de l'Académie des sciences*, which provide full text free of charge. Would that more publishers would do the same for such early papers, which are of immense historical significance but essentially zero commercial value!

I have derived a lot of amusement reading about examples of nominative determinism in the Feedback column of *New Scientist*. These concern studies where the author's name matches the subject, such as a paper about urinary incontinence by **A. J. Splatt** and **D. Weedon**, and a book about the polar regions by **D. Snowman**. Further on in this issue we have our very own example. **Mike Glazer** would like your help in identifying the pattern etched into a glass window in the Chemistry Department of University College London, where Kathleen Lonsdale had her office. Since someone went to the trouble of etching it, it must have had a great deal of significance.

Carl Schwalbe

BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
- 10% discount on exhibition stands at the annual BCA Spring meeting or a promotional poster at the annual BCA Spring Meeting.
- Free insert in the annual Spring Meeting delegate pack.
- Two free full registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly Crystallography News.
- Corporate Members will be listed in every Crystallography News and on the BCA website with clickable links to your organisation's website.

Corporate membership for 2014 is **£750.00**.

Corporate Members:

- Agilent
- Bruker
- CCDC
- Douglas Instruments Ltd
- ICDD
- Incoatec GmbH
- Molecular Dimensions
- Oxford Cryosystems
- PANalytical
- Rigaku

Benefits of Individual BCA Membership:

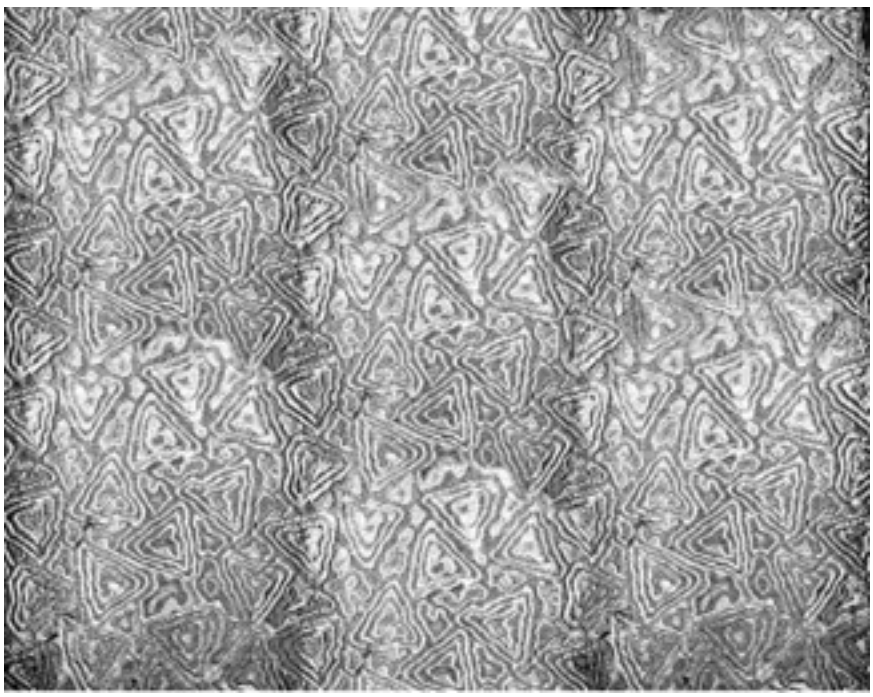
- The professional organisation for crystallographers in the UK
- A broad range of meetings organised by the BCA and its subject groups
- Preferential members' rates for such meetings
- Eligibility of students and postdocs for an Arnold Beevers Bursary award
- A copy of Crystallography News every quarter
- 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/**

Can you identify this?

THIS is a copy of a window at the Chemistry Department at University College London, where **Kathleen Lonsdale** had her office. Rumour has it that this represents a crystal structure, possibly a difference Fourier or something like that. We can see two possible unit cells.

If you have any ideas as to what this represents please contact **Mike Glazer** (glazer@physics.ox.ac.uk) or **Ian Wood** (ian.wood@ucl.ac.uk).



BCA Spring Meeting Reports

Named Lectures

BRAGG LECTURE

BRAGG Lecturers are normally chosen once every three years. The Bragg Lecturer has to be a doubly distinguished scientist, being selected by the Bragg Lecture Fund Committee but also expected to create a lecture that fits in with the theme of a BCA meeting. This year we were treated to a well-crafted and very relevant lecture by **Judith Howard**. Judith dedicated her lecture to the memory of her late colleague **Ken Wade** FRS (1933-2014). She reminded us how early the newly developed technique of X-ray crystallography was applied to biomolecules. Already in 1913 Nishikawa and Ono recorded diffraction from silk, and in 1926 Astbury obtained data from silk fibroin. Eighty years ago the first photograph from insulin was taken, 25 years later the structure was solved, and 50 years ago **Dorothy Hodgkin** received the Nobel Prize. Judith herself worked with Dorothy Hodgkin on neutron diffraction from insulin. As for the great innovations of the reciprocal lattice and the use of Fourier analysis, **P. P. Ewald** published his original diagrams in 1913; and **Kathleen Lonsdale** hand-calculated Fourier maps for hexamethylbenzene in 1928, confirming its planar and delocalised character. Judith herself worked on determining the charge density of benzene [*Chemistry – a European Journal*, 8, 3512-3521 (2002)]. Her group at Durham has never been afraid to design new apparatus when needed, e.g. to get temperatures down to 2K and to generate high pressure. A particular interest has been water in crystals. Often regarded as a nuisance by macromolecular crystallographers, it has been shown to form a significant amount of ordered structure in insulin and bacteriorhodopsin. As for the future, we can look forward to powerful new sources and wider impact of crystallography on cognate sciences.

Carl Schwalbe

LONSDALE LECTURE

THIS lecture provides the bridge between the Young Crystallographers' satellite meeting and the main meeting. This year **Henry Chapman** enlightened us about the super-hot (!) topic of X-ray free-electron lasers (XFEL). Their beams come in femtosecond pulses, can cut through steel and accomplish their diffraction before radiation damage annihilates the crystal. In a thrilling video Henry took us for a ride with the electrons through the Linac Coherent Light Source at SLAC. The only thing missing was those moving seats that you get at theme parks! Next, Henry corrected a misconception that I have long held: the main purpose in life of a crystal is to diffract radiation so that we can determine its structure.

Judith Howard

Henry Chapman and Elspeth Garman (Chair)

In fact, matter is essentially transparent to X-rays; hence we need a lot of X-rays (or a lot of matter). A typical synchrotron delivers 10^6 photons in ≈30 ps; for XFELs the numbers are 10^{12} photons in ≈30 fs. The tolerable dose for a cryocooled crystal on a synchrotron is ≈30 MGy. This amount of energy deposition would heat water by 6200K. It makes clear the advantage of outrunning radiation damage instead of trying to live with it. Henry showed how the formidable technical problems of delivering nanocrystals in a superfine jet, detecting their weak signals and merging the huge number of measurements have been solved. Since there is no need for cooling, there are no worries about the structural effects of cooling and addition of cryoprotectants. The occurrence of "diffraction before destruction" has been verified to better than 1.9 Å resolution. The method is well suited to time-resolved measurements, including irreversible reactions.

Carl Schwalbe

Plenary Lectures

BSG PLENARY

PETER Moody began the first session on Thursday by introducing **Neil Isaacs**, who presented an engaging talk entitled 'How Times Have Changed'. Neil took us on a fascinating journey starting in 1937 in the age without computer power. He described the beautiful experimental work of **Rosalind Franklin** and mentioned the major advance embodied in **Pehr Edman**'s method, which made it possible to sequence a protein at the speed of 1 residue per day and completely determine the sequence of lysozyme in 6 months. Neil showed us how advances in computing underpin much of modern structural biology with a look at the early days of refinement from developments in Fast Fourier Transform algorithms in 1965 with Cooley-Tukey through to structural genomics and the wwPDB.

Jonathan Chamberlain
University of Portsmouth

Neil Isaacs and Peter Moody (Chair)

CCG PLENARY

THE CCG Plenary Lecture was given by Prof **Paul Raithby** (University of Bath), who followed in the theme of the meeting by drawing on the developments of the field in the last century in order to consider what we might be able to achieve in the coming one. Paul illustrated the vast improvement in our crystallographic capabilities by referring to his own career: he started with precession photographs and a manual diffractometer, subsequently experiencing the introduction of automated diffractometers with point detectors, then area detectors, variable temperature and high pressure studies, and synchrotrons as radiation sources. Paul described the development of time-resolved crystallography to extend what had been a static technique. Pump-probe experiments can provide information on metastable states with lifetimes in the ns-ms range. The sample is hit with X-rays immediately after energy supplied by a laser boosts molecules into the metastable state. Conventionally, a chopper interrupts the beam from a synchrotron before too many molecules have left this state. Such waste of beam time and clock time is no longer necessary now that the Pilatus detector can gate and bin the data fast enough. The HATRX approach uses a Hadamard matrix to encode the probe sequence "on" or "off". Paul considered the potential of XFELs to study very complex systems on extremely fast timescales and speculated that crystallographers will be investigating considerably less ordered materials in the future.

Simon Coles and **Carl Schwalbe**
University of Southampton and Aston University/CCDC

Paul Raithby and Simon Coles (Chair)

IG PLENARY

FOR the title of his IG Plenary Lecture **Joel Bernstein** made a subtle but significant change to the title of the meeting: "Learning from the past and *trying* to look into the future" (italics mine). He cited three spectacularly wrong predictions by eminent people: (1) Our future discoveries must be looked for in the sixth place of decimals – A. A. Michelson, 1894. (2) X-rays will prove to be a hoax – Lord Kelvin, 1895. (3) I think there is a world market for maybe five computers – Thomas Watson, IBM president, 1943. Joel recounted anecdotes about three great pioneers of crystallography whom he knew personally: **P. P. Ewald**, **P. Debye** and **W. L. Bragg**. Bragg once poetically described a crystal as "a symphony of electrons". Joel reminded us of the importance of great scientific illustrators in the era before computer graphics. The drawings of proteins by **Irving Geis** and **Roger Hayward** were remarkably accurate, and even today their emphasis on the important features is instructive. While the first 100 years of crystallography were dominated by statics, the most spectacular progress in the future is likely to be in dynamics as we seek to understand the intermediates in chemical reactions, the nucleation of crystals, and the internal dynamics in jumping or exploding crystals.

Carl Schwalbe

Joel Bernstein and Cheryl Doherty (Chair)

PCG PLENARY

IVANA Evans introduced **Malcolm McMahon**, whose lecture had the exciting title of "Extreme Crystallography in a Flash". Malcolm gave three reasons to study materials under extreme conditions: to test theories of condensed matter, to discover new materials and to investigate forms of matter that may exist on exoplanets. Around 1990 the view was that such research would merely show that everything becomes metallic under high enough pressure. Now we know better! Putting an insulator under high pressure causes charge density to accumulate between ion cores; the bonding may become ionic in character. On the other hand, at high pressure sodium becomes transparent and an insulator. A pure sample of rubidium turns into a "host-guest" system with incommensurate "blue" and "red" chains that "melt" under different conditions. Potassium likewise shows host-guest behaviour, the host atoms having much smaller displacement parameters than the guests. Compared to europium under ambient conditions, high-pressure phases appear to have higher volume per Eu atom. This paradoxical result must be attributable to impurity atoms, most probably H atoms. It turns out to be harder to load clean Eu than clean alkali metals. The general conclusions concerning high pressure are that electrides are commonplace, as are incommensurate structures, and contaminants may get in. Future progress is likely to lead to ultrahigh pressures over ultrashort timescales. In the ensuing question-and-answer session the intriguing suggestion was made that the observed anisotropic transmission of seismic waves could be explained if the Earth's core were a single crystal!

Carl Schwalbe

Malcolm McMahon and Ivana Evans (Chair)

Early Career Researcher Prize Symposium

CCDC-CCG PRIZE

Lynne Thomas intrigued us with the title of her prize lecture, "Molecular Disorder and Materials Function – a Marriage made in Confusion". She reminded us that no crystal is perfect, and a diffraction experiment normally sees a time-average. Dynamic disorder involves correlated motions of atoms or molecules, while static disorder is frozen into the structure. Movement can be vital to function, and inefficiencies in packing can be useful. Complex crystallization conditions may lead to polymorphic forms with potentially favourable properties. Disorder and polymorphism can be encouraged by creating a mismatch of hydrogen bond donors and acceptors, introducing symmetric co-molecules and making hydrates or solvates. A systematic study of multi-component molecular materials exhibiting thermo-chromism based on combinations like 4-iodoaniline and 3,5-dinitrobenzoic acid has produced 31 complexes, 17 of which are ionic and colourless. The other 14 are coloured, and 11 of them show whole-molecule disorder!

Carl Schwalbe

Lynne Thomas

BSG PRIZE

SIMON Kolstoe presented the BSG prize lecture at the early career research prize symposium on Wednesday. He gave an excellent presentation about his work on the serum protein transthyretin and using structural biology in collaboration with the pharmaceutical industry to develop a drug to stabilize the protein tetramer and prevent its dissociation into amyloidogenic subunits. Transthyretin amyloidosis is a hereditary protein folding disease, where mutations in the transthyretin gene lead to an unstable protein. The largely β-sheet subunits dissociate and aggregate, leading to the formation of amyloid fibres that are deposited in the organs. Simon presented several nice structures illustrating the progression of the drug development, and explained the challenges of producing a molecule that can bind tightly to its target and also pass clinical trials! Several years of structural analysis and functional *in vivo* assays have yielded a molecule that out-performs other small molecules designed to stabilise the native tetramer. This compound is currently in clinical trials with the hope that it can be used to treat transthyretin amyloidosis.

Jonathan Chamberlain
University of Portsmouth

*L-R: Kate McHardy, **Simon Colstoe** and Vilmos Fulop (Chair)*

IoP-PCG-SCMP PRIZE

ROGER Johnson discussed polarity, chirality and axiality in multiferroics. He illustrated these important concepts with two examples: $MnSb_2O_6$ is chiral, polar magnetic and a possible multiferroic. $Cu_3Nb_2O_8$ is axial, chiral magnetic and multiferroic. There are two types of multiferroics. (1) When $T_{Fe} >> T_N$, the magnetic and polar order parameters are distinct and there is weak coupling. (2) When $T_{Fe} \approx T_N$, magnetic order induces electric polarisation and strong coupling. For us non-physicists in the audience Roger produced further examples. Polarity implies a clearly defined "up" and "down", e.g. a Duracell battery. Chiral objects cannot be mapped onto their mirror image, e.g. fusilli. The point symmetry of an axial object contains a unique rotation axis. Neutron powder diffraction measurements on the WISH instrument at ISIS have provided much useful information about structures containing Mn and Cu.

Carl Schwalbe

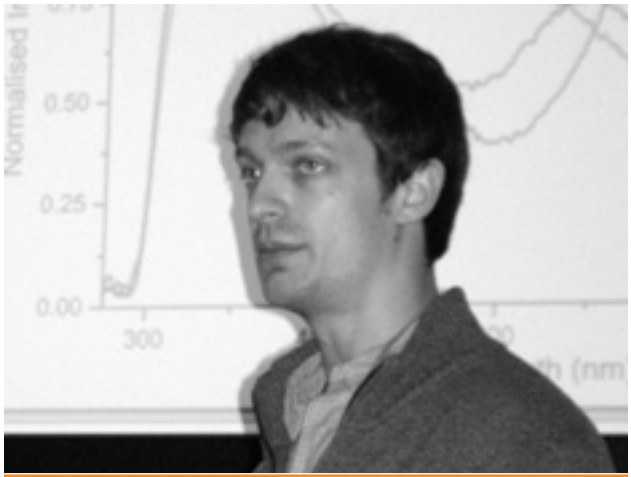
(photograph overleaf)

Roger Johnson

IG-YCG PRIZE

MATTHEW Bryant from Bath presented his results on tuning the optical properties of new organometallic systems. Pt(II) complexes with substituted tridentate 1,3-di(2-pyridyl)benzene (N^C^N) ligands show striking colour changes when simply exposed to moist air or a stream of dry gas. Water forms a hydrogen bonded network and facilitates overlap of Pt centres. Methanol also forms a hydrogen bonded network affecting Pt. Because the HOMO-LUMO gap is altered, the colours change from red to yellow to blue. Porosity in the red and blue forms allows easy ingress and escape of solvent. Matthew showed video images illustrating the dramatic effect of pressure on a material called MB57: writing "MB57" on it with a stylus left a clearly visible alteration in the luminescence.

Carl Schwalbe



Matthew Bryant

BCA Spring Meeting 2014

EXHIBITORS 1

The Young Crystallographers' Satellite Meeting

THE first session of the 2014 Young Crystallographers' Satellite Meeting kicked off with Iain Oswald, presenting the first plenary lecture on 'High Pressure Studies of Illicit Materials'. Iain described the difficulties of dealing with high-pressure data, collected in a diamond anvil cell, using mephedrone and cocaine as illustrative examples.

Matthew Bryant spoke next, showing the audience how he was able to tune the colour of some new organometallic materials, switching rapidly between red, yellow and blue complexes by adjusting orbital overlap through dehydration or exposure to methanol.

Continuing on the theme of crystallographic difficulties, **Sam Horrell** discussed some of the issues that macromolecular crystallographers encounter. One often-overlooked aspect is how to safely transfer your crystal from mother liquor to the diffractometer, for which Sam described the equipment available at the Diamond Light Source that controls environmental humidity in order to mitigate the problems.

Karim Sutton was up next, where he talked about bridging the gap between the small and big-molecule worlds. He applied the techniques used typically for very big molecules – MAD phasing – to 'quite big' molecules that give poor diffraction patterns, and was able to solve the structures for each case shown.

The first total scattering talk of the conference was given by **Serena Maugeri**, who made use of the diffuse components in X-ray and neutron diffraction patterns to investigate the local structures of iron filled nanotubes and calcium oxide/calcium carbonate nanoparticles.

Claire Hobday followed, talking about the effect of pressure on UiO-67, one of the most structurally robust metal-organic framework (MOF) materials. Claire showed that choice of hydrostatic medium in a diamond anvil cell really matters as smaller molecules can penetrate the framework on increasing pressure, sometimes resulting in a counter-intuitive expansion of the lattice.

The final speaker of the session was **William Bradshaw** who described one of nature's nastier organisms – the bacterium *Clostridium difficile* – and how his characterisation of a protein-cleaving enzyme, Cwp84, may be key to understanding its mode of infection, thus leading potentially to improved drug design.

ELSPETH Garman gave the second plenary lecture of the day, looking back at where crystallography has come from and the advances that have been made; how the field has progressed from a simple 2-atom structure to the recently-solved ribosome, consisting of 293,658 non-hydrogen atoms! Elspeth finished with a discussion of radiation damage in protein crystals and how the RADDOSE software can be used to calculate the extent of the damage.

Elliot Carrington talked about functionalised MOFs and their in-situ structures when exposed to carbon dioxide, using a gas cell to explore the sorption properties of these framework materials as a function of post-synthetic modification.

Colour-tuning made a reappearance, but this time on organic systems, as **Charlotte Jones** spoke about her research on using temperature to affect the thermochromic properties of some haloaniline/dinitrobenzoic acid co-crystals.

Anna Warren then gave a talk on the information, complementary to diffraction, which is provided by X-ray tomography and radiography. For many very small or opaque samples, it can be very difficult to spot the sample, which is important when considering factors like radiation damage. Anna showed how these samples can be located prior to a diffraction experiment using these techniques.

As the last speaker of the day, **Jeremiah Tidey** talked about a collection of high-pressure experiments on a family of palladium/platinum dithiacyclononanes. The different polymorphs investigated showed diverse compressibilities, having bulk moduli between 4 and 23 GPa.

THE second day of the YCG Satellite began with this year's Parkin lecture. This lecture is given by a young crystallographer who has made an outstanding contribution to crystallographic outreach. Claire Murray was the recipient of this year's award and gave the audience reasons as to why we should care about outreach. Aside from the contractual obligations to do so, the need to dispel media myths and the (hopefully) inherent love of crystallography, Claire's survey showed that there are some (rather worrying!) misconceptions about crystallography and that outreach is clearly more necessary than ever.

This was followed by **James Wright**'s talk on the structural transitions of a family of Ag-based coordination polymers. James showed how by means of in-situ and ex-situ powder diffraction it was possible to monitor the phase transitions driven by different external stimuli, including temperature and exposure to different solvent vapours. He subsequently detailed the structural consequences on the frameworks upon incorporation of different xylene isomers, showing the selective nature of these inclusions.

Simon Tanley then described the binding mode of the anti-cancer agent, cisplatin to a histidine group within lysozyme. The data showed that the cisplatin could be bound over several possible sites, leading to disordering of both the cisplatin and histidine.

Moving from protein disorder to hydrogen disorder, **Lucy Saunders** showed that in a pair of dinitrobenzoic acid polymorphs, thermally-induced disorder of hydrogen atom location occurred in one structure but not in the other. Lucy also warned of the dangers of not properly processing the raw diffraction images; this made the difference in identifying hydrogen positions accurately.

The last talk of the session was given by **Domenico Bellini** who described the first crystal structure of a HD-GYP phosphodiesterase from *Persephonella marina*. The structure revealed a novel trinuclear metal centre for hydrolysis of cyclic di-GMP, an important messenger involved in development, biofilm formation, motility and virulence.

TO end the YCG Satellite meeting, the first-ever debate was held, with the provocative subject, 'Are Crystallographers Still Necessary?' Arguing for the crystallographers was Simon Coles, with Graeme Winter taking the opposing view. Both made some interesting points; Graeme argued that (almost) no-one actually solves their structures anymore (thanks to George Sheldrick and others) and that it's usually better to let the computer make more of the decisions for you. Simon addressed the common criticism of 'stamp collecting', saying that a stamp collection can be a very valuable resource; indeed, a great deal of crystallographic analysis is possible because of the crystal structure collections hosted by the CCDC and the PDB. The point was raised by members of the audience that a difficulty arises in the differing definitions of 'crystallographer', with all sides agreeing that the work we do is valuable! The BCA meeting could continue…

Many thanks to all the speakers and meeting attendees who made this another great YCG Satellite meeting!

Nicholas Funnell
University of Oxford

Chairs' and Recipients' Reports

CRYSTAL ENGINEERING

THE crystal engineering session covered a diverse range of topics reflecting the interdisciplinary nature of the area. The session got off to an explosive start with **Colin Pulham** who described using the co-crystallisation technique to improve the physical properties of some widely utilised energetic materials such as thermal stability, decreased solubility, easier processability and reduced sensitivity. These have applications in many areas ranging from secondary explosives to propellants and gas generators. He discussed the crystal packing features which gave favourable properties such as the formation of hydrogen bonded layers reducing the sensitivity of molecules such as TATB and FOX-7. He even showed us some of the equipment they use for impact testing – pretty big kit! **Neil Champness** explored a range of architectures and discussed the methods for designing them. This included some photoactive MOFs and single molecule nanospheres which he imaged using TEM by placing them inside carbon nanotubes. He was also brave enough to demonstrate the use of non-diffraction techniques in imaging molecules and hydrogen bonds including weak C-H···O hydrogen bonds by placing molecules on surfaces and using a modification of AFM. **Kate Wittering** moved us from small scale crystallisations to attempts to scale up crystallisation processes into continuous crystallisation vessels towards continuous manufacturing. She discussed the polymorphic molecular complex of urea barbituric acid and how it is possible to select the polymorph by modification of the cooling crystallisation conditions. **Andrew Maloney** rounded up the session by again talking about some crystallisation, this time crystallising low-melting point primary amines *in situ* on a diffractometer. He investigated a series of compounds and discussed the balance between hydrogen bonding and dispersion forces in directing the crystal packing. He utilised the PIXEL method to rationalise this.

L-R: Colin Pulham (Edinburgh), Andrew Maloney (Edinburgh), Kate Wittering (Bath), Neil Champness (Nottingham), Lynne Thomas (Bath)

Lynne Thomas
University of Bath

NON-AMBIENT DIFFRACTION (I)

THE BCA spring meeting began with a series of excellent talks, both invited and contributed, on non-ambient diffraction. Steve Hull started off the session with a talk on *in-situ* neutron diffraction studies of battery and fuel cell materials, providing examples of analyses performed on both electrolytes for SOFCs and rechargeable batteries, and even entire fuel cells. This was followed by **Jorge Sotelo**, who talked about an in-situ gas adsorption X-ray diffraction study of single crystals of a Sc-based MOF. This study using high-pressure gas cells has allowed for the different gas adsorption sites in the frameworks to be determined. Gas sorption was also the theme of the third talk presented by **Inigo Vitorica**, this time focussing on a non-porous, crystalline silver coordination polymer. As in Jorge's talk, *in-situ* X-ray diffraction has allowed the adsorption properties to be studied, illustrating how adsorption can occur in spite of the presence of pore channels. Bringing the session to a close, **Bill David** gave a talk on *in-situ* diffraction of reversible hydrogen storage systems. These studies were performed using a combination of neutron and X-ray diffraction, and provided insight into the storage mechanisms for different types of systems, and their use in real world applications.

Overall, the high quality of these talks set a good standard for the rest of the meeting, shining light on a range of different tools available to scientists for non-ambient diffraction, and illustrating their potential to provide answers to some of the problems we currently face in the field.

M. L. Tate
Durham University

NON-AMBIENT DIFFRACTION (II)

THE second session on non-ambient diffraction began by two excellent talks highlighting the different effects high pressure has on organic and inorganic materials. Andrzej Katrusiak from the Adam Mickiewicz University in Poland gave a detailed lecture on the effects of high pressure on hydrogen bonding in organic compounds. He discussed the energetics of these, including unusual results on these lengthening under compression. This was followed by a talk from **Simon Parsons,** of the University of Edinburgh, presenting some insightful research into how great the changes in bonding in coordination complexes under pressure can be. Cases where either the coordination geometry or the coordination number change significantly with temperature were high-lighted, as was the effect of intermolecular interactions on their compressibility. The final talk in the session was given by **Nick Funnell**, from the University of Oxford, about the ferroelectric ordering of ice in an organic host with one dimensional channels, HHTP. This presented the first case of a host material in which the interactions of water molecules within a channel and between channels are balanced so that three dimensional ferroeletric order is achieved but at a temperature well below the melting point of water in the host.

Paul Saines
University of Oxford

APPLICATION OF NEUTRON DIFFRACTION IN CHEMICAL CRYSTALLOGRAPHY

IN this session the use of neutrons was explored for single crystal and powder samples across a variety of materials. **Amber Thompson** (University of Oxford) started the session with her talk entitled 'Just a spoonful of neutrons helps the chemistry move on…'. Amber highlighted the use of neutrons to locate missing hydrogen atoms in systems containing heavy and/or light elements with particular reference to disordered systems and unusual systems such as those containing dihydrogen bonding. **Dominic Fortes** (University College London) moved the session to mineral hydrates with his talk 'Analogue materials for high-pressure studies of planetary ices'. Dominic presented the elucidation of the crystal structure of a range of hydrates with unknown levels of hydration using X-rays, neutrons and a range of analogue materials in order to understand some high pressure phase hydrates found in the solar system. **Matt Cliffe** (University of Oxford) closed the session on a more disordered note with his talk entitled 'Frustration and disorder in simple molecular frameworks'. Matt presented his work on the phase transitions in analogues of AgCNO and the use of neutron total scattering experiments to study disorder and magnetism in AuCN and AgCN.

Dominic Fortes

Matt Cliffe

Sam Callear
ISIS, STFC

XRD IN THE PHARMACEUTICAL INDUSTRY (CCG & IG)

Co-chairs: **Peter A. Wood** *&* **Cheryl L. Doherty**

THIS session highlighted the importance of X-ray diffraction and crystal structures in the pharmaceutical industry with talks from a range of different perspectives. **Andy Dobson** (AstraZeneca) kicked off the session with a presentation of some case studies using XRD in the context of a major multi-national pharmaceutical company. Andy started by relating crystal forms and polymorphism to the packing of Lego bricks (N.B. other plastic brick-based construction toys are available!). This prompts the question – are there some bricks (or molecules) that are inherently difficult to pack and therefore prone to polymorphism, solvation or hydration? Andy showed how powder XRD, thermal gravimetric analysis (TGA) and gas vapour sorption (GVS) techniques can together be very powerful in understanding how tightly bound water molecules are in hydrate structures and at what conditions they may be lost from the structure. Some methods for obtaining crystals by sublimation were also mentioned (including the grandly named piece of equipment "Sublimus") as well as recently developed knowledge-based methods for assessing the risk of polymorphism.

Philippe Fernandes (Pharmorphix) next gave us some insight into the use of powder X-ray diffraction in particular within a Contract Research Organisation (CRO) environment. He demonstrated the use of XRD with a variety of complementary techniques to study variable channel hydrates of a pharmaceutical molecule. In particular the use of variable temperature and variable humidity experiments were used to study this complicated hydrate system. The complexity involved in understanding and fully characterising a series of closely related structures for this molecule, including indexing powder data and a discussion of the data quality needed, was also addressed.

Our final talk rounded the session off nicely with an academic research project focussed on issues in the pharmaceutical industry. **Mark Eddleston** (University of Cambridge) presented some fascinating insights into aspirin degradation mechanisms using a range of experimental techniques. Chemical stability is a crucial feature in pharmaceutical drug products and Mark demonstrated an intriguing link between the crystal structures of the parent drug and degradant with the observed chemical stability under accelerated conditions. In addition to XRD, Mark showed that AFM (Atomic force microscopy) and light microscopy are both valuable techniques in understanding the transformations that occur on aspirin crystal surfaces during degradation to salicylic acid. Mark also demonstrated that changes to the crystal structure, for instance by forming co-crystals of aspirin, impacts the chemical stability; hence offering the opportunity to tune the stability of a drug species.

L-R: Pete Wood (CCDC, CCG), Philippe Fernandes (Pharmorphix), Mark Eddlestone (University of Cambridge), Andy Dobson (Astra Zeneca), Cheryl Doherty (Pfizer and IG)

Peter A. Wood
CCDC

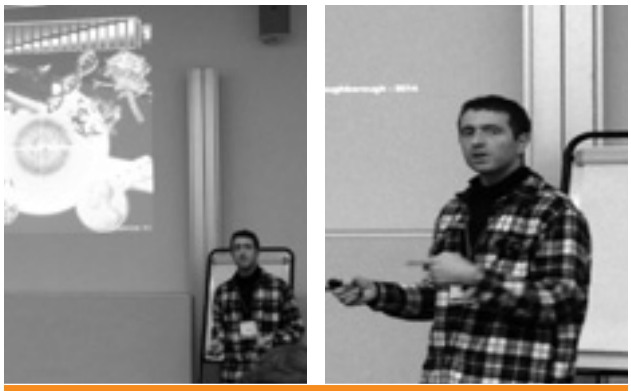
BSG SESSIONS

ALTHOUGH I attended the BCA – BSG Winter meeting in 2013, this was my first BCA Spring meeting. I was impressed by the turnout and slightly overwhelmed by the diverse subject areas covered by the delegates. Nonetheless I very much enjoyed the meeting, and the talks highlighted some exciting developments to expect in the future with the arrival of XFELs in Europe. We were also taken on a tour of the last 100 years of crystallography, an experience that I found particularly insightful being a newcomer to the field! Excellent talks came from those pushing the limits of macromolecular crystallography during which we were presented with many beautiful and complex structures.

The first talk of the *'Pushing the limits: Faster'* series was given by **Gebhard Schertler** who outlined the development of the SwissFEL project. The SwissFEL is currently under construction at the Paul Scherrer Institute at a cost of approximately CHF 280 million (~£190 million). Three experimental stations are being built to cater for various sample types. These will offer sample delivery jets, solid supports and capability to deal with three dimensional biological samples, allowing them to take advantage of the powerful light source, which will have a peak brilliance almost ten billion times that of a conventional third generation synchrotron! Gebhard discussed the need for femtosecond X-ray pulses in order to investigate ultra-fast processes such as bond reformation, giving the example of rhodopsin and G-protein coupled receptors. He also gave examples of data collected at the Linac Coherent Light Source (LCLS) using solid supports and obtaining diffraction data from two-dimensional crystals.

Gebhard Schertler

The second talk was from **Leonard Chavas** who discussed the European XFEL currently under construction in Hamburg. He highlighted the difficulty of producing large crystals needed for synchrotron macromolecular crystallography and the complications involved in using small crystals. He described the proposed setup of the XFEL and its capability of handling tiny crystals via sample delivery jets. A key selling point for the European XFEL will be its ability to deliver X-ray pulses at 20,000 Hz, almost 200 times faster than at the LCLS, providing much faster data collection. One part of his talk I found particularly interesting. Leonard mentioned the possibility of crystals grown *in vivo*, accompanied by an image of tiny crystals exploding from the gut of a young cockroach!



Leonard Chavas

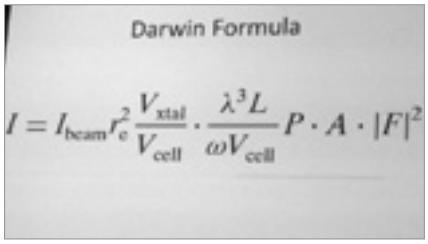
The final talk of the session came from **Petra Fromme** who showed us some exciting results collected using serial femtosecond nanocrystallography (SFX) at the LCLS on membrane proteins, specifically G-protein coupled receptors and photosystem I (one of the largest and most complex protein systems ever crystallised with 36 individual proteins and 381 cofactors!). It was amazing to hear how in spite of skepticism, the first SFX diffraction images were successfully collected in 2009 from photosystem I nano crystals. Petra showed us the beautifully complex structure that her group solved to a resolution of 3 Å, proving the principle of 'diffraction before destruction' using free electron lasers with femtosecond pulses. Other excellent structures that Petra displayed include the *Trypanosoma brucei* Cathepsin B (TbCatB) solved to a resolution of 1.9 Å using crystals grown *in vivo*.

Petra Fromme

Gwndaf Evans chaired the next session and **Colin Nave** was introduced as 'An expert who could do nearly as good a job as **James Holten** but cheaper'! Colin did an excellent job describing how we can capitalise on the information available from high coherent flux, high-density pixel detectors and small parallel X-ray beams. He revealed how shape-transforms can be used to help data interpretation and explained the principle of outrunning radiation damage through photoelectron escape which results in a lower effective radiation dose being deposited in very small crystals.

Gabriel Waksman

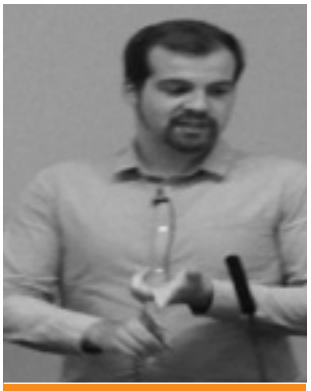
Gwyndaf Evans (Chair)



The second talk of the session was presented by **Robin Owen**, who discussed the current limits of the microfocus beamlines available at Diamond and what to expect in the future. He mentioned I24 which has a fully tunable, 8 x 8 µm beam as well as I04 which is using CRLs to achieve microfocus beams. Robin hit upon the problem of dealing with very small crystals, both mounting and locating crystals with the best diffraction. He provided data to reiterate the point that the best data is achieved when the beam size is matched to the crystal size in order to increase signal to noise (a nice illustration of the point described mathematically by Colin). His data showed diffraction collected from a 4 µm polyhedron crystal using both an 8 x 8 µm beam and a 5 x 5 µm beam. The smaller beam provided the structure with the best resolution (2.5 Å as opposed to 2.9 Å) due to a greater signal to noise. Robin concluded his talk with look to the future of the microfocus beamlines at Diamond noting that the beams will continue to get smaller with new advances such as 'dynamic apertures' allowing the beamsize to be optimized during data collection.

Robin Owen

Cornelius Gati presented the final talk of the session and described a method of implementing SFX at microfocus synchrotron beamlines. The example he used was TbCatB, a structure previously solved using SFX at the LCLS and described by Petra Fromme in the earlier session. Some of the most recent data collected at PETRA III used crystals, grown *in vivo*, measuring approximately 400-200 nm. The crystalline suspension was mounted using a standard cryogenic loop and contained approximately 5000 crystals. A series of helical line scans had to be used as it was impossible to target individual crystals. The final structure was solved to a resolution of 3 Å and was consistent with that obtained using data collected at the LCLS. With the insight into the future of synchrotron microfocus beamlines provided by Robin in the previous talk and the exciting new methods implementing SFX at microfocus beamlines displayed by Cornelius, I feel that synchrotrons still have much to offer us regardless of the forthcoming XFELs.



Cornelius Gati

Gabriel Waksman gave the first presentation of the 'Pushing the limits: Larger' session on Thursday morning. He described the process of pilus biogenesis in uropathogenic *E. coli*, a process that is absolutely required for their pathogenicity. Gabriel explained how his group has used X-ray crystallography to unravel the process of pilus assembly and secretion at the large usher complex on the outer membrane of these gram-negative bacteria. Co-crystallisation of the pilus subunit-chaperone complex as well as the usher complex has revealed how donor strand complementation and exchange mediates pilus elongation. With the aid of animations and some excellent high-resolution structures, Gabriel gave a good explanation of how structural biology as been used to elucidate this complex mechanism.

Gabriel Waksman

John Schwabe (Chair)

Russell Wallis next gave an excellent presentation about the structure of C1 protein and its role in the initiation of the classical complement pathway. This was yet another great example of X-ray crystallography being used to unravel complex protein mechanisms, in this case shedding light on the early stages of complement activation. Russell presented several images showing the hexameric, collagenous C1q homo-oligomer and the C1r and C1s proteases that are encased within the bouquet like structure. He described how by studying the very similar protein MBL, which is part of the analogous lectin pathway of complement activation, the binding site of C1s on the collagenous C1q domain was discovered.

Russell Wallis

Finally **Leonid Sazanov** presented his work determining the structure and mechanism of respiratory complex I, the first and largest enzyme of the respiratory chain. This huge L-shaped protein consists of 44 subunits with extensive membrane and hydrophilic domains. Leo explained how his group managed to crystallise subunits of the complex from both *E. coli* and *T. thermophilus* gradually managing to build up a picture of the entire complex. He described the challenges they encountered, years of optimising crystallisation conditions to lower anisotropy and provide higher resolution structures. Leo also presented the entire *T. thermophilus* complex I structure that his group has recently solved; it is the largest asymmetric membrane protein structure solved to date. The work that Leo presented has provided a structural basis for understanding the mechanism of electron transfer and proton translocation by Complex I.

Leonid Sazanov

The final session (below) on *'Pushing the limits: Slower'* is the subject of a separate summary by the Chair, John Helliwell.

PUSHING THE LIMITS: SLOWER – THE X-RAY LIMITS

The paradigm of "structure is needed to define function in biology" leads to a thirst via appropriate techniques to achieve this, irrespective of sample state. Thus, crystal structure analysis by X-rays works well in furthering this paradigm but hits limits. It is not effective in many cases, becoming slow or obviously impossible to give the desired structural details. Neutrons are exquisite probes of proton ionisation states of amino acids and so neutron macromolecular crystallography can provide these. Cryo EM and single particle imaging can free up the need for crystals as well as deal with mixtures i.e. non homogeneous populations, whereas a crystal contains a relatively much more homogeneous population (ie apart from static disorder 'local' effects'). Atom and molecular dynamics also can underpin function. Solid-state NMR finds application in defining ligand dynamics in membrane targets. This session brought together experts spanning these techniques and their applications.

Matthew Blakeley from the Institut Laue-Langevin in Grenoble described:-
Neutron macromolecular crystallography: current developments and highlight applications.

The traditional problem for this technique has been of low neutron fluxes, which led to needing very big crystals (eg the 25mm^3 myoglobin crystal used in the pioneering study of **Benno Schoenborn** in 1969 at Brookhaven USA using a monochromatic thermal neutron beam into a single counter 4-circle diffractometer). Since then, the technique has made major strides using quasi Laue diffraction at reactor-based sources or time-of-flight Laue diffraction for spallation sources, such as the now approved nMX instrument at ESS and operational new instruments at SNS USA and J-PARC Japan. Matthew highlighted the sustained efforts these last 15 years at Grenoble with new image plate detectors, new instrument locations nearer to the reactor and a deuteration microbiology facility. Most recently the quasi-Laue diffractometer LADI-III has a new beam guide, a N_2 cryostream and a wider choice of wavelengths, allowing crystals as small as 0.05mm^3 and opening the doors to many new projects categories such as cryo-trapping enzyme intermediates. Data collection time for Benno Schoenborn's project would no longer be a year but a fraction of a day. Much larger molecular weights are accessible too. The open discussion included our guest from Arizona, **Petra Fromme**, who posed the challenge for nMX and the future neutron facilities of the Photosystem-II with its near 300 Å unit cell. Overall then the field of nMX is making good headway in technically challenging areas.

Alan Roseman from the University of Manchester described:- *What to do with non-homogeneous molecular populations: complementing crystallography with EM.*

By conveying ideas of mixed populations of zebras and wildebeest Alan vividly introduced us to an immediate advantage of single particle EM in biology, that of dealing with inhomogeneous populations which would likely defeat crystallisation. He summarised the field including breakthrough 'back thinned' direct electronic detectors which have recently led to much better resolution of electron potential maps with clearly seen amino acid side chains. Alan highlighted new techniques from his work for digitally isolating subcomplexes from within heterogeneous specimens, using local correlation functions. He illustrated the clear benefit of this with projects being studied in his Lab.

Finally **Anthony Watts** from the University of Oxford and also Rutherford Appleton Laboratory described:- *Functionally relevant dynamics of bound ligands at their target sites in membrane proteins*.

In the context of membrane bound GPCRs being such important drug targets for the pharmaceutical industry Tony highlighted through various examples the power of solid state NMR. As well as not needing crystals the use of conditions close or identical to in vivo was stressed; the context here being that crystallisation necessarily may well require conditions for crystallisation away from in vivo either through pH or a complex mix of additives. The sensitivity of NMR to protein dynamics through linewidth analyses was very powerfully illustrated. In the discussion we had chance to quiz Tony about the instrumentation approaches adopted in Europe (distributed facilities in general) and that in Japan at the NMR park in Yokohama (comprising 40 high field NMR machines built initially for their 'Protein 3000' structural genomics project).

L-R: John Helliwell, Alan Roseman, Matthew Blakeley and Tony Watts

There were very good discussion periods after each talk involving the audience, and which comprised members of the BSG, CCG and PCG thereby making it an excellent across-the-science-disciplines microsymposium.

John Helliwell
University of Manchester

Overall I found the conference extremely enjoyable. The diverse range of talks has shown that even after a century, crystallography continues to progress and push the boundaries even further. The introduction of much more powerful radiation sources and microfocus beams are making the need for large, difficult to produce crystals redundant and allowing the examination of much larger protein complexes. The speed at which these new sources will be able to deliver X-ray pulses will also give a much clearer picture of the dynamics of protein interactions, which is of particular importance for the development of novel drugs. I would absolutely recommend the conference to any other PhD students working in macromolecular crystallography and I am looking forward to the next meeting!

Report written by
Jonathan Chamberlain, University of Portsmouth).

Photography by
John McGeehan (BSG Secretary).

GETTING A JOB (IG & YCG)

THIS session was a joint session organised by the IG and YCG. It was aimed at younger researchers to give insights into what career options might be open to them.

It kicked off with a short presentation from **Marc Payne** (BP) who began by talking about his career paths after his PhD. He spoke of the opportunities available at BP and the recruitment process that possible employees would have to go through to get the job, with a lot of hints and tips for what can be done at each stage through this recruitment.

After Marc, **Simon Coles** (Southampton) gave a presentation, with a similar introduction talking about the career paths he had taken up to where he is now. Simon spoke more broadly about the opportunities that may be open to you as an academic, with useful information on different paths that may be taken for funding.

L-R: Cheryl Doherty, Simon Coles, Marc Payne and Anna Warren

The main highlight of this session was the audience participation. The session was designed so researchers could interact and ask questions relevant to them, gaining insights into the different types of career paths open to them. Many useful points were raised, with both Marc and Simon answering these questions from two different perspectives.

There was a big emphasis on creating an excellent online profile for yourself through websites such as LinkedIn and ResearchGate, with many members of the audience agreeing that they would definitely look at these profiles when short listing perspective employees for interview.

The wide range and number of questions that were asked during this discussion emphasised the usefulness of this session for younger researchers.

Anna Warren and **Cheryl Doherty**
Diamond Light Source and Pfizer

MAGNETIC STRUCTURE (PCG)

THIS year one of the PCG group sessions was given over to a very successful and informative microsymposium on magnetic structure determination chaired by Emma McCabe.

There is little consensus over the best way to describe the symmetry of a magnetic structure. **Andrew Wills** started the session trying to unite the two main approaches for classifying magnetic structure in the solid state, that of irreducible representation and that of magnetic space groups. He highlighted the complementarity between the two approaches and called for a unification of these "dysfunctional family members".

This was followed by two talks on systems exhibiting novel magnetic behaviour. **Alex Gibbs** presented work on the hexagonal perovskites Ba_2MTeO_6 (M = Ni, Cu, Zn) which have both rich magnetic and structural phase diagrams. **Paul Saines** presented his results on unusual dipolar mediated long range magnetic ordering in metal organic framework materials.

Paolo Radaelli bought the session to a close with a look at how practically complex magnetic structures might be used to store and retrieve information with particular emphasis on the magnetoelectric effect. He highlighted the need not just to determine a magnetic structure but also to understand the polarity of that magnetic structure with respect to the polarity of a given structural domain.

Mark Senn (Diamond)

Bursary Reports

FROM start to finish the 2014 BCA Spring meeting was a great experience. My first opportunity to attend a BCA meeting gave me great insight into the variety and depth of research that occurs in the British crystallographic community. Not only did I find very relevant presentations that directly relate to my PhD project, but many refreshing talks that introduced other aspects of crystallography of which I was less aware. This highlighted the many applications of crystallography and how it helps shape the understanding of many different scientific problems.

The meeting started with a very dynamic and interesting YCG session, where the chemical plenary speaker, **Iain Oswald**, kick-started with the challenges experienced when dealing with high-pressure diffraction data and how to overcome these issues, for example by using direct space methods for structure solution of the new phases of some of the illicit materials he currently investigates. This was followed by many great presentations by other young crystallographers, such as that of **Karim Sutton** on the application of MAD phasing for structure determination of small molecules, **Elliot J. Carrington**, who talked about *in-situ* gas adsorption diffraction experiments on Metal-Organic Frameworks or **Lucy Saunders**' work on imaging proton-disorder systems. To finish off the YCG session, a debate on whether crystallographers are still necessary led by **Simon Coles** and **Graeme Winter**, raised some interesting questions about how crystallographers should evolve as a community alongside new technological developments.

It was curious to see how this debate related nicely to the different plenary lectures, which covered how crystallography has evolved in the last 100 years, and how it will progress into the future. It was nice to see how times have changed and how, thanks to the efforts of many great crystallographers, we have got to the place we are now, where it is possible to elucidate a crystal structure in a matter of hours or even minutes. However, it was made clear that embracing the advantages of faster computing capacities and more powerful and novel methods of performing diffraction experiments, should not stop us keeping a critical awareness of some of the issues that come with the increasing automation of the field.

What this BCA meeting transmitted to me is the wide range of research that can now be undertaken precisely thanks to these engineering advancements. As is the case for the different *in situ* environments in which diffraction experiments can now be performed or the possibility to understand dynamic mechanisms using crystallography thanks to faster data collection capabilities. It is also worth highlighting too some of the remarkable advancements that were covered in the last session on complementary non-diffraction techniques. For example, the presentations of **Martin Dove** and **Jerome Wicker**, covering the use of RMC to elucidate short-range order and machine-learning algorithms to predict crystallisation propensity, respectively, can help us understand beyond our diffraction experiments and explain even more scientific phenomena.

I would like to take this opportunity to thank the BCA and ABBF fund for the financial support to attend this meeting, and hope many other young researchers can enjoy the benefits of these bursaries in the years to come.

Jorge Sotelo
University of Edinburgh

BEFORE the 2014 BCA spring meeting kicked off at the University of Loughborough, the Young Crystallographers group (YCG) put on another excellent satellite meeting with a variety of topics covered. Claire Murray gave the Parkin lecture on crystallography outreach and why it is important that our scientific community actively partake in this. The reasons for outreach were particularly eye-opening, especially given the fact that a lot of the public and even other scientists gave crystal healing and glass as answers when asked what is the first thing that comes to mind when you hear the word crystal. The work the BCA and YCG are doing for outreach were mentioned a number of times during the meeting and it is crucial to get crystallography out there to grow our community further. The satellite meeting came to an end with a provocative and thought provoking discussion on 'Are Crystallographers still necessary?' Simon Coles and Graeme Winter gave their arguments for and against the topic. I was on the side that crystallographers were still necessary and so were the rest of the audience, with the main discussion point being, what is the definition of a crystallographer? Something for us all to ponder.

The topic of the BCA spring meeting was 'Looking to the future, Crystallography at 100, learning from the past' due to this year being the international Year of Crystallography and 101 years since W L Bragg solved the structure of sodium chloride and came up with Bragg's law. All of the plenary speakers used this opportunity to look at the roots of how crystallography started and how it is has changed quite considerably due to the advances in computing and technology. As a relatively young crystallographer it was really important for me to learn the history of our science and who the major pioneers were. Not just looking at the past, this meeting was also a chance to look to the future and to describe the major advances which are still to come; and especially for macromolecular crystallography the most important one will be the XFEL's. The creation of these will lead to faster data collection times on nano crystals and more structural dynamic results will be possible as the photon power can lead to pulses in the femtosecond time window. It became clear to me as a protein crystallographer that neutron protein crystallography is also important to study proteins in a complementary way, as well as the techniques of EM and NMR being very important in particular categories such as non-crystallisable proteins, complexes and for the study of dynamics.

A very useful addition to the scientific programme was the session on 'Getting a job' as I am in that position where I have completed my PhD and looking towards the next step in my scientific career. The session gave great advice from the academic sector and from a large multi-national company, BP. The key advice was to sell yourself as much as possible and to use conferences such as the BCA spring meeting to show off your skills and talk to supervisors so you become memorable, for all the right reasons. I hope I did that.

Overall, the range of speakers and topics covered in this meeting made it an enjoyable and worthwhile learning experience. This coupled with the opportunity to network with fellow students and supervisors makes the BCA spring meeting a must for all students.

Simon Tanley
University of Manchester

CRYSTALLOGRAPHY meetings are like Christmas gatherings; eagerly awaited, many familiar and friendly faces and lots of delicious food: the BCA Spring Meeting in Loughborough was no exception. The week started with the Young Crystallographers Satellite Meeting where many enthusiastic crystallographers get the chance to present their work and is always something that catches my attention. The day consisted of ten short talks and two plenary lectures. An excellent plenary lecture by Iain Oswald entitled 'High pressure studies of illicit materials' got the meeting underway and set the tone for a plethora of exciting talks to come. Secondly, a captivating presentation by Matthew Bryant from the University of Bath described his work on the solvent induced structural rearrangement in novel organometallic complexes with great videos to illustrate the structural changes. Consequently he was a worthy winner of the YCG Prize.

A buffet dinner and poster presentation followed the first day; the conversation and drink were flowing and it was a great way to refuel and re-energise ready for the next three days. A 9 am lecture can be something that people dread but the first talk on the second day of the Satellite Meeting was enjoyed throughout the room. The enthusiasm and passion from **Claire Murray** about Crystallography Outreach was welcomed and it was a great interactive talk about how crystallography is perceived by the general public. Personally I was surprised about how many members of the general public think crystals are large shiny objects. It clearly shows that outreach is important and it is vital that we spread our knowledge to all generations.

After two days of the Satellite Meeting, the main event began with many of the sessions being well attended. The section 'Non-ambient Diffraction' was an area of particular interest to me as it is closely related to my work. I particularly enjoyed **Simon Parsons**' presentation describing his work on structure-property relationships of transition metal complexes. This provided a great insight into how we can use other techniques e.g. UV-visible spectroscopy to complement high pressure crystallographic studies.

Another area which caught my attention was related to the use of XRD in the pharmaceutical industry. Unlike many of the other talks, these talks saw industrial researchers describe how a combination of XRD and other analytical techniques can be used to solve industrial problems. **Andrew Dobson** from AstraZeneca explained how XRD along with TGA (Thermal Gravimetric Analysis) and DVS (Dynamic Vapour Sorption) can be used as analytical tools for understanding the properties of different forms of pharmaceutical solids.

There could not really be a BCA Spring Meeting in 2014, the International Year of Crystallography, without presentations on how crystallography originated and developed. **Elspeth Garman** (in the Satellite meeting), **Paul Raithby**, **Judith Howard**, **Joel Bernstein** and **Neil Isaacs** (in the main meeting) gave informative presentations on crystallography: past, present and future.

As is traditional, the meeting ended with a conference dinner with an elegant three course meal followed by a Ceilidh dance which always provides great entertainment and was a fantastic way to end the 2014 BCA Spring Meeting.

Alice O'Connor
University of Nottingham

BCA Spring Meeting 2014
EXHIBITORS 2

IT was hard to believe that it had been two years since the last BCA Spring Meeting, but I guess time flies when you're busy solving crystal structures. This year the meeting was held at Loughborough University; up until now conferences had only taken me as far as Warwick so I was looking forward to being able to tick another place off my 'visited' list.

In keeping with tradition, the meeting kicked off with the Young Crystallographers' Group Satellite, which gives early career crystallographers the chance to present their research in a relaxed environment. It was also my turn to face the daunting prospect of delivering my first ever conference talk, but thankfully crystallographers are a friendly bunch! The talks covered a diverse range of topics and everyone did an excellent job. Those presenting posters also got the chance to sell their research, by means of a flash presentation, but with the added pressure of the Countdown clock. The Satellite meeting included two plenary lectures, the first by **Iain Oswald** on 'High Pressure Studies of Illicit Materials' and the second by **Elspeth Garman** entitled 'Crystallography@100: Whither Goest Thou?'. This year the Parkin Lecture was given by **Claire Murray** ('Crystallography Outreach. Why?'), and I think she inspired us all to get out there and make sure the world knows what crystallography is all about! A particular highlight of the Satellite was the concluding session, where **Simon Coles** and **Graeme Winter** battled it out to answer that burning question: Are Crystallographers Still Necessary? Very brave, I think, in a lecture theatre full of crystallographers! No prizes for guessing how the majority voted, but I think the debate did prove that the answer to the question is very much dependent on our interpretation of the term 'crystallographer'.

This year's main meeting encompassed the past, the present and the future of crystallography – rather a lot to cover in just a few days, but it was achieved with great success. Each of the plenary lectures focused mainly on the last 100 years but also provided some insight into where the field may be heading. There was surprisingly little overlap between each of the lectures, and it was great to hear about so much history as well as some more personal accounts and thoughts. The sessions of the main meeting focused on the latest developments and also on our move away from using crystallography purely to determine structures. I attended the two sessions on Complementary Non-Diffraction Techniques, which really demonstrated how we can use additional techniques alongside diffraction in order to see the 'bigger picture'. As my own research lies in the area of multi-component crystallisation, the session on Crystal Engineering was of particular interest. **Colin Pulham** began with an explosive talk (sorry…) on co-crystallisation as a means of tailoring the properties of energetic materials, and discussed how some of the structural features of the co-crystals are favoured for various key properties. He concluded his talk with a slide designed to embarrass the session chair, **Lynne Thomas** – much to her dismay (and our amusement) – and with this Lynne moved us swiftly on to the next speaker. **Neil Champness** gave us a fantastic talk covering several different areas of his research, including the construction of nanoscale spheres and the organisation of molecules on surfaces, all using crystal engineering principles. Next, **Kate Wittering** introduced us to the polymorphic multi-component system of urea and barbituric acid and discussed the transfer of the system into the continuous flow environment, and the session was concluded by **Andrew Maloney** with a talk on the competition between hydrogen bonding and dispersion interactions. When you are focused on your own research it is often easy to forget how interdisciplinary 'crystal engineering' is, but this session really highlighted this.

Of course, it is never 'all work and no play', and Wednesday evening brought us a lovely three-course conference dinner which was followed by the presentation of prizes to the well-deserving winners. We then waited in anticipation for our evening's entertainment to begin; during my, albeit short, time in crystallography, I am yet to attend a crystallographic meeting without a ceilidh, and thankfully on this occasion we were not disappointed!

It is great to be starting out in crystallography during a particularly exciting time in the field, especially during this designated International Year of Crystallography, where we have the perfect opportunity to look back on and learn about all the advances during the last century. One particular quote from the meeting has stuck in my mind: "It's tough to make predictions, especially about the future" – only time will tell, but I am sure the future of crystallography will be just as exciting as the past!

Chick Wilson's Research Group (University of Bath) – a rare photo of the whole group, taken at the conference dinner

Charlotte Jones
University of Bath

THIS year's BCA spring meeting was held in the sprawling and sporty campus of Loughborough University from the 7th-11th April. The meeting was my first conference and a chance to meet many distinguished crystallographers and listen to talks on cutting edge research in many different crystallographic fields and the use of complementary techniques to diffraction.

Before the main meeting, the Young Crystallographers Group satellite meeting was held. This included many young and enthusiastic researchers and very engaging plenary speakers including **Iain Oswald** (University of Strathclyde) who discussed the difficulties of handling high pressure crystallographic data and how to obtain high quality refinements using both single crystal and powder x-ray diffraction.

When the main meeting kicked off, I thoroughly enjoyed the crystal engineering session chaired by **Lynne Thomas**.

Colin Pulham (University of Edinburgh) gave a fascinating talk on the cocrystallisation of energetic materials, which was filled with many interesting pictures and short films. He showed us how he could tune their explosive nature – using crystal engineering, a trick already used frequently by the pharmaceutical sector to help increase stability/solubility of drugs. By co-crystallising the explosives with other small molecules, they can stabilise the energetic materials and thus be transported more easily. Following Prof Pulham's talk was the coordination polymer chemist **Neil Champness** (University of Nottingham). His talk entitled "From Frameworks to Spheres – Exploiting the Coordination Bond" explored MOF chemistry in recent years, focusing on photoactivity and magnetism. He began by highlighting the many possible architectures that are possible with such simple building blocks and how crystal engineering can create structurally beautiful and useful systems. He showed us a Re/Cu containing coordination polymer which can undergo an irreversible photoinduced charge transfer process due to the photoactive Re and redox active Cu^{2+}, underlining how the coordination chemistry can be used to design innovative photoactive materials.

Two PhD students also spoke about their research in this session. **Kate Wittering** (University of Bath) spoke about her work involved with the Centre for Continuous Manufacturing and Crystallisation with her talk entitled "Continuous-flow Crystallisation of Multi-component Systems of Pyrazine Carboxamide: A World Health Organisation Essential Medicinal Compound for Tuberculosis Treatment". She explained why it would be useful to have a continuous flow crystallisation system as opposed to a batch crystallisation and how she has optimised the crystallisation of pyrazine carboxamide using a continuous oscillatory baffled crystalliser. The final speaker was **Andrew Maloney** (University of Edinburgh), whose talk, entitled "Competition between Hydrogen Bonding and Dispersion Interactions in the Crystal Structures of the Primary Amines", explained the importance of intramolecular interactions in the crystal packing of primary amines. He spoke about the phenomenon of melting point alternation between odd and even alkane chains and how he could relate this to differences in hydrogen bonding and chain packing firstly using a purely geometrical approach with CrystalExplorer. To validate this geometrical approach, he followed this up with by calculating the energetics of these interactions using the PIXEL method.

The conference was a very social affair, with plenty of time to talk to other delegates and integrate into the crystallographic community. In particular the YCG and main meeting poster sessions were a great opportunity to meet people, discuss research and explore areas of research with which I am not very familiar. Of course, the conference dinner was the biggest social occasion held on the final evening of the meeting, where food, wine and dancing were enjoyed with great company!

I would like to thank the BCA for financial assistance to attend this conference; I really do feel it has helped develop my postgraduate research experience.

Claire Hobday
University of Edinburgh

THE BCA conference 2014 provided a good chance to mingle with others in the field and possibly to learn something new and apply it to our own research interests. The first part was the Young Crystallographers' satellite meeting, initiated by an interesting Plenary by Ian Oswald on high pressure crystallography, and how to overcome some of the inherent issues therein. It was followed by talks given by students on the results they have obtained through their own research.

The talk "Big Methods for small molecules" by **Karim Sutton**, from the University of Oxford was particularly interesting. It featured the use on small molecules of an approach (MAD) more regularly used for solving protein structures. The proof of concept for the technique was a multiple wavelength study on a well diffracting sample containing a bromide ion. The differences in anomalous scattering between the wavelengths were then used to solve the phase problem. It will be good to see how well the technique progresses as it is used for other more complex structures.

One of the themes of the talks this year seemed to be high pressure crystallography and/ or metal-organic frameworks (MOFs), and this topic was nicely broached by **Claire Hobday** from the University of Edinburgh, in a talk in which she described the use of penetrating compression media for increasing the mechanical stability of MOF structures under high pressure.

The YCG Biological Plenary given by **Elspeth Garman** was an eye-opening look into the fragility of crystals and the potentially destructive nature of crystallography, shown with an amusing cartoon for a bacterium being zapped with an x-ray gun and losing an eye. The talk also introduced a means of predicting dose levels for crystals (RADDOSE) which would prove useful for improving data quality in unstable crystals.

After the YCG poster session and a much needed sleep, the YCG continued on Tuesday morning with the Parkin lecture, this year a call to arms for crystallography outreach and public engagement given by **Claire Murray**. The talk included data from public surveys about what people thought crystallography was (largely either crystal healing or to do with drugs) and concluded with the message that we need to be more involved with putting our interests into public view. I would tend to agree with this and also some of the comments made in the discussion that followed, that it is surprising how few people really understand what crystallography is, when some physical sciences such as theoretical physics are so prevalent in the public consciousness.

The YCG concluded with a light hearted debate between **Simon Coles** and **Graeme Winter** on the subject "are crystallographers still necessary?". Graeme took the stance that crystallographers are not really necessary any more due to the increasing capabilities of the refinement programs for solving structures and (in the future) writing full reports for you; and so really the only true crystallographers these days are people like **George Sheldrick** who write the programs we all use. Simon Coles' rebuttal was that the blindly clicking approach only works up to a point; but when confronted with unusual data, it is up to crystallographers to make sense of it and through knowledge and understanding of the science, produce a structure that could not have been found by a trained monkey. The debate was followed by questions that turned into audience participation, largely due to the

evocative subject matter. The interesting point was raised that many of us do not consider ourselves simply crystallographers any more, but more commonly either chemists, biologists, physicists or materials scientists (apologies if I have missed anyone out). I can't say that this feeling really applies to me, but I can understand how, as a feature of its incredibly diverse usefulness, the field has spread into so many areas of science that it would be naive to assume all people that use the technique are crystallographers.

On Tuesday, the BCA conference opened with the Lonsdale lecture given by **Henry Chapman** on the use of free electron lasers for the determination of macromolecular structures using datasets collected in the short time before the intense beam causes the crystal to explode. The "diffraction before destruction" in combination with a continuous flow liquid delivery system means that previously unobtainable structures are now within the realms of possibility. I am looking forward to hearing more in future about the capabilities of XFELs as they continue to change the way it is possible to do crystallography.

In the dynamic processes and reactions session, **Mark Warren** introduced the new Pilatus detectors on beamline I19 at the Diamond Light Source and their incredibly fast collection times. By using gating instead of a mechanical chopper, dynamic changes in photo-activated crystals can be captured in time-resolved single crystal experiments.

Giles Flowitt-Hill
University of Edinburgh

(redacted by the Editor from the original text).

THIS year's annual meeting of the German Mineralogical Society (DMG) will be held for the first time at the University of Jena, Germany. We cordially invite you to join this event from 21-24 September 2014.

Organized under the motto "Minerals at Focal Point" the conference aims at bringing together researchers from all fields of our multifaceted discipline mineralogy. The meeting program advertises thus a wide range of topics in or at the crossroads of the fields crystallography, **applied mineralogy**, **petrology**, and **geo-/cosmochemistry**.

The organization of the 2014 DMG meeting coincides with the 100th anniversary of the journal "Chemie der Erde/Geochemistry", which was originally founded in Jena. On the occasion of this event a special volume is under preparation that will be handed out to the attendees of the conference. The meeting offers also a half-day excursion to the close-by former Uranium mining district at Ronneburg.

We are looking forward to your attendance and contributions and welcome you in the city of light.

With kind regards,
On behalf of the organizing committee.

Invited speakers

Prof. Dr. G. Diego Gatta
Universita' degli Studi di Milano (Milano/IT)

Prof. Dr. Mihály Pósfai
University of Pannonia Veszprém (Veszprém/HU)

Dr. Hella Wittmann-Oelze
Helmholtz-Zentrum-Potsdam (Potsdam/DE)

Prof. Dr. Klaus Keil
University of Hawaii (Honululu, HI/US)

MAIN SPONSOR
NETZSCH

Prize Winners

THE four winners of Early Career Prize Lectures have been mentioned earlier, along with summaries of their lectures. More tangible (and often liquid rather than crystalline) prizes were given out after the Conference Dinner. Thank-you messages were conveyed to Lee Brammer for putting together such an interesting and well-balanced programme, to the various people who helped him, and to HG3 and the Loughborough University staff for making the meeting run so smoothly. Prizes were awarded as follows:

CCG Prize, poster CCG16 **Scott McKellar**

CrystEngComm Prize, poster CCG31 **Rajni Miglani Bhardwaj**

IUCr Prize, poster CCG17 **Lucy Saunders**

Honourable mention, poster CCG20 **James A Arnold**

Honourable mention, poster BSG9 **Anna M Davies**

RSC Solid State prize **Matthew Tate**

SCMP-PCG Prize **Mark Senn**

PANalytical Thesis Prize **Alexander Hearmon**

YCG Best Flash Presentation **Louise Hamdy**

YCG Durward Cruickshank Prize **Anthony Phillips**

Computational Prize **Pascal Parois**

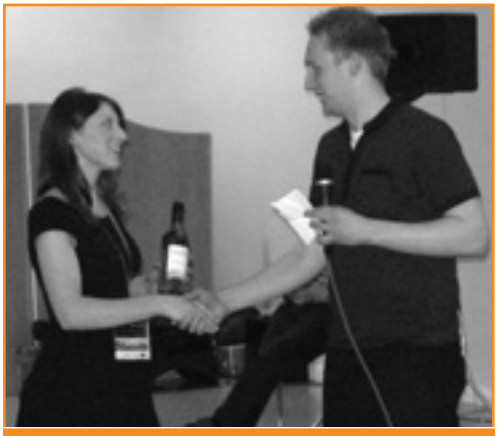
Exhibitor Passport **David Rendle**

Where it was possible to get photographs of the winners, these are presented. Unfortunately, some winners were both shy and fleet of foot, resulting in an artistic study of retreating backs!

Scott McKellar

Lucy Saunders

Rajni Miglani Bhardwaj



Louise Hamdy

Summary Financial Statements for year ended 31 December 2013

Examining Accountant: R A Young, BSc. FCA
The Young Company, Ground Floor, Unit 2b, Vantage Park, Washingley Road, Huntingdon, Cambridgeshire, PE29 6SR.

These are consolidated accounts based on the unaudited financial statements and include the BCA, BSG, IG, CCG, CCG School funds and YCG, expressed in pounds sterling (£)

INCOMING RESOURCES:

	2013	2012
Grants and sponsorship	19,545	11,591
Donations	21,362	967
Annual conference	–	91,293
Meetings of groups	45,850	7,882
Crystallography News	17,100	17,100
Membership Subscriptions	14,662	18,209
Investment income	5,800	6,263
Interest received	33	68
TOTAL INCOME	**124,352**	**153,373**

EXPENSES:

	2013	2012
Direct charitable expenditure (2)	79,250	123,173
Management and administration (3)	13,305	28,477
TOTAL EXPENDITURE	**92,555**	**151,650**

	2013	2012
NET INCOME:	**31,797**	**1,723**
Unrealised gains (losses) on investment assets	18,971	5,691
NET MOVEMENT IN FUNDS	**50,768**	**7,414**
Balances brought forward at 1 January 2013	207,016	199,602
Balances carried forward at 31 December 2013	257,784	207,016

ASSETS:

Fixed assets	2013	2012
Tangible assets	5	5
Investments	137,972	119,811
Total	**137,977**	**119,816**
Current assets		
Debtors	11,057	23,778
Cash at Bank	125,361	79,026
Total	**136,418**	**102,804**

CREDITORS:

Amounts falling due within 1 yr	(16,063)	(15,359)
Amounts falling due after 1 yr	(548)	(245)
NET ASSETS	**257,784**	**207,016**

INCOME FUNDS:

	2013	2012
Restricted funds (4)	131,608	119,517
Unrestricted funds (4)	126,176	87,499
Total	**257,784**	**207,016**

NOTES TO THE SUMMARY FINANCIAL STATEMENTS

1. ACCOUNTING POLICIES

These summary statements are based on financial statements which have been prepared under the historical cost convention, with the exception of investments which are included at market value. The financial statements have been prepared in accordance with the Statement of Recommended Practice, "Accounting and Reporting by Charities" published in March 2005 and applicable accounting standards.

All incoming resources are included in the Statement of Financial Activities when the charity is legally entitled to the income and the amount can be quantified with reasonable accuracy. All expenditure is accounted for on an accruals basis and has been included under expense categories that aggregate all costs for allocation to activities. Investments are stated at market value at the balance sheet date.

Tangible fixed assets are stated at cost less depreciation. Depreciation is provided at rates calculated to write off the cost of fixed assets, less their estimated residual value, over their expected useful lives.

2. DIRECT CHARITABLE EXPENDITURE

	2013	2012
Subscription to International bodies	11,278	11,191
Annual conference (5)	–	85,655
Meetings of groups	6,254	7,949
Crystallography News + Newsletters	15,740	13,229
Course fees and accommodation	41,453	–
Grants and sponsorship	3,300	1,981
Awards & bursaries	50	1,818
Arnold Beevers Bursary Fund	1,175	1,350
Total	**79,250**	**123,173**

3. GOVERNANCE

	2013	2012
Administration fees	5,581	13,883
Administration expenses	1,090	6,557
Accounting fee	4,500	4,500
Insurance	540	530
Bank and security charges	193	2,129
Special Interest Group Administration	15	20
Council members' expenses	1,287	812
Website Costs	99	46
Total	**13,305**	**28,477**

The full BCA accounts for 2013 are available as an e-mail attached file from the BCA administrative office.

4. STATEMENT OF FUNDS	Brought Forward	Incoming Resources	Resources Expended	Transfers	Gains (Losses)	Carried Forward
UNRESTRICTED FUNDS						
General Fund	**87,499**	**63,647**	**(43,941)**	**–**	**18,791**	**126,176**
RESTRICTED FUNDS						
Arnold Beevers Bursary Fund	9,111	210	(1,175)	–	–	8,146
IUCr bursary fund	30,231	–	–	–	–	30,231
Dorothy Hodgkin prize fund	8,675	30	–	–	–	8,705
Chemical group teaching school	27,869	44,821	(40,299)	–	–	32,391
Chemical group fund	4,893	4,357	(314)	–	–	8,936
Industrial group fund	21,490	8,956	(5,794)	–	–	24,652
Biological Structures group fund	14,333	2,331	(500)	–	–	16,164
Durward Cruickshank fund	1,531	–	–	–	–	1,531
Young Crystallographers Group Fund	1,384	–	(532)	–	–	852
Subtotal	**119,517**	**60,705**	**(48,614)**	**–**	**–**	**131,608**
Total of Funds	**207,016**	**124,352**	**(92,555)**	**–**	**18,971**	**257,784**

Treasurer's Report 2013

THIS was an unusual year for the BCA in that there was no Spring Meeting and instead the ECA held ECM28 in Warwick. Despite concerns that this would have a negative financial impact on the Association, this has not been realised, with the generous donation of a share of the surplus produced by the ECM28 meeting boosting our accounts.

Overall we had a surplus of £50,768 during the year ended 31 December 2013, and the Association has no material guarantees or commitments which could affect its future solvency.

The general fund had a surplus of £38,677 including an increase of £18,971 in the value of the investments and the donation of the ECM28 surplus. The reserve funds operated by the Groups and the Association had an overall surplus of £12,091. The income from our investments brought in £5,833 this year, a small decrease on last year due to a reduction in yields on the investment portfolio.

The major risks to which the Association is exposed are with regard to the cost of the Spring Meeting and its effects on the Association's major reserves. To mitigate those risks the Association has all its investments placed with an independent professional management company. Our investment portfolio was valued at £137,972. Bank interest rates continue to be at historically low levels, so income from interest is substantially lower than a few years previously. The Council's review of the reserves indicates that we should always be striving to generate more income to enable us to plan and encourage even higher levels of educational and scientific activity.

Crystallography News continues to contribute to the income of the BCA. We are grateful to its advertisers and sponsors who have continued to generously support our activities. We are as always grateful for those who contribute to the newsletter and to **Carl Schwalbe** for editing and overseeing its production.

Subscriptions to international bodies were £11,278, covering our membership of the IUCr and also our subscription to the European Crystallographic Association.

We have sponsored a number of events related to the Bragg centenary and the International Year of Crystallography over the year.

I would like to thank everyone who has helped me in my role this year, in particular the other Officers, members of Council, Nicola and the team at HG3, and our accountant Ray Philpott at The Young Company for all their help throughout the year.

Pamela Williams
Treasurer

Education & Outreach Update

Contact: education@crystallography.org.uk

THE last few months have been very busy for the Education and Outreach Coordinators, with many events taking place or being organised with an active attempt to improve our online presence.

In light of the launch of the International Year of Crystallography (IYCr2014) we created a new BCA Education website (learn.crystallography.org.uk) which we released in January to coincide with the launch of the IYCr. The website was aimed as a resource for this year, including links to events and advertisement, but it was also meant as a general teaching resource with information about all aspects of crystallography. We decided to create a website that could be used for many years to come, not purely as a website for the IYCr. There is still much more information that can be added and we plan to continue to develop this fantastic resource. If you see that there is something related to your research that would be interesting to the general public and we're currently missing it, get in touch! We also have a Twitter account (@Whatsinacrystal) and a Facebook page (www.facebook.com/britishcrystallography) where we are constantly adding links to new crystallographic gems that we find.

In December we held a meeting at the CCDC in Cambridge for parties interested in getting involved in public engagement in the UK for the IYCr. We had around 30 delegates from a range of institutes and organisations and a few active individuals, and it was great getting everyone together to hear about everyone's ideas and whether we could collaborate on any projects. We agreed that the BCA education website would be the host for a calendar of UK events for IYCr2014.

One of the main outcomes of the meeting is a collaboration with the Royal Society of Chemistry in their Global Experiment which will be launched in June. Every year the Royal Society of Chemistry hold a Global Experiment which is designed with easily accessible materials that schools and children can get involved with. They post their results and findings onto a website which allows results all over the world to be compared. This year the Global Experiment will be on recrystallisation, where 5 easily available compounds have been chosen with guidance on how to grow crystals of each. Once results begin to be published online, students can compare the findings worldwide, to see whether things such as temperature, humidity etc have an effect on crystal growth. There is no closing date for this event and it will run for a full year giving the maximum opportunity for people to participate.

One of our biggest events for the IYCr was the Big Bang Fair at the Birmingham NEC in March. This event saw over 75,000 visitors over 4 days, where we held our 'Structure of Stuff is Sweet' stand. The stand was funded by STFC for the second year and we received additional funding from ISIS (travel and subsistence) and Diamond (who provided our attractive yellow T-shirts!). We had around 40 volunteers who helped out, and they seemed to enjoy themselves as much as our visitors. In advance of the event we had also liaised with the IUCr, who sent along someone to help out as well as IYCr materials and glitter bugs, which we displayed as a cubic close packed array of bugs! We estimate that we spoke to more than 12000 people during our time at the Big Bang fair. These numbers are (rounded down) estimates, but we collected some data that showed we were seeing more than 531 visitors/hour! Massive thanks go to all our volunteers who helped during the 4 days; without this help the event would not have been possible, or as successful as it was!

At the moment we have one more major event planned for the coming year, the Cheltenham Science Festival in June. We will be holding two events at Cheltenham, the first of which is an interactive stand for over-16s with hands-on activities similar to the Big Bang Fair. The second event will be a panel discussion jointly sponsored by the British Society of Immunology entitled 'The Immune System: Your Inner Army' (http://www.cheltenhamfestivals.com/science/whats-on/2014/the-immune-system-your-inner-army/).

Two speakers have already been confirmed for this: **Susan Lea** from the University of Oxford and **Clare Bryant** from the University of Cambridge. They will discuss how crystallography is useful for deciphering information about your immune system.

Please keep updating us on any events that you may be running in your local area and we can put them in the calendar of events on our website. Also keep an eye on this, our twitter feed and our Facebook page to find out about other events which may be happening near you! We have a pack of resources based around our Big Bang Fair activities which are freely available to you if you feel like having a go yourselves! Just get in touch and we'll be happy to give you some useful pointers.

At this year's BCA AGM, **Claire Murray**, **Lynne Thomas** and **Anna Warren** stepped down as the Education and Outreach Coordinators – we'd like to thank all of our volunteers and supporters and the BCA council for their help during our year in the post. **Sam Callear** from ISIS has now taken the reins so expect to hear lots from her over the next year as we continue the momentum through the IYCr2014. In light of the fact it is a big year we are all looking forward to working closely together over the remainder of the year to ensure the smooth running of the up and coming events.

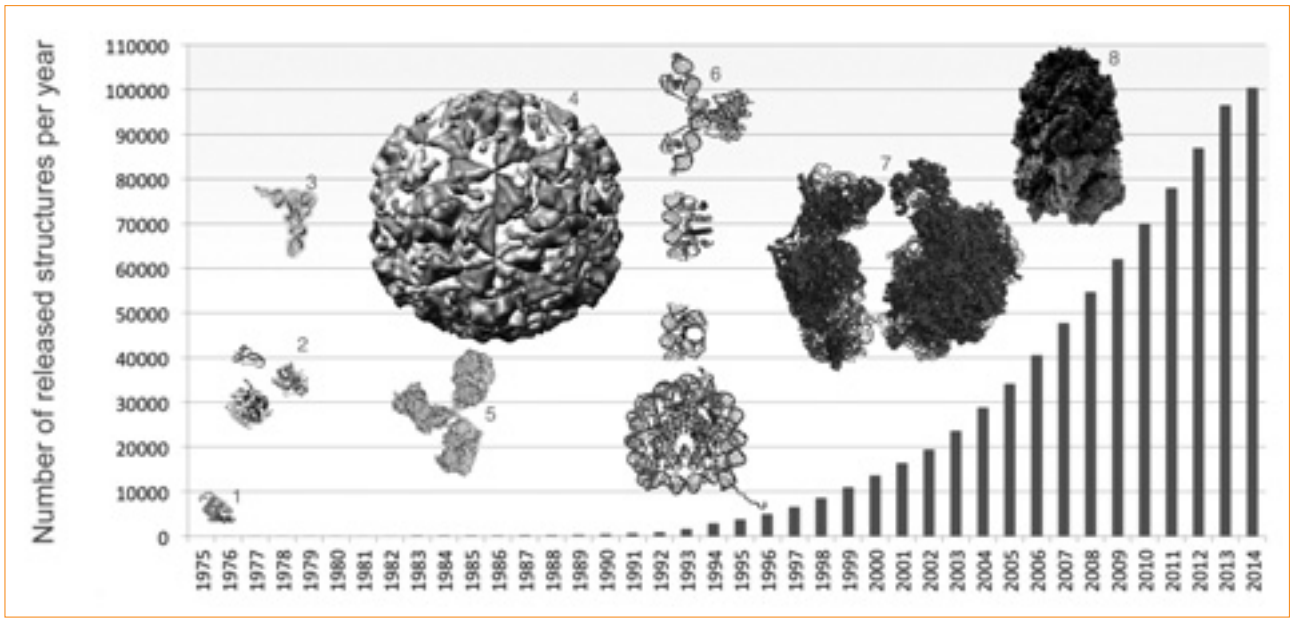
Sam Callear

Protein Data Bank: 100,000 structures

THE Worldwide Protein Data Bank (wwPDB) today announces that it has released to the community its 100,000th macromolecular structure. Established in 1971, this central, public archive of experimentally-determined protein and nucleic acid structures has reached this important milestone thanks to the efforts of structural biologists throughout the world.

Future challenges

The scientific community eagerly awaits the next 100,000 structures and the knowledge these will undoubtedly bring. However, the increasing number, size and complexity of biological data being deposited in the PDB and the emergence of hybrid methods, which use a variety of biophysical, biochemical, and modelling techniques to determine the shapes of biologically relevant molecules, all present major challenges for the management and presentation of structural data. wwPDB will continue to work with the community to meet these challenges and to ensure that the archive maintains the highest possible standards of quality, integrity and consistency.



Validation reports available for all X-ray structures in the PDB

THE Worldwide Protein Data Bank (wwPDB) partners are pleased to announce that validation reports for all X-ray crystal structures in the PDB archive are now publicly available.

"The new validation reports are sure to become an indispensable resource for all X-ray crystallographers. Most importantly, we hope they will be really useful for all the end users of structural models, who increasingly need to critically assess and compare PDB entries," said **Anastassis Perrakis**, Netherlands Cancer Institute, whose research focuses both on analysing macromolecular structures relevant for cancer, and also on developing the tools needed to decipher these structures.

The reports implement the recommendations of a large group of community experts on validation and include the results of geometric checks, structure-factor assessment and ligand validation. The reports include results from tried and tested software including MolProbity, Xtriage, Mogul, EDS and various CCP4 programs. They summarise the quality of the structure and highlight specific concerns by considering the coordinates of the model, the diffraction data and the fit between the two. Easily interpretable summary information that compares the quality of a structure with that of other structures in the archive is also provided.

Validating structures prior to publication and deposition

The new X-ray structure-validation reports have been provided to depositors as part of the structure-annotation process since August 2013. More recently, a stand-alone wwPDB X-ray structure validation server was launched (http://wwpdb-validation.wwpdb.org/). The server allows crystallographers to check early, intermediate and near-final models on demand and helps identify any potential problems that need addressing prior to structure analysis, publication and deposition.

"The stand-alone validation server will run exactly the same validation tests that have recently been introduced for the annotation of new depositions", says **Randy Read** of Cambridge University. Read chairs the wwPDB X-ray Validation Task Force (VTF) that has produced detailed recommendations to the wwPDB about how macromolecular crystal structures should be validated[1]. *"With the stand-alone server, crystallographers won't have any last-minute surprises when they deposit their structures just before submitting the paper"*, Read adds.

Accessing validation reports for archived structures

Validation reports for X-ray structures archived in the PDB are accessible from the following FTP sites:

- **ftp://ftp.wwpdb.org/pub/pdb/validation_reports/** (wwPDB)
- **ftp://ftp.ebi.ac.uk/pub/databases/pdb/validation_reports/** (PDBe)
- **ftp://ftp.pdbj.org/pub/pdb/validation_reports/** (PDBj)

The reports have been developed in the context of a larger initiative, the new wwPDB Deposition and Annotation system (http://wwpdb.org/system_info.html), which was created to unify the annotation tools and practices used across all wwPDB deposition centres and for all common structure-determination methods.

About wwPDB

The wwPDB (http://wwpdb.org) is the international partnership that manages the PDB archive. It consists of: the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB; http://rcsb.org) and BioMagResBank (BMRB; http://bmrb.wisc.edu) in the USA, the Protein Data Bank in Europe (PDBe; http://pdbe.org) and the Protein Data Bank Japan (PDBj; http://pdbj.org). Together, the wwPDB partners are committed to ensuring high standards of quality, integrity and consistency of this uniquely important archive and to make it freely available for the benefit of scientists worldwide.

[1] Read R. J., Adams P. D., Arendall III W. D., Brünger A. T., Emsley P., Joosten R. P., Kleywegt G. J., Krissinel E. B., Lütteke T., Otwinowski Z., Perrakis A., Richardson J. S., Sheffler W. H., Smith J. L., Tickle I. J., Vriend G., and Zwart P. H. A new generation of crystallographic validation tools for the Protein Data Bank. *Structure,* **19**, 1395-1412, 2011. DOI: 10.1016/j.str.2011.08.006

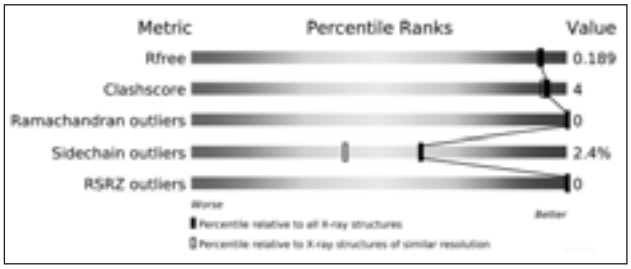


Figure 1: *The validation reports provide at-a-glance summary information that compares the quality of a model with that of other models in the archive.*

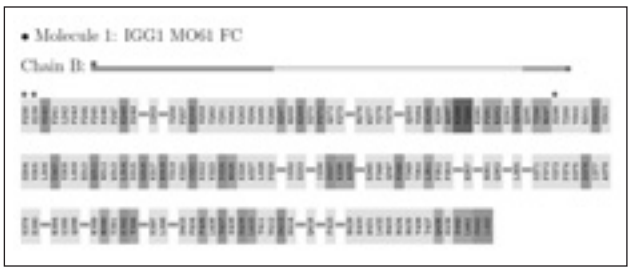


Figure 2: *The reports contain residue-property plots. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ>2).*

2014 Ludo Frevel Crystallographic Scholarship

The ICDD Announces the Recipients of the 2014 Ludo Frevel Crystallographic Scholarship

February 11, 2014

THE ICDD Ludo Frevel Crystallography Scholarship Committee has selected thirteen recipients for the 2014 Scholarship Program. These recipients were selected, on a competitive basis, from seventy-eight commendable applications received by the ICDD Scholarship Committee. The recipients are:

Agris Bērziņš, University of Latvia, Riga, Latvia.
On the differences of Crystal Structures for Compounds with almost the same Chemical Structure: Case of Benperidol and Droperidol

Kunpeng Cui, National Synchrotron Radiation Lab, Univ. of Science & Tech. of China, Hefei, Anhui, China.
In-situ Studying Crystallization and Precursors during Short-term Extension Using Synchrotron X-ray Scattering

Juli-Anna Dolyniuk, University of California, Davis, CA, USA.
New High-Efficiency Thermoelectric Materials Based on Transition Metal Clathrate Frameworks

Sofia Marah Frias, National Institute of Geological Sciences Quezon City, Philippines.
Characterization of Hydrothermal Alteration Mineralogy using Portable XRD/XRF and Laboratory-Based XRD

Bahareh Khalili Najafabadi, University of Western Ontario, Ontario, Canada.
New Metal-Phosphido Precursors for Metal-Phosphide Nanocluster Assembly

Kyle McDevitt, Alfred University, Alfred, NY, USA.
New Ceramic Materials for Solid Oxide Fuel Cells

***Gift Mehlana**, University of Cape Town, Cape Town, South Africa.
Crystal Engineering of Pyridyl Benzoic Acids

Cristina Motillo, McGill University, Quebec, Canada.
Mechanistic Studies of Solvent-free Transformations of Metal Oxides into Porous Metal-Organic Frameworks

Guzman Peinado, Facultad de Química, Udelar, Novosibirsk, Montevideo, Uruguay.
Preparation, Structural Study and Evaluation of Physical Properties of Nanostructured Diacetate Based MOFs

Clare Rowland, Northwestern University, Evanston, IL, USA.
Synchrotron Studies of Melting Behavior in Nanocrystalline Materials

Thanh Thao Tran, University of Houston, Houston, TX, USA.
From Crystallographic Architecture to Centricity Control of Novel Alkaline/Alkaline-earth Lead Fluoride Carbonate Materials

Benjamin Trump, Johns Hopkins University, Silver Spring, MD, USA.
Dimensionality in the Misfit Series (MX)(1+δ)m(TX2)n as a Chemical Handle to Tune Physical Properties

Tedi-Marie Usher, North Carolina State University, Raleigh, NC, USA.
Advanced Diffraction Techniques: Structure-Property Relationships in Complex Perovskites

*2012 Recipient

The ICDD will present each of these students with a check in the amount of $2,500 to assist in the continuation of studies in their selected fields of crystallographic research. Scholarship awards are made possible by donations from both individuals and corporations. One hundred percent of all donations to the scholarship fund are applied to student funding, as defined by the program's charter. The Ludo Frevel Scholarship Program is a registered non-profit charity, and all donations are tax-deductible. Please consider making a personal or corporate donation to the fund today.

Donate here: **www.icdd.com/frevel/index.html**

News from the Groups

AS in previous years, the Young Crystallographers Satellite meeting took place directly before the BCA Spring Meeting 2014, which was held at Loughborough University. We have come to expect a very high calibre of oral and poster presentations and this year did not disappoint. One such example was the Parkin Prize Lecture, delivered by Claire Murray from Diamond Light Source, who outlined clearly and passionately why outreach is vitally important, both for scientists and non-scientists (and for the young and not-so-young). As proof of the quality of the abstracts submitted to speak in the satellite meeting, some applicants were in fact pinched to speak at the main meeting instead!

The YCG committee awards two prizes each year. The first is for the best flash poster presentation, which recognises the important ability to sell your research concisely and effectively. This was won by **Louise Hamdy** from the University of Bath. The second YCG award is the Durward Cruikshank prize, which is a £250 prize awarded to a Young Crystallographer who has made an outstanding contribution in any area of crystallography. The prize is judged on poster and oral presentations as well as all-round contributions during the BCA Spring Meeting. This year the recipient of the award was **Anthony Phillips** from Queen Mary University of London, who chaired the debate session (entitled "Are Crystallographers Necessary?"), gave a talk in the main meeting (entitled "Comparing the Dynamics of Co-ordination Polyhedra in a Metal-cyanide Framework") and additionally co-organised the programme for the YCG meeting. Anthony has also been involved in crystallographic teaching and outreach during his time on the YCG committee as the former PCG representative.

On the YCG committee there were five new members appointed. Two new YCG officers join the committee – **Scott McKellar** replaces **Anna Warren** as the YCG Chair and **Claire Hobday** takes on the role of YCG Secretary, replacing **Lauren Hatcher**. The CCG, PCG and IG group representative positions are now filled by **Jorge Sotelo**, **Jerome Wicker** and **Anneke Klapwijk** as **Helen Mason** and **Anthony Philips** step down. **Kate Wittering** takes a sideways step from IG representative to ordinary member, replacing **Issy Kirby**. They join the existing committee of **Nicholas Funnell** (vice chair), **Pascal Parois** (webmaster), **Anna Polyakova** (BSG representative), **Sam Horrell** (ordinary member), **Sarah Gurung** (ordinary member) and **Lucy Saunders** (ordinary member).

As discussed at the YCG AGM, there were a number of crystallography outreach activities over the past year, such as the extremely successful Big Bang Fair in Birmingham which saw thousands of school children learning about crystals and diffraction at the BCA's "The structure of stuff is sweet" stand. Members of the YCG from the universities of Bath, Liverpool, Oxford and Reading also helped run the BCA 'What is a crystal?' stand at two consecutive Diamond Light Source open days in March. There was a good turnout of sixth formers from local schools who were not only attracted by the supply of sweets but by the structures that could be made using them! Visitors to the stand also got first hand crystal growing experience and the chance to see some live 'diffraction'.

In her final report as treasurer, **Lauren Hatcher** reported the good news that the YCG had been successful in obtaining a grant of £800 from The Biochemical Society. This money was awarded to help promote biological crystallography to the wider public. In light of this the YCG have decided to use this money towards helping the BCA Education and Outreach Team attend the Cheltenham Science Festival in June. Here two events have been planned, the first of which is an interactive stand for over 16s with hands on activities similar to the Big Bang Fair. The second event will be a panel discussion jointly sponsored by the British Society of Immunology entitled 'The Immune System: Your Inner Army' (http://www.cheltenhamfestivals.com/science/whats-on/2014/the-immune-system-your-inner-army/). We feel this is a great event for the YCG to use this money for, with many of the members of the YCG helping out as volunteers.

We are always happy to hear any feedback or suggestions from any of the members of the YCG, so please contact us on: ycg@crystallography.org.uk .

XRF Meeting 2014

The Next XRF meeting is on 18th June 2014 at the University of Leicester.

Registration is now open on the HG3 BCA admin site.
A limited number of FREE STUDENT PLACES are available at this meeting. To apply please E-mail the Group Treasurer with your name, E-mail address and Institution for details of how to apply for a FREE place.

NOTE: THE STANDARD REGISTRATION FORM DOES NOT SUPPORT FREE PLACES AND STUDENTS USING IT WILL BE CHARGED CONCESSION FEES.

Fees: after 17th May – £84 or £42 concessions.

Provisional programme

A unique chance to see major manufacturers of handheld and portable equipment [including Bruker, Thermo (Niton) Oxford Instruments, Spectro, Olympus (Delta) and more...] demonstrating their instruments in two workshops.

09:30 **Registration, Coffee and Exhibition**

10:00 **Welcome**

10:10 **Handheld XRF workshop** – Bruker, Thermo (Niton), Oxford Instruments, Spectro and Olympus (Delta).

11:15 **Exhibition and Coffee**

11:45 **An evaluation of FP-XRF to assess metals in boat paint fragments** Kevin Solman, Plymouth University.

12:05 **Presentation and open discussion of results from DOT-1 sample – distributed at last year's meeting**, Ros Schwarz.

12:35 **Introduction of DOT-2**, David Beveridge.

12:45 **Prize session:** Your chance to spend a few minutes telling us about your most difficult sample.

13:00 **Lunch**

14:00 **Portable XRF workshop.** Bruker, Spectro, and more...

15:00 **Exhibition and Tea**

15:30 Title tbc, Garry Smith, Scimed.

16:00 **XRF chlorine calibration using sample preparation by fusion**, Mathieu Bouchard, Corporation Scientifique Claisse.

16:30 **XRF on a micro scale. How EDX, coupled with SEM, can provide elemental data to solve product and research problems**, Andy Scothern, Saint Gobain.

17:00 **Close**

Puzzle Corner

A CENTURY OF CRYSTALLOGRAPHY

1. Name the six crystallographers (4 male, 2 female) chiefly associated with major advances in the following scientific subjects:

- **A.** X-ray diffraction
- **B.** Nature of the Chemical Bond
- **C.** Vitamin B12
- **D.** Boron hydrides
- **E.** Electron microscopy and nucleic acid-protein complexes
- **F.** Ribosome

2. What do these six crystallographers (and the scientific subjects) have in common?

3. The six decided to have a celebratory dinner, sitting at a circular table. The eldest took the first seat, and the others then sat sequentially in order of decreasing age. The dinner was held in the land of Oz. Who sat directly opposite Dorothy?

4. A significant date was chosen for the dinner, by summing all the 4-digit numbers for the six years associated with their common accomplishments, plus an extra 100 (to celebrate a centenary of crystallography), giving a 5-digit number, which was read as a date in the 20th century (dd-m-yy). What was that date?

5. What "ex-ray" phenomenon was observed on that date by a gathering of 2600 crystallographers?

6. Where, and for what purpose, were the 2600 crystallographers gathered?

Suggest a suitable noun to describe a gathering of crystallographers, e.g. a CONGRESS of crystallographers.

This anniversary puzzle has been contributed by **Jim Trotter**

Answers to March 2014 Word Search

THE answers are presented in two ways: (1) with columns designated left to right as a, b, …, o and rows top to bottom as 1, 2, …, 15; (2) on the original grid using typography.

Open Lab hosts and SESAME members in **bold** on the grid:
ARGENTINA b12-b4;
IVORY COAST e3-e7 & i9-m13;
MOROCCO c10-c4;
SOUTH AFRICA j11-j7 & b12-g12;
URUGUAY l7-f13;
BAHRAIN h5-n11;
CYPRUS n13-i8;
EGYPT d13-h13;
IRAN e3-h6;
ISRAEL e3-j3;
JORDAN n10-n5;
PAKISTAN o6-h6;
PALESTINIAN AUTHORITY a13-k3 & m7-e7;
TURKEY d4-d9.

SESAME Observers in *italics* on the grid:
BRAZIL n1-i1;
CHINA g9-g5;
FRANCE f14-a14;
GERMANY o14-o8;
JAPAN h10-l14;
PORTUGAL a13-a6;
RUSSIAN FEDERATION a1-g1 & o2-f2;
SWEDEN g14-l14;
UNITED KINGDOM b15-n15.

R	*U*	*S*	*S*	*I*	A	*N*	E	*L*	*I*	*Z*	*A*	R	*B*	Y
M	B	O	N	N	*N*	*O*	*I*	*T*	*A*	*R*	*E*	*D*	*E*	*F*
I	Y	S	J	I	S	R	A	E	L	N	S	W	O	G
N	A	O	T	V	R	A	L	L	A	N	K	A	P	F
A	N	C	U	O	W	A	B	I	E	P	S	C	N	L
L	I	C	R	R	C	*N*	N	A	T	S	I	K	A	P
A	T	O	K	Y	T	I	R	O	H	T	U	A	D	M
G	N	R	E	C	T	*H*	V	S	T	R	T	R	R	*Y*
U	E	O	Y	S	Y	*C*	P	C	U	W	A	M	O	*N*
T	G	M	E	T	T	I	*J*	G	O	R	A	I	J	*A*
R	R	L	V	N	J	K	U	*A*	S	A	P	Y	N	*M*
O	A	F	R	I	C	A	E	L	*P*	M	S	Y	H	*R*
P	X	U	E	G	Y	P	T	B	Y	*A*	A	T	C	*E*
E	*C*	*N*	*A*	*R*	*F*	*S*	*W*	*E*	*D*	*E*	*N*	I	T	*G*
F	*U*	*N*	*I*	*T*	*E*	*D*	*K*	*I*	*N*	*G*	*D*	*O*	*M*	*A*

The postal town and beamline scientist are ALLAN g4-k4 (Allan, Jordan and David Allan from Diamond).

The winning entry was submitted by **Jim Trotter**.

Answers to December 2013 Element Puzzle

H, At, P, Pb, Y, Ni, Es, W, Yb, Eu, Ar, Rh, O, F, C, Re, Y, Se, Ti. The message is "HAPPY NEW YEAR OF CRYSTallography."

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.

15-18 June 2014
EPDIC14. European Powder Diffraction Conference, Aarhus, Denmark.
http://epdic14.au.dk/

15-19 June 2014
6th International Workshop on Crystal Growth Technology, Berlin, Germany.
http://iwcgt-6.ikz-berlin.de/

16-19 June 2014
16th International Workshop on Physical Characterization of Pharmaceutical Solids, Prague, Czech Republic.
http://www.assainternational.com/workshops/iwpcps-16/

16-20 June 2014
Fifth Workshop on Neutron Scattering Applications in Structural Biology, Oak Ridge, TN, USA.
http://neutrons.ornl.gov/conf/gcnb2014/

18-22 June 2014
1st International Symposium on Halogen Bonding (ISXB-1), Porto Cesareo, Italy.
http://www.isxb-1.eu/

22-27 June 2014
Hybrid Electronic & Photonic Materials and Phenomena. Gordon Research Conference Hong Kong, China.
http://www.grc.org/programs.aspx?year=2014&program=hybridelec

22-27 June 2014
Bioinspired Materials: Exploiting Biological Concepts and Strategies in Functional Synthetic Materials, Gordon Research Conference, Newry, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=bioinsp

23-26 June 2014
XXIV Symposium of the Specialized Group on Crystallography and Crystal Growth (GE3C), Bilbao, Spain.
http://www.ehu.es/en/web/ge3c2014

22-27 June 2014
Three Dimensional Electron Microscopy, Gordon Research Conference, Girona, Spain.
https://www.grc.org/programs.aspx?year=2014&program=threedim

24-27 June 2014
15th Tetrahedron Symposium, Challenges in Bioorganic and Organic Medicinal Chemistry, London.
http://www.tetrahedron-symposium.elsevier.com/index.html

30 June – 4 July 2014
5th Edition of MAUD Workshop, Combined Analysis Using X-ray and Neutron Scattering, Caen, France.
http://www.ecole.ensicaen.fr/~chateign/formation/MAUD%20Training%202014.pdf

2-4 July 2014
Seminar on Advanced X-ray Powder Diffraction Techniques and Applications, Dresden, Germany.
http://www.panalytical.com/event/XRDdresden.htm

2-13 July 2014
Bachelor Summer Program (physical computing, large scale facilities, biochemistry), Université Joseph Fourier, Grenoble, France.
http://www.ujf-grenoble.fr/international/bachelor-summer-program/

7-11 July 2014
International Conference on Highly Frustrated Magnetism 2014, Cambridge.
http://hfm2014.tcm.phy.cam.ac.uk/

9-10 July 2014
Neutrons & Food 3, Paris, France.
http://neutronsandfood.com/

9-11 July 2014
Emerging Photon Technologies for Chemical Dynamics – Faraday Discussion 171, Sheffield.
http://www.rsc.org/conferencesandevents/rscconferences/

12-13 July 2014
Thin Film and Small Scale Mechanical Behavior: Gordon Research Seminar, Bentley University, Waltham, MA, USA.
http://www.grc.org/programs.aspx?year=2014&program=grs_thnflm

13-17 July 2014
Membrane Transport Proteins: Structure, Function, Physiology, and Targets in Disease, Gordon Research Conference, West Dover, VT, USA.
http://www.grc.org/programs.aspx?year=2014&program=membtrans

13-18 July 2014
Small Scale Mechanical Behavior: Observations, Insights and Analyses: What's New in the World of Micro Mechanics, Gordon Research Conference, Bentley University, Waltham, MA, USA.
http://www.grc.org/programs.aspx?year=2014&program=thinfilm

13-18 July 2014
Atomic & Molecular Interactions: Energy Conversion Processes and Chemical Reactions in Clusters, Solution, Surfaces, Interfaces, and Biological Systems, Gordon Research Conference, Easton, MA, USA.
http://www.grc.org/programs.aspx?year=2014&program=atomic

13-18 July 2014
Nanostructure Fabrication: Nanostructures in Information Technology, Energy Conversion, and Nanoelectromechanical Systems, Gordon Research Conference, Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=nanofab

17 July 2014
Symposium celebrating Barkla, Bragg and Shechtman, Liverpool.
http://www.ifb2014.com/UKTI-Market-Event-SE-Asia-e48.html

20-25 July 2014
Colloidal Semiconductor Nanocrystals: From Fundamental Physics to Functional Materials, Gordon Research Conference, Smithfield, RI, USA.
http://www.grc.org/programs.aspx?year=2014&program=collsemi

20-25 July 2014
Structural Nanomaterials. Gordon Research Conference, Hong Kong, China.
http://www.grc.org/programs.aspx?year=2014&program=strucnano

21-25 July 2014
ICSOS'11: 11th International Conference on the Structure of Surfaces, Coventry.
http://icsos11.iopconfs.org

21-25 July 2014
41st International Conference on Coordination Chemistry, Singapore.
http://www.iccc41.org/

26-27 July 2014
Diffraction Methods in Structural Biology, Gordon Research Seminar, Lewiston, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=grs_diff

27 July – 1 August 2014
Diffraction Methods in Structural Biology: Faster, Smaller, Better: Novel Technologies for Diffraction Experiments in Molecular Biology and Drug Discovery, Gordon Research Conference, Lewiston, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=diffrac

28 July – 1 August 2014
Denver X-ray Conference. 63rd Annual Conference on Applications of X-ray Analysis, Big Sky, MT, USA.
http://www.dxcicdd.com/

30 July – 2 August 2014
Bicontinuous Cubic Phases Conference, Noosa, Queensland, Australia.
http://cubicphase2014.org/

31 July – 2 August 2014
Molecular Modelling 2014: From biomolecules to materials, Lamington National Park, Queensland, Australia.
http://compbio.chemistry.uq.edu.au/mm2014/index.htm

1-31 August 2014
Virtual Conference on Computational Chemistry.
http://sites.uom.ac.mu/vccc2014/

3-8 August 2014
18th International Biophysics Congress, Brisbane, Australia.
http://www.iupab2014.org/

3-8 August 2014
Conductivity & Magnetism in Molecular Materials: Understanding and Controlling Emergent Properties. Gordon Research Conference, Lewiston, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=conduct

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

9-15 August 2014
2014 PSI Summer School on Condensed Matter Research (13th edition) Exploring time, energy and length scales in condensed matter, Zug, Switzerland.
http://indico.psi.ch/conferenceDisplay.py?confId=2672

10-14 August 2014
248th ACS National Meeting & Exposition, San Francisco, CA, USA.
https://www.acs.org/content/acs/en/meetings/fall-2014.html

10-15 August 2014
DNA Topoisomerases in Biology & Medicine: from Molecular Structure to Drug Targeting. Gordon Research Conference, Newry, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=dnatop

10-15 August 2014
Multiferroic & Magnetoelectric Materials: Designing for Multifunctionality. Gordon Research Conference, Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=multiferr

12-16 August 2014
Topological methods for expert systems in materials science, Samara, Russia.
http://sctms.ru/train/school/?lang=en

14-16 August 2014
The Role of Magnetic Symmetry in the Description and Determination of Magnetic Structures, Hamilton, ON, Canada.
http://magcryst.org/meetings/cmsworkshop2014/

17-23 August 2014
Biomineralization: Where Geology Meets Biology: The Inorganic-Organic Interface, Gordon Research Conference, New London, NH, USA.
http://www.grc.org/programs.aspx?year=2014&program=biomin

20-29 August 2014
Neutron Scattering Applications to Hydrogen Storage Materials, Berlin, Germany.
http://www.helmholtz-berlin.de/events/hydrogen-school-2014/index_en.html

23-26 August 2014
Transcription and Chromatin. 11th EMBL Conference, Heidelberg, Germany.
http://www.embl.de/training/events/2014/TRM14-01/index.html

25-29 August 2014
FEL2014. Free Electron Laser Conference, Basel, Switzerland.
http://www.fel2014.ch/

25 August – 3 September 2014
EMU School 2014 – Planetary Mineralogy, Glasgow.
http://eurominunion.org/?p=571

28 August – 6 September 2014
ECS1. First European Crystallography School, Pavia, Italy.
http://ecs1.azuleon.org/

1-5 September 2014
IMA 2014 - 21st General Meeting of the International Mineralogical Association, Gauteng, South Africa.
http://www.ima2014.co.za/

1-12 September 2014
18th JCNS Laboratory Course – Neutron Scattering 2014, Jülich / Garching, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/LabCourse/_node.html

7-13 September 2014
Soft-Inter2014: Soft Interactions in Biological and Biomimetic Self-assemblies, Saint Malo, France.
http://soft-inter2014.sciencesconf.org/

13-17 September 2014
SISN 2014 Learning Days School Session 1, Bolzano, Italy.
http://nmi3.eu/index.php?article_id=437

14-17 September 2014
2nd International Science at FELs Conference, PSI Villigen, Switzerland.
http://science-at-fels-2014.eurofel.eu/

14-17 September 2014
Annual Meeting of the German Biophysical Society, Lübeck, Germany.
http://www.biophysical-congress.de/

14-19 September 2014
XTOP 2014: The 12th Biennial Conference on High-Resolution X-Ray Diffraction and Imaging, Grenoble, France.
http://xtop2014.org/

14-20 September 2014
ICCBM15. 15th International Conference on the Crystallisation of Biological Macromolecules, Hamburg, Germany.
http://www.iccbm15.org/iccbm15.xhtml

15-19 September 2014
Polarised Neutrons for Condensed-Matter Investigations Conference, Sydney, NSW, Australia.
http://nmi3.eu/news-and-media/calendar/show-individual-event.html?back=yes&eventid=165

15-19 September 2014
Crystallography in Material Science: Novel Methods for Novel Materials, Warsaw, Poland.
http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=368&Itemid=137

16-19 September 2014
ISIC19. International Symposium on Industrial Crystallization, Toulouse, France.
http://www.isic19.fr/

16-19 September 2014
Mid-European Clay Conference 2014, Radebeul near Dresden, Germany.
http://www.mecc2014.de

17-19 September 2014
Physical Chemistry of Functionalised Biomedical Nanoparticles. Faraday Discussion 175, Bristol.
http://www.rsc.org/ConferencesAndEvents/RSCConferences/FD/FD175/index.asp

19-22 September 2014
SISN 2014 Learning Days School Session 2, Grenoble, France.
http://nmi3.eu/index.php?article_id=437

20-27 September 2014
BioCrys2014. FEBS Practical & Lecture Course, Oeiras, Portugal.
http://biocrys2014.itqb.unl.pt/

24-26 September 2014
ESS Science Symposium: "Surface and Interface Reconstruction: A Challenge for Neutron Reflectometry, Munich, Germany.
http://tum.converia.de/frontend/index.php?sub=16

25-27 September 2014
17th Heart of Europe Bio-Crystallography meeting (HEC-17), Berlin, Germany.
http://www.helmholtz-berlin.de/events/hec/

29 September – 3 October 2014
ICANS XXI – 21st Meeting of the International Collaboration on Advanced Neutron Sources, Mito, Ibaraki, Japan.
http://j-parc.jp/researcher/MatLife/en/meetings/ICANS_XXI/index.html

5-8 October 2014
Summer School: Theory and Practice of Modern Powder Diffraction, Ellwangen, Germany.
http://www.kofo.mpg.de/iycr/index.html

5-10 October 2014
10th World Conference on Neutron Radiography, Grindelwald, Switzerland.
http://indico.psi.ch/conferenceDisplay.py?ovw=True&confId=2019

7-10 October 2014
GTBio 2014, Grenoble, France.
http://www.afc.asso.fr/index.php?option=com_content&view=article&id=189:gtbio-2014&catid=45:les-colloques&item=85

16-17 October 2014
Crystal (cl-)Year, Turin, Italy.
http://www.nettab.org/2014/CCY/

19-23 October 2014
JCNS Workshop on neutron instrumentation, Munich-Tutzing, Germany.
http://fisica.cab.cnea.gov.ar/hacesra10/index.php/9-novedades/51-first-circular-jcns-workshop-on-neutron-instrumentation-2

26-28 October 2014
2014 Pittsburgh Diffraction Conference, Athens, GA, USA.
http://www.pittdifsoc.org/

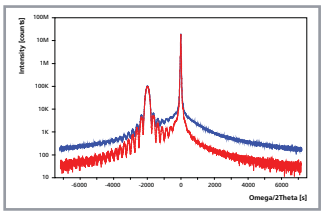
27 October – 3 November 2014
Solution scattering from biological macromolecules. EMBO Practical Course, Hamburg, Germany.
http://events.embo.org/14-sas/index.html

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

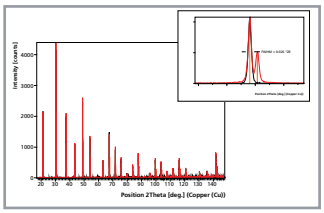
EMPYREAN

The world of X-ray diffraction is no longer flat

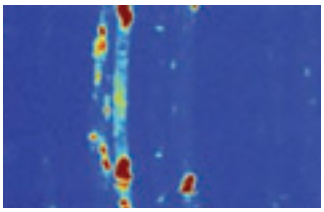
0D



1D



2D



3D

The only XRD platform that does it all

- Powders
- Thin films
- Nanomaterials
- Solid objects

The new Empyrean from PANalytical is truly innovative, with cutting-edge technology in every aspect. Empyrean brings the idea of the perfect XRD platform to life:

- The widest range of samples
- The highest data quality on every sample, no compromises
- Exceptional tube performance
- The highest performance goniometer
- 2nd generation PreFIX for optics and sample platforms
- PIXcel^{3D}: the only detector for 0D, 1D, 2D and even 3D applications
- Unmatched area detector dynamic range, linearity and resolution
- See inside your samples with the world's first 3D detector

PANalytical Ltd.
7310 IQ Cambridge,
Waterbeach,
Cambridge,CB25 9AY
t +44 (0)1223 203480
f +44 (0)1223 203490
info@panalytical.com
www.panalytical.com

Cutting-edge technology. Ultimate commitment.

The Analytical X-ray Company

PANalytical

range

expertise | development | range | quality | support

The right solution to fit your application





We know that one size doesn't fit all; which is why our wide range of low temperature devices offers various temperature bands and delivery methods.

Whether your needs are single crystal or powder diffraction, small molecule or macromolecular, no other company is better placed to advise you on the right product for your application.

Contacting Oxford Cryosystems will initiate a comprehensive exploration of your needs so that the right product is selected for the application, optimising both budget and performance requirements.

See our full range of products at **www.oxcryo.com** or call us on **+44 1993 883 488** to discuss your specific requirements.

OxfordCryosystems

it's what makes us cooler