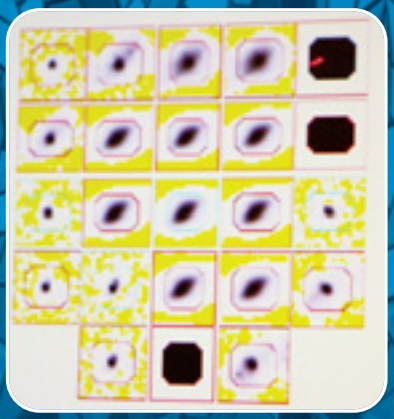
Crystallography News

British Crystallographic Association

Issue No. 130 September 2014
ISSN 1467-2790



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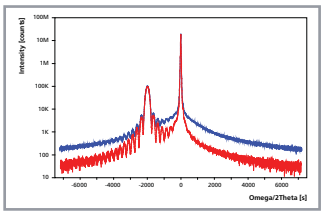

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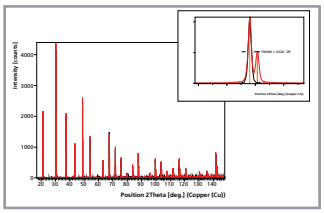

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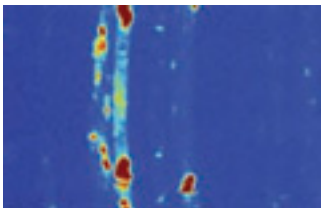

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by Bowmans, Leeds. Text should preferably be sent electronically as MSword documents (any version - .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.
Please ensure that items for inclusion in the December 2014 issue are sent to the Editor to arrive before 25 October 2014.

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This month's cover:

ACA meeting photos by Peter Mueller and Joan and Carl Schwalbe

From the President

I was out with some friends of ours at the weekend and their four-year old daughter was very busy 'collecting' stones from wherever she could find them. Admittedly they mostly came from the National Trust-tended gravel paths in Avebury, but she insisted in carrying her heavy bag of stones around with her for the whole day. Of course she is not alone in finding interesting things when out and about and taking them home; I have a very poor piece of quartz that looks like a huge back tooth from a beach in Cornwall, and some quite tarnished fools gold cubes chipped out of slates in Scotland sitting on my office bookshelves. They are far from perfect specimens but the important thing for me is the memories of summer holidays that they evoke. It seems to me that crystals often fulfil this reminding role – particularly through jewellery – but for us crystallographers I am certain there are specific crystals that tell a story of lucky finds, memorable experiments and interesting science. It is a bonus for us that our samples are also often extremely beautiful!

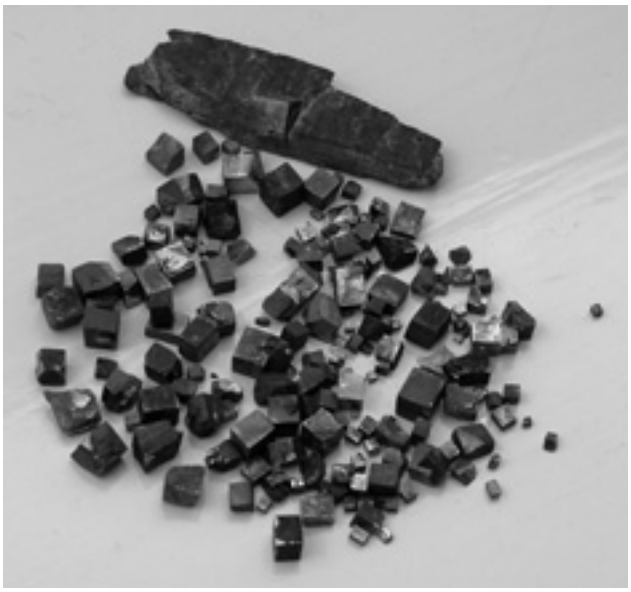
Although as I write, the IUCr conference has yet to take place, perhaps some of you will have been out collecting specimens in Canada this year while over there for the 23rd IUCr Congress and General Assembly. For those of us lucky enough to be able to go I hope that we will have also collected good memories of an excellent conference and I look forward to reading some of your recollections in the meeting reports sections of later issues of *Crystallography News*. Carl, our *Crystallography News* Editor, tells me that he is going on a trip to the wilds of the Gaspe Peninsula after the conference – somewhere where apparently there isn't any food. I'm planning a week beside the Bay of Fundy where they only seem to eat Lobster…

The 2015 BCA Spring Meeting in York is coming together nicely with the first announcement included in this issue of *Crystallography News*. The Programme Committee is planning an extensive program with a workshop theme running alongside the main sessions and we are hoping to be able to offer more opportunities for contributed talks. Please do take a look at the programme, make a note of the dates in your diaries and consider what you might like to offer to present at the meeting. I am delighted that Professor **Sir Tom Blundell** has agreed to give the Dorothy Hodgkin lecture at the meeting. Tom was one of Dorothy's students and will be giving a talk titled, "Dorothy Hodgkin, structural biology and drug discovery".

Continuing where I left off in my last column, education and outreach and other public engagement activities are continuing apace. We had a stand at the Cheltenham Science Festival and at the southwest's Big Bang Fair in Exeter last June. The same month saw crystallography showcased in the garden, the University of Oxford's Botanic Garden to be precise, and we may be taking our Crystallography stand to the Gravity Fields Festival in Grantham later in September. We are also working with the photographer **Max Alexander** to create an exhibition of crystallographers for display in the Royal Albert Hall and elsewhere in the Autumn. Nature have published a special issue on Crystallographic Milestones (see **www.nature.com/milestones/milecrystal/index.html**), the 2014 Royal Society of Chemistry Global Experiment is on the art of crystallisation (see **www.rsc.org/learn-chemistry/collections/online-experimentation/collaborative-chemistry/global-experiment-2014**) and I hear a rumour that our immediate past president **Elspeth Garman** will be appearing on Radio 4's "The Life Scientific" later in the year. As ever, the best way to keep up to date with all these events is via the BCA Education and Outreach web site (**learn.crystallography.org.uk/crystallography-events**) and twitter feed (**twitter.com/Whatsinacrystal**).

I'm off to pack my bags and print my boarding cards for Canada whilst, in the weird time-shifted column that I must write, I simultaneously hope that you have all had relaxing holidays over the summer. Enjoy reading this edition of *Crystallography News!*

David Keen



'Rusty' iron pyrites crystals collected by the BCA President from a Scottish beach.

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

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

From the Editor

THIS issue features the contribution made by BCA members to the excellent American Crystallographic Association meeting held in scenic Albuquerque, New Mexico, from May 24 to 28. Some scenes appear on the cover, and details appear later in this issue along with more photographs. John Helliwell had the immense honour of opening the entire meeting with the Patterson Lecture. He is shown receiving the Patterson Award from ACA President Martha Teeter and delivering his lecture. John took us through the burgeoning application of synchrotron radiation in macromolecular crystallography, basing his lecture both on deep personal experience and on generous acknowledgement of designers and beamline scientists. (Incidentally, 2014 has an association with Patterson: it marks the 80th anniversary of A. L. Patterson's paper that first showed how to create a vector map. Such a vector map becomes easier to interpret if a few "heavy" atoms are present. I have just published an article in *Crystallography Reviews* about the impact of the Patterson function on elemental abundance in small-molecule crystal structures). Chaired by Peter Wood and George Lountos, a very interesting session presenting "Industrial Research from Young Scientists" included exciting contributions from BCA members. The speakers and chairpersons are shown on the cover. We also enjoyed a good helping of wit and wisdom from Harry Powell. Although the science was first-rate and the atmosphere both at the conference and around Albuquerque was welcoming, there was one disappointment: the attendance was lower than at previous ACA meetings. We hope that this decrease, which we had also noticed at our own Spring Meeting, is due to the IUCr Congress in Montreal, with people who could only afford one meeting saving up their "loonies" (Canadian dollar coins) for the big meeting.

Our President's article may cause some readers to worry that Joan and I will be suffering hardship as we tour the scenic Gaspé Peninsula after the IUCr Congress. In fact, we'll be staying one night on a stretch of shoreline so remote that there's not even a convenience store within miles; and we'll have to collect sufficient food at the last town we encounter. The rest of the time there will be plenty of good hearty Quebecois fare on offer, but our survival will depend on our ability to speak French in this very Francophone part of Canada. A characteristic regional dish is poutine, French fries topped with curd cheese and gravy. As we sample this delicacy, we'll think of Dave, condemned to a diet of lobster. Incidentally, "Poutine" is also the way French Wikipédia spells the surname of the Russian President.

There will be no excuse to miss our Spring Meeting in 2015. A preliminary announcement of the programme appears on these pages. You will see that once again there is a stellar lineup of speakers. Much care has been taken to devise sessions that have appeal across the Groups. We are confident that all kinds of crystallographer will find a great deal to interest them.

As has become customary in our September issue, we carry a report on the recent meeting of the South West Structural Biology Consortium. This meeting was the lucky 13th in the series, and from the report it is clear that a lot of excellent science was presented and discussed in a collegial spirit. Since we don't get similar reports from other parts of the country, there must be something special about the South West – I wonder if it's the cider!

In keeping with the spirit of the International Year of Crystallography, BCA members have put on a variety of stimulating events to acquaint non-crystallographers with crystallography. Anyone who reads the report will see that busy people have given generously of their precious time to provide the personal contact that makes these events so memorable. Particular credit goes to **Sam Callear**, our Education and Outreach Coordinator, to the enthusiastic Young Crystallographers, especially **Lynne Thomas** and **Anna Warren**, and to eternally-youthful crystallographers like **Mike Glazer**. There still is plenty more to do, and additional volunteers will be welcome.

Our June issue described important enhancements recently made to the Protein Data Bank by the scientists curating it. Their counterparts at the Cambridge Crystallographic Data Centre have also been busy. This issue includes an announcement about the improved Web-based system for depositing structures into the Cambridge Structural Database. Importantly, whether your new structure is published in *Nature* or deposited in the CSD, it will be rewarded with a DOI for easy identification.

I began to write this column shortly after the humbling by Germany of Brazil's football team. This event has left me with the feeling that Brazilians would have ended up much happier if some of the money they lavished on stadium improvements had bought a free-electron laser instead.

With the Scottish independence referendum set to take place shortly after this issue appears, to stimulate forward planning in the event of a "yes" vote I have written an article describing how three crystallographic associations have handled the need to span two nations. The American Crystallographic Association included Canada from its inception. The Czech and Slovak Crystallographic Association stayed together after the amicable separation of the two countries. Even though Croatia and Slovenia remained on generally good terms after the acrimonious and bloody breakup of Yugoslavia, their crystallographic associations divided but still hold an annual joint meeting.

Finally, as the crystallography community celebrates the 100th-ish anniversary of great events, I have a very personal 50th anniversary to mark. It was in October 1964 that I joined the research group of **William N. Lipscomb** and became a crystallographer. He was an inspiring supervisor, and crystallography has inspired me ever since.

Carl Schwalbe

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- Influence on the development of crystallography and the BCA

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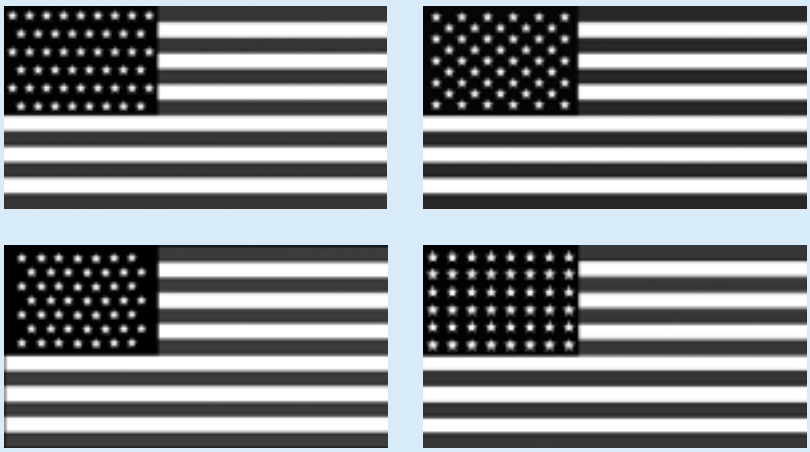
Puzzle Corner

ELSEWHERE in this issue we contemplate the possibility of Scotland leaving the United Kingdom. Things could be different in the United States. In a non-binding plebiscite held in 2012, a majority of Puerto Ricans voted to become a state. This year a bill has been signed into law providing funds to hold a binding referendum. Thus in the foreseeable future an extra star may have to be added to the American flag. A simple grid of 3 x 17 stars is plainly unsuitable, but a more nearly equidimensional arrangement is shown below. Adjacent to it is the current 50-star flag. Also shown are the 49-star flag used briefly when Alaska but not yet Hawaii had become a state, along with the 48-star version used between 1912 and 1959. For a mathematical analysis of designs for various numbers of stars see the website http://danbliss.blogspot.co.uk/2011/11/51-star-flag.html .



What is the symmetry of the union (the star field) in each design? What if the stars were 6-pointed?

(An answer to our challenging June Puzzle Corner will appear in the next issue.)

BCA Spring Meeting March 30th-April 2nd 2015

From the BCA 2015 Programme Committee

THE BCA 2015 Spring Meeting programme is rapidly taking shape with sparkling lectures, scientific sessions and workshops already in place, thanks to the hard work of the Programme Committee. The programme spans a diverse range of scientific sessions covering topical crystallography within each of the BCA groups. The 2015 BCA Named Lectures have been confirmed: the Dorothy Hodgkin Lecture will be presented by Prof Sir Tom Blundell FRS and the Lonsdale Lecture by Prof Simon Parsons. A number of plenary speakers are also already confirmed.

We have increased the biological structures component of the meeting so that it spans all 6 parallel sessions. The layout of the York Exhibition Centre also allows us to run workshops simultaneously with sessions, allowing plenty of choice for delegates.

This year we have scheduled two sessions to capture the recent surge in outreach and education activities by the BCA. There will be an educational lecture during the Young Crystallographers' Satellite Meeting given in a double act by Prof **Mike Glazer** and Prof **Bill Clegg** on the use of International Tables for Crystallography, as well as a session within the main meeting dedicated to the subject of teaching crystallography.

The website http://york2015.crystallography.org.uk/ is live!!!!

Biological Structures Group (BSG)

BSG Plenary. Tuesday pm.
Prof **Gideon Davies**, University of York.
Chair: ***E J Dodson***

BSG sessions

Tuesday Session 1. Drug design.
Chair: ***Dave Brown*** (Kent).

Tuesday Session 2. Data acquisition.
Chair: ***Elspeth Garman*** (Oxford).

Wednesday Session 4. Data Mining – wealth & pitfalls.
Chair: ***Kevin Cowtan*** (York). Kevin.Cowtan@york.ac.uk

Thursday. Session 5. Simultaneous use of EM and MX data.
Chair: ***Garib Murshudov*** (LMB, Cambridge).

Thursday Session 6. Low-resolution refinement.
Chair: ***Keith Wilson*** (York)

BSG Joint Session with Chemical Crystallography Group (CCG)

Wednesday Session 3. Ligand Chemistry.
Chair: ***Ehmke Pohl*** (Durham).
[See details below.]

BSG Workshops under active consideration
CCP4mg. Stuart McNicholas (York), **Keith Wilson**
DIALS. David Waterman (CCP4).
EM and X-rays. Jorge Navaza (Bilbao).
PDBe Roadshow. Sameer Velankar (EBI) –or another EBI person.

Chemical Crystallography Group (CCG)

CCG Plenary. Tuesday lunchtime:
Colin Groom, CCDC.
Chair: ***Simon Coles***

Session 1: Data Avalanche

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

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

Session 2: Automation

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

Developments in areas such as detectors, sources and computing provide powerful drivers for automation in chemical crystallography. Automation also offers exciting opportunities to carry out new systematic scientific studies. This session could include work relating to hardware and/or software to handle higher throughput of structures and results of studies arising from such developments.

Session 3 (Joint with BSG): Ligand Chemistry

Chair: ***Ehmke Pohl*** (Durham University),
Co-chair: to be confirmed

This session is focussed on the interface between chemical

and macromolecular crystallography where structural information from the entire range of crystallography is used to analyse, understand and optimise small-molecular to protein interaction. We welcome presentations describing novel methods and experimental techniques, as well as current examples of important protein-ligand systems.

Session 4: **Problem Data**
Chair: ***Stephen Moggach*** (University of Edinburgh),
Co-chair: ***Jamie Gould*** (University of Liverpool)

Recent advances in crystallographic software and hardware have resulted in significant advances within many areas of crystallographic research. These include time-resolved studies, experiments involving different sample environments and the extraction of detailed information from between the Bragg reflections. We welcome presentations on methods which involve extracting crystallographic information from such sample environments on what are (or once were) referred to as 'problem data'.

Session 5: **Would you publish this?**
Chair: ***Bill Clegg*** (University of Newcastle),
Co-chair: ***Gary Nichol*** (University of Edinburgh)

Keynote: **Larry Falvello** (University of Zaragoza)

This session will have an unusual format. After an opening talk by Professor Larry Falvello from the points of view of a crystallographer, author, and editor, anyone present can briefly describe a structural result that raises the session title question for the audience to discuss. We'll be requesting contributions in advance to avoid total chaos - more detail to follow!

Session 6 (Joint with PCG): **Complementary Calculations**
Chair: ***John Claridge*** (University of Liverpool),
Co-chair: ***Simon Parsons*** (University of Edinburgh)

The use of computational methods has made great strides, both in structure determination, prediction of new structure types and their response to stimuli, providing insight and guidance to experimental studies. We welcome presentations on computational methods used to complement traditional crystallographic techniques to give a deeper understanding of crystal chemistry and physics.

Industrial Group (IG)
Plenary speaker TBA

Wednesday

Session 1 Topic: **Catalysis and advanced characterisation**

Catalysis is estimated to be involved in 90% of all chemical processes and in the creation of 60% of the chemical products available on the market, but still it is rarely analysed at the atomic scale. The need to understand catalysis at this level is driven by both economic and environmental concerns; therefore there is a global interest in optimising the synthesis of new catalytic materials and in understanding the fundamental process of catalysis. In this session we will explore how advanced characterisation techniques are driving innovation in this hugely important sector.

Session 2 Topic (Joint with PCG): **Liquids and Amorphous Materials**
Chairs: Dr ***Christoph G. Salzmann*** (University College London) & Dr ***Spoorthi Dharmayat***

Lacking any long-range order, liquids and amorphous materials are notoriously difficult to characterise structurally. From a technological and scientific point of view they are, however, immensely important classes of materials. The vast majority of chemical reactions is carried out in the liquid state and amorphous materials, such as amorphous silicon, are widely used in industry, for example, in thin-film transistors and photovoltaic cells. This session will highlight some of the recent advances in this area ranging from structural characterisations to the applications of these materials.

Physical Crystallography Group (PCG)
PCG Plenary: Professor **Tony Cheetham** (University of Cambridge)

Phase transitions in metal organic frameworks
Chair: ***Matt Tucker*** (ISIS/Diamond)

Session 1: **"Beyond the elastic line –Resonant and Inelastic diffraction"**
Chair: Dr ***Mark Senn*** (Diamond)

Keynote: **Steve Collins** PBS (Diamond)

This is an interdisciplinary session designed to bring crystallographers together with researchers who come from a background in resonant and inelastic scattering. The aim of the session is to explore the possibilities in crystallography beyond "conventional" charge scattering, and speakers with a background in spectroscopy or an element of spectroscopic measurements in their work are strongly encouraged to apply.

Session 2: **Challenges and technical advances in powder diffraction**
Chair: Dr ***Paul Saines*** (University of Oxford)

Powder diffraction plays a crucial role in the characterisation of functional materials including studies in-situ and at extreme conditions; especially in the many cases where single crystals are unavailable. This session will examine recent developments in techniques and instrumentation alongside cutting edge results in this important field.

Session 3: **"Structural insights into ferroic materials"**
Chair: Prof. ***Phil Lightfoot*** (University of St Andrews)

Keynote: Prof **Pam Thomas** (University of Warwick).

Materials that display ferroelectric, ferroelastic or

(ferro)magnetically ordered states are of widespread technological interest. The nature of these phase transitions, the symmetry breaking that occurs and the possibility of coupling these ferroic orders are the focus of this session.

YCG Satellite meeting:-

Monday pm and Tuesday am

BSG YCs' Plenary speaker: **Susan Lea**
Chair: ***Sam Horrell***

PCG/IG YCs' Plenary speaker: **Bill David**
Chair: ***Jorge Sotelo***

The YCG will have an *International Tables Teaching Session:-*
"Space groups - the final frontier"
Part 1: A voyage into orbit – **Bill Clegg**, Newcastle University
Part 2: Into deep space – **Mike Glazer**, Oxford University

Dorothy Hodgkin Lecturer: Prof Sir **Tom Blundell** FRS

Lonsdale Lecturer: Professor **Simon Parsons**

In summary here are the names of the Group Plenary speakers confirmed thus far:-

BSG Plenary: **Gideon Davies**
CCG Plenary: **Colin Groom**
PCG Plenary: **Tony Cheetham**

Deadlines
The deadline for oral abstract submissions, including submission for the YCG Satellite Meeting, is **Monday 12 January 2015**. The final deadline for poster abstracts is **Monday 2 March 2015**.

The full Programme Committee is:-

- **John R Helliwell** (Chair)
- **Eleanor Dodson** (BSG)
- **Keith Wilson** (BSG)
- **Mike Probert** (CCG)
- **Pete Wood** (CCG)
- **Spoorthi Dharmayat** (IG)
- **Judith Shackleton** (IG)
- **Emma McCabe** (PCG)
- **Paul Saines** (PCG)
- **Horst Puschmann** (Computing and software)
- **Scott McKellar** (YCG)
- **Lucy Saunders** (YCG)
- **Claire Wilson** (BCA Secretary)
- **Richard Cooper** (BCA Vice President)

Dates, Links & Abstract Submission
All the latest information concerning the meeting, including the programme, registration and abstract submission, will become available at the meeting website in due course.

John R Helliwell, Chair of BCA 2015
john.helliwell@manchester.ac.uk
and
Richard Cooper, BCA Vice President
richard.cooper@chem.ox.ac.uk

York Exhibition Centre

American Crystallographic Association Annual Meeting

AS usual in the year of an IUCr Congress, the ACA brought forward its meeting from late July to late May and chose a southern location to take advantage of the more temperate climatic conditions. This year's venue was the Albuquerque Convention Center. Although participants arriving early for the workshops were greeted with uncharacteristically cool showery weather, the sun returned soon enough. Then we had the expected heat, with humidity low enough that it felt comfortable. The Convention Center has just finished the first half of a $20 million renovation programme. The part we occupied looked new and fresh. Our eyes were led to the main entrance by a cheerful mosaic (pictured on the cover), giving a suggestion of blue skies and colourful landscape.

In his Patterson Lecture **John Helliwell** started by reminding us that the 1987 book "Patterson and Pattersons" edited by **J. P. Glusker** et al. and published by Oxford University Press still is a good source of historical insights about the great man and his function. John proceeded to his main topic, the development of synchrotron radiation for macromolecular crystallography. Starting with proof of principle on a "roll your own" crystal of lysozyme wrapped in Mylar, he described how more intense sources made it possible to determine more challenging samples, culminating in virus structures. The introduction of rapid tuning made it possible to obtain good anomalous difference Patterson maps from SeMet proteins. This advance also had spin-offs for chemical crystallography, e.g. work led by **Madeleine Helliwell** which used anomalous scattering to distinguish Ga and Zn, which are adjacent in the Periodic Table. By the mid-1980s new ring concepts were developed and undulators were designed, but some scientists needed to be convinced that crystals could withstand the intense beam they produced. By using the Laue method it became possible to collect a data set in msec from a single bunch. Transient electron density in the active site of hydroxymethylbilane synthase was revealed. The structure of β-crustacyanin, the source of the colouration in lobster shells was determined, taking advantage of the Xe high pressure absorption edge. These concepts were transferred to neutron crystallography by combining "all the talents": the Laue method, Daresbury software, the Grenoble reactor neutron source, and Japanese image plates for neutrons. Thus the protonation state of concanavalin A was worked out at 0.94 Å resolution. John finished by looking to future synchrotron radiation sources and X-ray lasers.

With the topic of "100 Years of Crystallography" the Transactions Symposium followed. **Cora Lind-Kovacs** described outreach activities with the crucial word "fun". These ranged from examining differently coloured quartz crystals and growing crystal gardens to crystallizing lysozyme under guidance from teachers who themselves had been instructed via Skype. Other activities involved fun with diffraction and fun with symmetry. A US crystal growing competition will start in October. Additional events are described at http://www.iycr2014.org/aca/home .

Next, **Martha Teeter** told us about women in crystallography. Thanks to the fair-mindedness of great crystallographic pioneers like the **Braggs** and **J. D. Bernal**, women were given training and career opportunities in crystallography earlier than in most other fields of science. This fine record has been complemented by a recent survey. Questionnaires were sent to 90 female ACA members over the age of 50; answers were returned by 24 of them. Topics under investigation included the origin of participants' interest in science in general and crystallography in particular, the role of mentors, and whether their careers were conventional or unconventional (about 50:50). Of the 24 participants, 19 had children and faced the need to reconcile family and work.

Alexander McPherson directed our attention to the surprisingly long history of protein crystallization. Already in 1840 **Friedrich Hünefeld** crystallized haemoglobin by squeezing worms and letting the drops evaporate. Near the end of the 19th century crystallization was applied as a purification method, and techniques were developed that are still used today. In 1892, by controlling temperature and salt concentration and by using alcohols, the agricultural scientists **Osborne** and **Sumner** crystallized a wide variety of seed globulins. In 1898 the physiologists **Hopkins** and **Pincus** crystallized egg albumin by controlling pH. In the 20th century further important proteins were purified. Eventually these crystals attracted the attention of crystallographers, albeit with no idea about how to obtain the structure. Thus in 1935 **Bernal**, **Crowfoot** and **Fankuchen** obtained X-ray diffraction from a protein crystal (pepsin). The further development of macromolecular crystallography, beginning with structure determinations for myoglobin and haemoglobin, is well known; but it still seems miraculous that all the prerequisites for speedy progress (recombinant DNA technology, cryocrystallography, synchrotrons, area detectors, high speed computers, automated procedures) came together at about the same time.

Helen Berman discussed databases, starting with the reasons for their existence: safe storage, a one-stop shop, preventing accidental duplication and unlocking knowledge through comparisons. She illustrated the concept with three databases: the Protein Data Bank, the Cambridge Crystallographic Data Centre and the International Centre for Diffraction Data. There is a common data pipeline: creation, deposition, processing, validation, distribution, analysis and visualisation. The funding models differ, but all three databases have to deal with an increasing torrent of data and face challenges about future support.

Among the afternoon sessions "Industrial Research from Young Scientists" was particularly attractive because of the subject matter, the strong BCA participation and the enthusiasm of the presenters. **Rajni Bhardwaj** introduced the antipsychotic drug olanzapine, which causes problems for pharmaceutical scientists because it can crystallize in metastable forms and many different solvates. Experimental or theoretical work alone is insufficient; but by combining extensive experimental screening with crystal energy landscapes, insight can be obtained. Statistical modelling and

PIXEL calculations help to explain the packing in different physical forms, and structural relationships between crystal structures help to provide a mechanism for desolvation.

Jacob Trotta presented the polymorphism of dehydro-aripiprazole (dAPZ), which is also an antipsychotic drug. It has 5 polymorphs, 2 polymorphic methanol solvates and a monohydrate. The melting points and heats of fusion were obtained by differential scanning calorimetry, and the stability of various forms was evaluated with slurry experiments. Stability was found to follow density. Polymorphs of the related molecule aripiprazole (APZ), which only differs by one double bond, include both dimers and catemers. The polymorphs of dAPZ include only dimers, but there is a diversity of conformations.

Ghazala Sadiq also discussed a polymorphic system, p-aminobenzoic acid (PABA), but with the objective of obtaining a desirable form. The alpha polymorph is commercially available and stable above 13.8°C, but it has poor morphology. The beta form had only been nucleated from aqueous slurry at 5°C but never from organic solvents. A search of the Cambridge Structural Database gave 71 hits, of which 46 were cocrystals. Examination of the interactions suggested that nitromethane might be a suitable organic solvent for crystal-growing. Although it still produced the alpha form, the resulting needles were of much better quality.

Puja Pathuri turned our attention to drug design by fragment screening. The target is a very important enzyme, HCV-NS3/4a. This multifunctional protein is indispensable for replication of hepatitis C virus through its involvement in polyprotein processing, RNA replication and viral assembly. Small molecule inhibitors that bind to its protease active site have been found, but some quasi-species are resistant to them. Making use of the crystal structure of the full length protein, fragments were offered to the protein and the resulting structures were screened for binding at the protease-helicase interface. The first fragments in any trial are likely to bind very weakly; and with an ability to detect binding of 10 mM inhibitors, X-ray crystallography is better than any other method. In the present study a ≈500 μM hit was found. This structure was optimised to fill a small pocket and to induce a twist that better followed the binding site. Mutant generation confirmed the mechanism.

Christopher Bianchetti made us think in a new way about the selectivity of enzymes with respect to the hydrolysis of biomass. While our mind-set tends to appreciate an enzyme that performs one function spectacularly well, to the exclusion of anything else, his application area requires the exact opposite, multifunction enzymes. Plant biomass comes to a processing facility from a variety of sources. Its cellulose needs to be broken down, but so too must the hemicellulose and lignin accompanying it. This can be achieved by adding a cocktail of many enzymes, but the cost and the complication of the process can be reduced by combining more than one active site in one protein. Automating the step from gene to protein and testing the resulting enzyme for activity shows promise for widening the range of applicability.

Two lectures particularly caught my attention on the second day. Having spent a lot of time in the 1970's and 1980's working on dihydrofolate reductase (DHFR) inhibitors, I was fascinated to see how neutron diffraction and ultrahigh-resolution X-ray diffraction have advanced our understanding of this vital enzyme. Even more impressively, this was only a spare-time project for **Qun Wan** at Oak Ridge. Crystal quality and size were improved by microseeding and macroseeding. Neutron data to 2.0 Å were collected on DHFR with bound folate and $NADP^+$. The results clarified the protonation state of ionisable groups: N3 of folate is protonated but N5 is not, and Asp27 of DHFR is ionized. The region around Met20 is very dynamic, enabling water on a partially occupied site to form a hydrogen bond to N5.

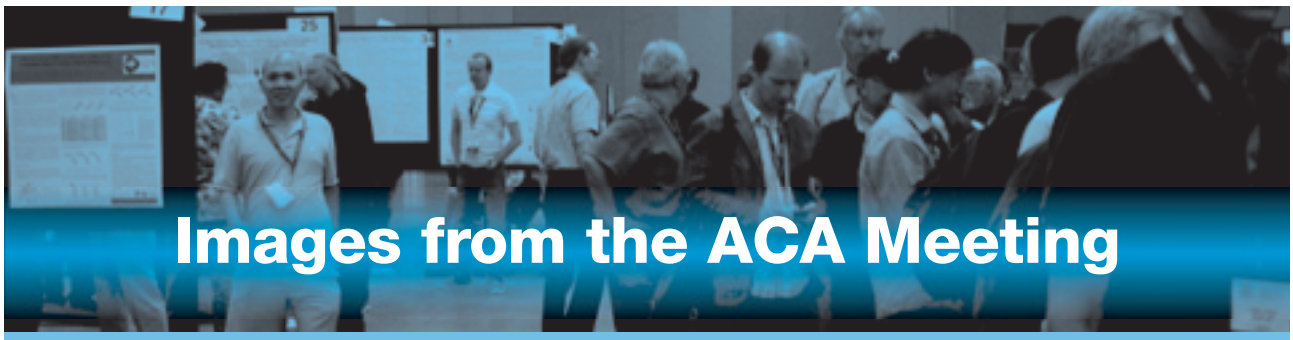
Harry Powell began a "blackboard session" about iMosflm with two maxims of wide applicability, particularly for postgrads and postdocs. (1) You took months to clone/express/crystallize your protein, so take some time to think about your data. (2) You may fail; if your Principal Investigator had been certain of success, he'd have done it himself. As an example Harry took a structure of trypsin inhibitor, possibly with trypsin, that gave better statistics in C2 than in $P4_3$, but only the latter yielded a molecular replacement solution (with no trypsin). Pseudo-merohedral twinning was suspected. Hints and tips included the following suggestions. Since Mosflm uses the headers, it is worthwhile looking at them. If some numbers look wrong, they probably are wrong and will mislead Mosflm unless corrected. Scaling programs hate reflections obscured by the beam stop. The human eye is very good at evaluating symmetry in simulated precession photos.

On the final morning a "Cool Structures" symposium was held once again, presenting structures thought to be "cool" but not necessarily measured at low temperature. **Muwei Zhang** started the session by describing the symmetry-guided synthesis of highly porous MOFs. The crystal structure of zinc acetate was taken as a starting point, to be turned into a framework with linkers. However, the rational design of MOFs is challenging because sometimes the same metal and the same ligand may give different frameworks, or frameworks may interpenetrate. Careful attention to framework topology has enabled the design and synthesis of Zr-MOFs with exceptional stability.

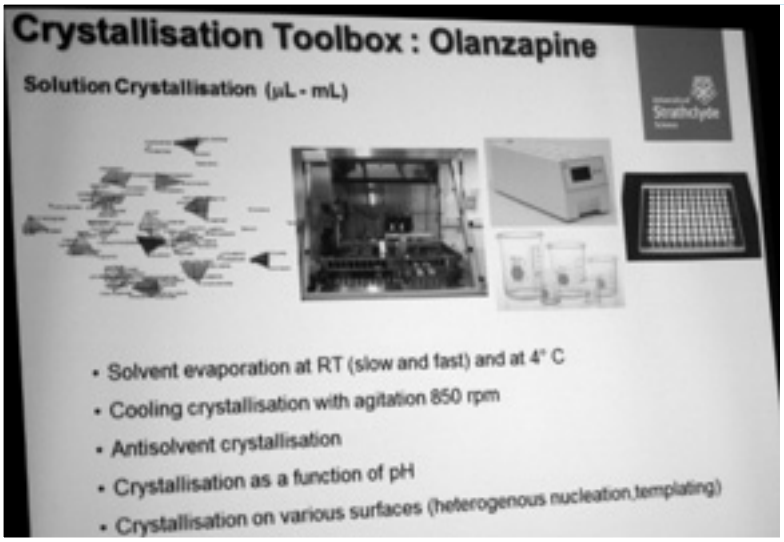
I gave the last lecture before lunch. Perhaps because of my slightly salacious subtitle "A Marriage or a Ménage à Trois", not too many people left early to beat the queues. I compared carboxylate salts of amines where crystal structures are known for both the 1:1 salt and the cocrystal of this salt with an extra molecule of neutral carboxylic acid.

The General Interest session in the afternoon was… interesting. The final presentation by **Larry Falvello** entitled "When the Unseen Hydrogens are the Most Interesting Atoms in the Structure" retained a large audience. Nowadays it is expected that a high-quality structure determination will include the location of all hydrogen atoms. Examining a series of more or less distorted transition metal citrate hydrate cubanes, Larry and coworkers found this a difficult-to-impossible task. Neutron diffraction on D19 at ILL provided some useful information. A manganese complex containing 30 water molecules, 21 of which were Mn-bound, demonstrated complete exchange of D_2O for H_2O at all 30 sites upon exposure to a D_2O atmosphere. There are no channels, but chains of hydrogen-bonded water molecules, "water wires", are present. The difficulty of finding H atoms provides evidence for partial occupancy of the H sites in these chains in accordance with a double-well potential and/or a Grotthuss mechanism. The latter mechanism was percipiently postulated by the nobleman Freiherr **Christian Johann Dietrich Theodor von Grotthuss** already in 1806. In modern terms, it involves one H_2O passing a proton to the next water O atom, which in turn passes a different proton to the next O atom, and so on.

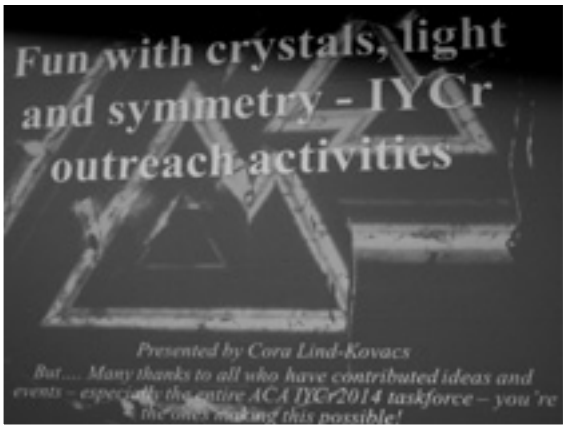
Carl Schwalbe

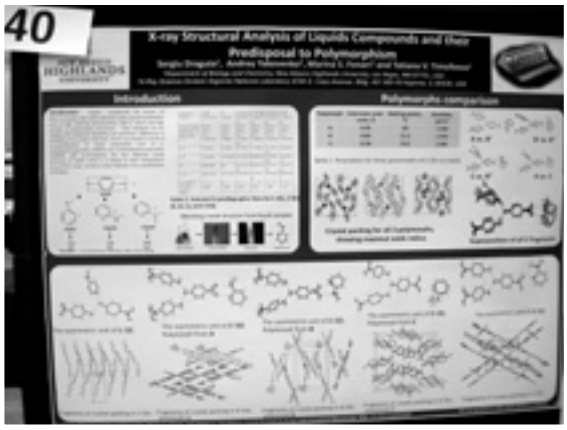


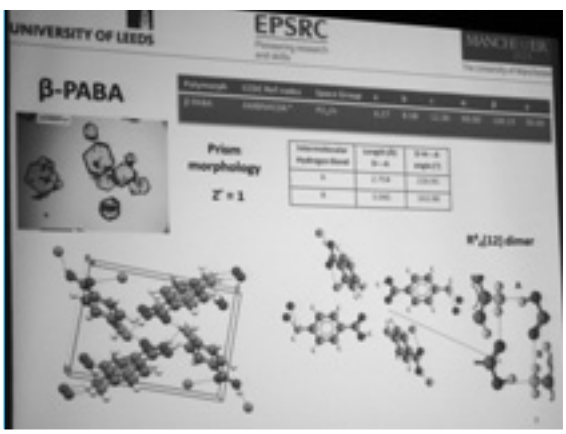
Images from the ACA Meeting

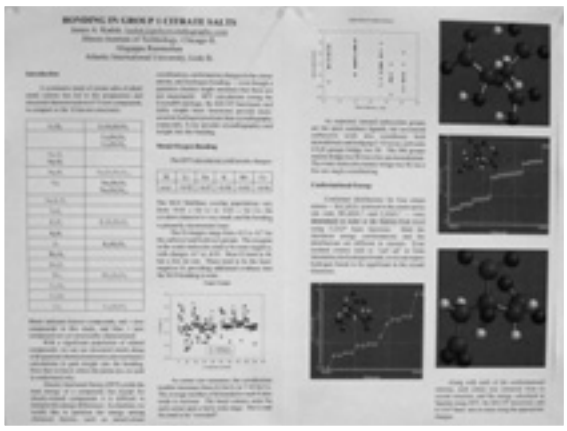



Rajni Bhardwaj









Southwest Structural Biology Consortium

THIS year's annual meeting of the South West Structural Biology Consortium (SWSBC) was held in Bath on June 23-24. For the 13th time researchers from the South West region convened to discuss the latest developments in structural biology. The meeting with over 100 delegates was hosted by the Department of Biology & Biochemistry at the University of Bath and organized by Susan Crennell and Jean van den Elsen.

The SWSBC meetings are a platform for PhD students, postdocs and group leaders at an early stage in their careers to present their work to a larger audience and to enable them to network with other scientists across the region, whilst enjoying the local hospitality. There were 13 talks from junior researchers and 48 poster presentations, with a large and involved audience despite the unsually warm and sunny weather. The high quality of the talks and posters, especially those from junior researchers, was very encouraging and demonstrated that the structural biology community in the South West is thriving. Congratulations to **Shalini Iyer**, a postdoctoral researcher from the University of Bath, who won first prize for her poster on the structure and function of aminopeptidase P-1 from *C. elegans.* Second prize was for **Catherine Back** from the University of Bristol, for her poster on the structure and function of *Streptococcus* adhesion CshA, and **Halina Mikolajek** from the University of Southampton came third with her poster on the structural basis of eEF2K activation by calcium/calmodulin. Representatives from 4 companies sponsoring the meeting also presented updates on recent developments in structural biology technologies.

Dr **Ivo Tews** from the Centre for Biological Sciences at the University of Southampton and Dr **Charles Ballard** from CCP4 provided an overview of the current state of the CCP4 suite and gave an update on some exciting future plans. The program for the next CCP4 workshop was also revealed. This year's plenary speaker, Dr **Marisa Martin Fernandez** from the Central Laser Facility at the Rutherford Appleton Laboratory in Oxford gave an interesting talk on the potential of fluorescence lifetime imaging –resonance energy transfer as a tool for studying the architecture of large molecular complexes. She described the use of this technique to reveal intriguing insights in the molecular details of the aggregation states of the human epidermal growth factor receptor (EGFR1/HER1) and the complex mechanisms by which these molecular clusters might regulate the onset of EGFR signalling.

*The prize for the best poster was presented to Dr **Shalini Iyer** (left) by Dr **Chris Pudney** (right)*

We can look back at another successful meeting, made possible by generous sponsorship from CCP4, the BCA Biological Structures Group and the commercial exhibitors, and we look forward to the next meeting, which will be held at the University of Sussex.

Susan Crennell and **Jean van den Elsen**
University of Bath

SWSBC 2014 group photo

Education & Outreach Update

IN June the BCA Education and Outreach team attended the Times Cheltenham Science Festival. This was our first time attending this festival and it was a great success targeting a different audience to our previous events – these ranged from family groups to the retired! We held two events during the weeklong festival. The first of these was in collaboration with the British Society of Immunology, and was entitled 'The Immune System: Your Inner Army'. This comprised of a fantastic hour-long discussion session chaired by Vivienne Parry with Prof Susan Lea (University of Oxford) and Prof Clare Bryant (University of Cambridge) explaining how important crystallography is to elucidating the structures of many of the proteins which are used in deciphering how our immune system works. They both gave fantastic explanations of crystallography and the immune system, with the audience asking some very informative questions at the end. The structures of the compounds were explained using 3D printed models to explain how certain molecules behave and function due to their shape with the help of Jamie Heather (UCL).

Our second event was held over the weekend, where we had an interactive stand for visitors over 14 years old who could come and get involved. The stand was based on our "Structure of Stuff is Sweet" exhibit developed for the Big Bang Fair. It was incredibly popular and we were constantly being bombarded with enthusiastic visitors! We taught our visitors how to carry out diffraction experiments using the Lego beamline, and how they can grow their own crystals, teaching them how to crystallise the enzyme lysozyme. Finally we explained why this technique is so important to elucidating the structure of materials, and why it's key to know these structures to understand how a material might function. This

weekend event would not have been possible without our fantastic and endlessly enthusiastic volunteers, so our thanks go to **Claire Wilson**, **Jonny Brooks-Bartlett**, **Peter Canning**, **Nick Funnell**, **Mike Glazer**, **Matt Tucker**, **Sam Callear** and **Helen Playford**.

These events require a huge amount of support, without which it would not be feasible to attend. We are therefore hugely thankful to STFC, ISIS, Astex Pharmaceuticals, the Young Crystallographers Group and Rigaku.

Lynne Thomas and **Anna Warren**

The next BCA Outreach event will be on the ***24th and 27th September at the Gravity Fields Festival in Grantham***. On Wednesday 24th September **David Price** from Diamond Light Source will be giving a talk about the science carried out at DLS and the BCA stand will have its usual hand-on activities to complement his talk for the school children attending. On the 27th September there is a Family Science Day where Grantham will be transformed with science workshops, displays, exhibitions and story-telling for all the family. For more information, or if you are interested in volunteering for either or both of the dates please get in contact with us on education@crystallography.org.uk .

As always, if you're interested to learn more, check out our website (learn.crystallography.org.uk), Facebook (British Crystallographic Association Education and Outreach) or Twitter (@Whatsinacrystal) accounts and get in contact with us on education@crystallography.org.uk .

Sam Callear
BCA Education and Outreach Coordinator

Illuminating Atoms

AN upcoming photography exhibition in the Royal Albert Hall called 'Illuminating Atoms' will explore the science and the people behind crystallography in the UK. These photographs will be on display to attendees at concerts between Monday 4th November 2014 to Sunday 7th December 2014. There will also be three open days on Saturday 15th, Sunday 16th and Saturday 29th November for members of the public and curious crystallographers to view the wide range of portraits and reportage shot by photographer Max Alexander.

The idea of the exhibition is to reflect the vibrant nature of crystallography in the UK and so it covers both established scientists and young crystallographers, as well as covering crystallography in academic laboratories, industry and central facilities. The exhibition has been very kindly sponsored by STFC, Wellcome Trust, GlaxoSmithKline, Astra Zeneca and Diamond Light Source, and we are very grateful to them for their assistance.

It is hoped that after November the exhibition will tour about the UK and BCA members will be updated about this in future *Crystallography News* editions. The BCA website will be updated regularly in the run up to the exhibition but the pictures alongside are a sneak preview just for BCA members!

Claire Murray

Media Supporting IYCr2014

OUR International Year celebrations have stimulated the dissemination of crystallographic information in various media.

Nature Milestones in Crystallography has just launched. Produced with support from the IUCr and the worldwide network of neutron and X-ray sources, the supplement has been timed to coincide with the International Year of Crystallography, and features 25 topics that have been specially selected to highlight the breadth of crystallography.

The American Crystallographic Association History Project showcases and preserves the history of crystallography and X-ray diffraction through online access, articles in ACA RefleXions quarterly newsletter, and archival at the Niels Bohr Library and Archives in College Park, MD. The History Portal is accessible at http://www.amercrystalassn.org/history_home .

Recent additions include the following 3 items:

The 1988 Nobel Laureates Symposium

Held during the ACA meeting in Philadelphia, the session was chaired by Linus Pauling and featured lectures by five Nobelists – Sir John Kendrew, Dorothy Crowfoot Hodgkin, William N. Lipscomb, Herbert H. Hauptman, and Jerome Karle – as well as introductory and concluding comments by Pauling.

Alexander McPherson, **"Let Us Now Praise Famous Men"**

Alex accepted the 2013 Fankuchen Award on behalf of Richard E. Dickerson at the 2013 ACA meeting in Honolulu, HI and presented a lecture summarizing the work of Dickerson and other 20th century crystallographers.

Thomas C. Terwilliger, **"Molecular replacement and model-building using distant homology models as templates"**

In this video of his ACA Kenneth Trueblood Award presentation Tom describes a combination of modeling and electron density fitting, and introduces a technique he calls "morphing".

The American Crystallographic Association and American Chemical Society have co-produced a 40-minute webinar entitled “Crystallography Frontiers: How Chemistry Reveals the Wonder of Everyday Materials”. The two very likeable presenters, **Cora Lind-Kovacs** and **Jim Kaduk**, refer to the structures of a variety of materials ranging from diamond, graphite and peanut butter to high-tech catalysts and drugs. Thereby they painlessly introduce quite a lot of crystallography to people with background knowledge of chemistry. ACS webinar archives are available as an exclusive benefit for ACS members, but at the time of writing I was able to access this video via the ACA website **http://www.iycr2014.org/aca/home** , and clicking button number 6 in the box “ACA Celebrates International Year of Crystallography”.

Readers of *Crystallography News* will remember an article about phytochemicals and crystal structures that appeared in the December 2012 issue. This has now been expanded into a book, ‘Molecules, Medicines and Mischief: A Year on the Chemical Trail around Cambridge University Botanic Garden’ by **Gwenda Kyd** (text) and **Mo Sibbons** (photos); Vervain Publishing; 164 pages; ISBN 978-0-9928998-0-6; £12.99. This book includes information on 26 plants from the Chemicals from Plants Trail, each of which contains a structure which is in CSD. The 26 entries are separated by “any year” diary pages to form “a year on the chemical trail”. For stockists or to order online go to **www.cambridge-bach.co.uk/vervain-publishing** .

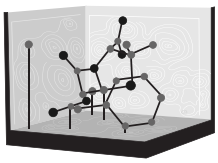
Carl Schwalbe

Another Durham School to take place next year

THE renowned Intensive Schools on X-ray Structure Analysis have inspired emulation by other crystallographic societies throughout the world. They are remembered by their alumni with a mixture of affection for the warm and collegial atmosphere and pride at having mastered a breadth and depth of knowledge that they might previously have thought to be unattainable.

Information about next year’s Intensive School, to be held once again at Durham University, is given below. The timing and location will be particularly convenient for participants. The School will finish on March 29th. The BCA Spring Meeting will commence with the YCG Satellite Meeting, as usual, on the afternoon of March 30th at York University, just 123 km away – little more than walking distance for fit Young Crystallographers!

Dorothy Hodgkin Commemoration Symposium



Dorothy Hodgkin
SOMERVILLE COLLEGE

UNIVERSITY OF OXFORD

2014 international year of crystallography

The Dorothy Hodgkin Commemoration Symposium will be hosted by UNESCO, the IUCr and Somerville College in Oxford on Wednesday, 29th October. The symposium will mark the 50th anniversary of Dorothy Hodgkin's Nobel Prize for Chemistry, and you are warmly invited to attend.

The Symposium will feature a number of distinguished speakers, among them **Professor (Sir) Venki Ramakrishnan**, winner of the Nobel Prize for Chemistry in 2009.

Key topics will include the legacy of Dorothy Hodgkin, the development of crystallography over the past century, how it is addressing pressing global issues today, particularly in health and medicine. Women in science will also be a key focus.

Please register your interest at **development.office@some.ox.ac.uk** and further details will be forthcoming.

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

BCA Industrial Group Autumn Meeting

"Crystallography in Industry"

The Royal Institution, London
12-13 November 2014

More information will become available at
https://sites.google.com/site/bcaindgrp/meetings/autumn-meeting-2014 .

The Cambridge Crystallographic Data Centre - Making it easier to deposit data into the CSD

The Cambridge Crystallographic Data Centre (CCDC; www.ccdc.cam.ac.uk) launched a new improved service in June 2014 to make it easy and fast for researchers to deposit their structural data at the CCDC.

THE CCDC creates and distributes the Cambridge Structural Database[1] (CSD), the world's repository of small molecule crystal structures, so that the crystallographic community can store and share their structures with scientists across the globe. Since the inception of the CSD nearly 50 years ago the CSD has grown considerably and now contains over 730,000 entries; the complexity of these entries is also on the increase. As the size of the CSD has grown, so too has the number of depositions, revisions and publications that go alongside the entries in the CSD. Today nearly 10,000 different individuals deposit data at the CCDC every year – a record 9622 structures were processed into the CSD during the month of May 2014 alone. This figure demonstrates how much the crystallographic community has advanced since 1990 when fewer than 9,000 small molecule crystal structures were published in the entire year. With all these structures and so many depositors storing data at the CCDC, it is essential there is a quick easy process to deposit data and ensure that high quality, comprehensive structural data is made more readily available to the scientific community.

The new deposition process

The CCDC launched its new CSD web-based data deposition facility (www.ccdc.cam.ac.uk/deposit) on the 23rd June 2014 to address these challenges, making the whole process of depositing small molecule data faster, easier and more intuitive[2]. The service incorporates the CCDC's enCIFer syntax checking and editing functionality to enable straightforward review and correction of deposited CIFs. This makes the process more efficient for depositors, and also ensures the integrity of the data stored at the CCDC for the world's community of structural chemists. To further ensure the quality of the crystallographic data and to help with the peer review process, the inclusion of structure factors is now a prominent part of the deposition. In addition to this, users are able to review, edit and add to the metadata during the process. This ensures the quality of the metadata received and provides the community with a more enriched CSD entry. The CCDC has plans to build on this new deposition process in the coming months; one of the many enhancements on the horizon is to incorporate sophisticated CCDC diagram generation code.

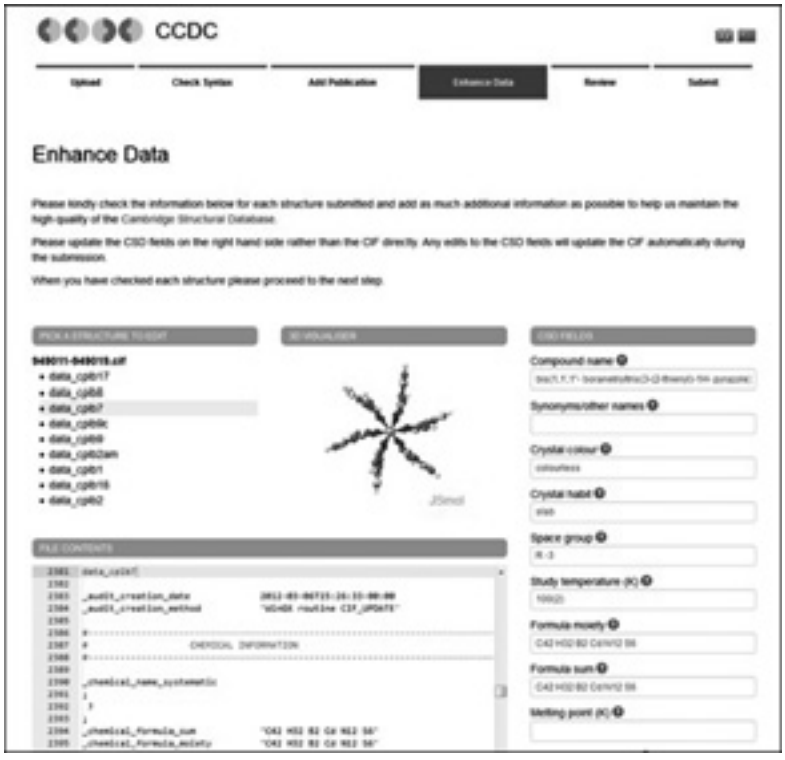


Figure 1: The new deposition process allows users to easily check and update the metadata during the process.

"Depositors will be delighted to discover how quick and easy it is to deposit their data with the CCDC now that the new, interactive, web-based data deposition facility has been launched. The IUCr is particularly pleased that the new process highlights the importance of including structure factors in the deposition process which should help to ensure the quality of the reported science" said **Peter Strickland**, Managing Editor at the IUCr.

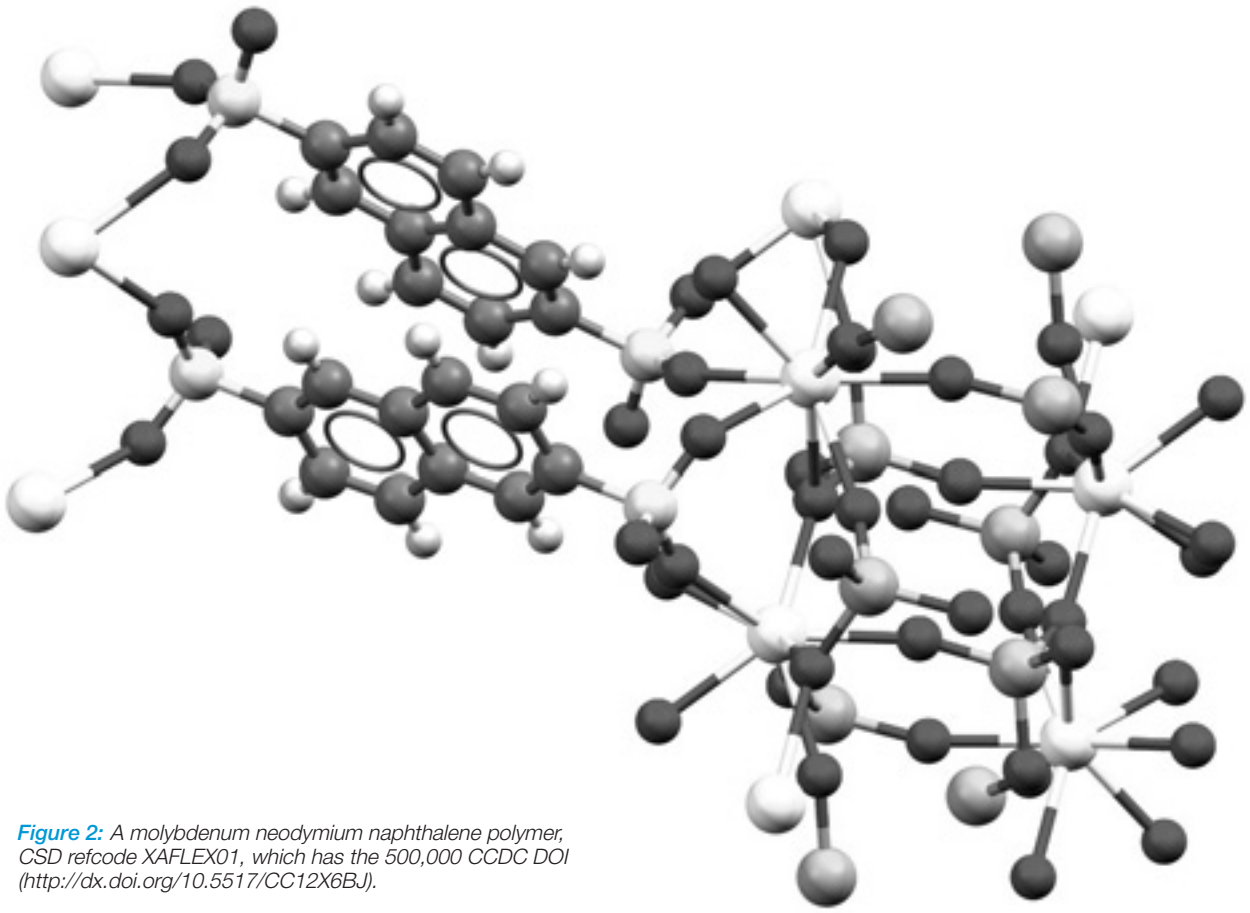


Figure 2: A molybdenum neodymium naphthalene polymer, CSD refcode XAFLEX01, which has the 500,000 CCDC DOI (http://dx.doi.org/10.5517/CC12X6BJ).

Maximising accessibility of crystallographic data

The new deposition form is just one of the latest developments of an ongoing process to maximise accessibility of crystallographic data from the CCDC. We have been working with DataCite (**http://www.datacite.org/**), and in March 2014 the CCDC started assigning Digital Object Identifiers (DOIs) to datasets of crystal structures deposited with the CCDC[3]. Now over half a million CCDC data DOIs have been assigned. Not only do DOIs provide a stable linking mechanism that helps ensure the preservation of data, they also provide a way to increase the discoverability of data. For example, the CCDC will be utilising the workflow that was developed between DataCite and Thomson Reuters to populate the Data Citation Index (**http://wokinfo.com/products_tools/multidisciplinary/dci/**). The metadata available through DataCite also allow authors in the CSD to add data to their researcher or institutional IDs to make sure the appropriate credit is received for data as well as publications.

The CCDC is committed to adding to the array of free services that are available to the scientific community, to aid the discoverability of research data. With the April 2013 launch of CSD-Xpedite[4], the new infrastructure used to manage depositions and process entries into the CSD, the CCDC is now prepared for the rapid growth of the CSD into the next decade. The crystallographic community is now able to experience some of the benefits of this new architecture with the release of CCDC DOIs and the new deposition process. Furthermore the CCDC is looking forward to expanding the opportunities for crystallographers world-wide to gain high value insights from their experimental data.

[1] F. H. Allen, *Acta Cryst.*, B58, 380-388, 2002 "The Cambridge Structural Database: a quarter of a million crystal structures and rising" DOI: 10.1107/S0108768102003890

[2] http://www.ccdc.cam.ac.uk/NewsandEvents/News/Pages/NewsItem.aspx?newsid=29

[3] http://www.ccdc.cam.ac.uk/NewsandEvents/News/Pages/NewsItem.aspx?newsid=28

[4] http://www.ccdc.cam.ac.uk/NewsandEvents/News/pages/NewsItem.aspx?newsid=23

Suzanna Ward
Manager – Cambridge Structural Database, CCDC

The PANalytical Award supports young scientists

PANalytical is a Corporate Member of the BCA and one of the world's leading suppliers of analytical X-ray instrumentation and software. The company embarked on an initiative to reward young scientists that have demonstrated innovative thought to their research when using an X-ray analytical technique with a €5,000 prize. There are no restrictions on the manufacturer of the X-ray equipment that was used.

Ms. **Ana Cuesta**, affiliated to the Department of Inorganic Chemistry, University of Málaga (Spain) was elected as winner of the PANalytical Award 2013 for her splendid investigation of yeelimite, the most important phase in calcium sulfoaluminate cements. She is currently working on her PhD thesis and plans to invest the prize money in furthering her education.

The winner of the first PANalytical Award in 2012, Dr. **Thomas Bennett**, appreciated the international recognition of his work in X-ray diffraction, provided by the award. *"Shortly after the award, I was elected to a highly competitive research fellowship at Trinity Hall, University of Cambridge. I was able to use the PANalytical award as evidence of my international standing, which can prove crucial in setting young academics apart from one another."*

The PANalytical Award has now been launched for the third year in a row. The winner of the award would have published a paper that appeared in print during the period from 1 January 2013 until 1 December 2014 and that demonstrates groundbreaking thinking in a topical field. The prize will be decided by a selection committee that includes established research scientists unaffiliated to PANalytical.

Applying for the award is easy via www.panalytical.com/award, with a closing date of 1 December 2014. Correspondence or questions about the award can be addressed to award@panalytical.com .

Sybille Franken
PANalytical

UK delegates waiting for the start of the IUCr General Assembly

(L-R:) Richard Cooper, Claire Wilson, David Keen, Alex Griffin, Sandy Blake

THE Congress of the International Union of Crystallography is not just an occasion for exciting science and pleasant socialising. Many items of routine business, such as reports from the IUCr Commissions, need to be formally adopted; and every so often the monotony is broken by a contentious item. The venue for the IUCr Congress six years hence is always hotly contested; and, in addition, a new slate of officers has to be elected. These administrative tasks are accomplished in General Assembly sessions extending over 3 evenings. The UK has the benefit of 5 votes, making us one of the heavyweight delegations, but that power can only be wielded if we put forward our full complement of 5 delegates.

At the Montreal Congress this was not easy since these meetings ran alongside the poster sessions. Therefore we were allowed to appoint alternate delegates who could take over when primary delegates had to be elsewhere. Our first 5 delegates are shown here in a happy mood, along with one of the extremely rare glasses of beer exclusively on offer to delegates at a generally dry conference.

(Picture posted on Twitter on August 6 by **David Keen**)

Young Crystallographers Group Update

OVER the last few months, the Young Crystallographers Group (YCG) has been busy planning for the YC satellite meeting, which will be held on the 30th March 2015, directly before the BCA Spring Meeting. We have two excellent plenary speakers in the form of Prof **Susan Lea** (University of Oxford) and Prof **Bill David** (University of Oxford/ISIS). Prof Lea is a Professor of Chemical Pathology with research interests in structural biology and host-pathogen interactions. Prof David has a range of interests, most recently publishing high-profile work on hydrogen production from ammonia. Together, these plenary talks will touch on biological, chemical, physical and industrial crystallography themes and provide a great start to what we are sure will be a broad and exciting meeting. In addition, Prof **Mike Glazer** (University of Oxford) and Prof **Bill Clegg** (Newcastle University) will be delivering a two-part lecture on space groups, where they will take the audience on a journey through crystallographic symmetry and the use of International Tables. Lastly, the 2015 Lonsdale Lecture, taking place in the main meeting, will be delivered by Prof **Simon Parsons** (University of Edinburgh), whose research interests include absolute structure, twinning and high-pressure crystallography, to name a few.

University of Edinburgh's School of Chemistry at the 'Crystal Chemistry' stand

The YCG would like to remind delegates that there are Arnold Beevers Bursary funds available for students and postdocs to attend the conference (**http://crystallography.org.uk/prizes/bursaries/abbf-bursaries**). Finally, a reminder to the readers of *Crystallography News* that attendance of the YCG Satellite meeting is not exclusive to 'young' crystallographers – all ages and research disciplines are most welcome!

In addition to meeting planning, YCG committee members have been doing their bit at outreach events such as the Cheltenham Science Festival (discussed on page 13) and the Edinburgh International Science Festival. Over the first two weeks of April, the University of Edinburgh's School of Chemistry set up the 'Crystal Chemistry' stand and had great success in bringing crystallography closer to more than 12,000 visitors.

Monica Hoyos-Flight and **Sophie Thurlow** took charge of the organisation of the stand and numerous volunteers, including the YCG committee members **Claire Hobday** and **Jorge Sotelo**, ran a wide variety of hands-on activities and workshops to show kids and adults alike the many wonders crystallography has brought to us in the last 100 years. From growing their own crystals to understanding the process of diffraction, using laser pens and diffraction gratings, visitors engaged with great enthusiasm in the different activities. In particular, the Chocolate Alchemy workshop was very popular, giving everyone a tasty opportunity to appreciate the different properties of the polymorphs of chocolate. Overall, the Crystal Chemistry stand was very well received and when visitors were asked to vote on their favourite event of the festival, Crystal Chemistry came out on top!

Scott McKellar
University of Edinburgh

Scottish Independence Referendum

ON September 18 our Scottish members will take part in one of the most important votes in our lifetimes: the Scottish independence referendum. While the fate of the BCA if Scotland becomes independent is unlikely to be uppermost in voters' minds, it can still be useful to Scottish scientists, and to the wider BCA, to consider three examples of cross-border crystallographic activity.

The American Crystallographic Association is different in one important respect: its foundation in 1949 came a full 173 years after the separation of its member countries, Canada and the United States. Thus the political relationships were firmly established. However, the ACA had to address a question that would also be relevant to the BCA: how to create an equitable relationship between a less populous member nation (Canada, 35 million) and a much more populous one (USA, 314 million). The ACA has a Canadian Division which elects its own officers and operates much the same as a Special Interest Group (SIG) in that they help organize sessions of interest to the Canadians (almost all of which overlap with sessions of interest to the full membership) and they sponsor a Poster Prize in memory of Louis Delbaere. They also have a full voting seat on the ACA council as one of the six Council Officers – they have to find their own candidates – and only Canadian members can vote for that position.

The problem of disparities between the Canadian and US dollars is more apparent than real. The ACA finesses the currency issue by using credit cards for dues and meeting fees – basically the same way as for dues/registration from anyone outside the US. A greater difficulty is the question of tax relief if a Canadian member makes a donation to one of the ACA funds, which are registered as US charities. According to a Canadian accountancy firm's tax guidance website, charitable donations by Canadians to US charities may qualify for Canadian tax relief, but the donor has to have US-source net income that is taxable in Canada.

When Czechoslovakia underwent its "velvet divorce", the populations of the two component republics were more similar: Czech Republic (10.5 million) and Slovakia (5.4 million). The Czech and Slovak Crystallographic Association (CSCA) remained a unified body. However, two institutions particularly renowned for their excellence in crystallography, the Charles University and the Academy of Sciences, were both located in Prague; and there still appears to be a degree of Czech dominance in this transnational society. The President, Vice-President and Secretary of the CSCA all come from the Czech Republic. The Regional Committee is more balanced, with 4 Czech and 3 Slovak representatives; but the 7 most recent annual "Kolokvium – Struktura" meetings organised by the CSCA have taken place in the Czech Republic.

The disintegration of Yugoslavia was very far from amicable and broke the country into multiple pieces. Prior to this convulsion the Yugoslav Centre of Crystallography functioned under the auspices of the Yugoslav Academy of Sciences, located in Zagreb. Clearly this has given Croatian crystallography a strong heritage. In the successor nations the crystallographers of Croatia (population 4.3 million) and Slovenia (2.1 million) maintained the closest relationship. Even so, they did not stay together in a unified society. With its membership of approximately 100 the Croatian Crystallographic Association (CCA) is strong enough to make a successful bid to host the European Crystallographic Meeting in 2015, which will be held in Rovinj, not far from the border with Slovenia. On the other hand, the Slovenian Crystallographic Society (SCS) became a division of the Slovenian Chemical Society. The CCA and SCS still hold a joint "Slo-Cro" meeting every year, its venue alternating between the two countries.

These three examples give us something to ponder in the event of a "Yes" vote for Scottish separation. I am grateful to **Judith Flippen-Anderson** for information about the ACA.

Carl Schwalbe

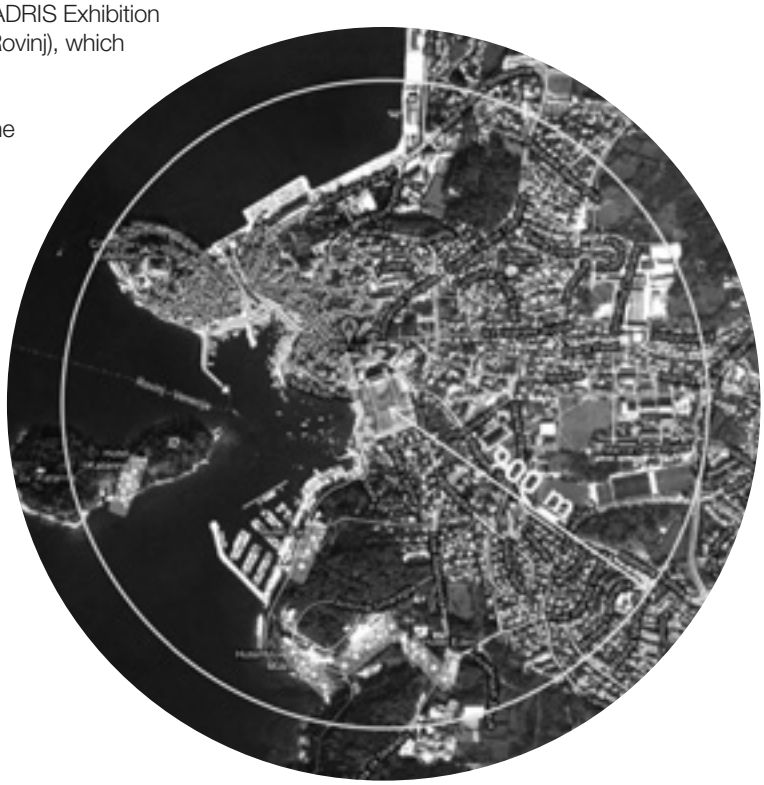
The 29th European Crystallographic Meeting

Venue

NEXT year's ECM will be held in a town that can be regarded as the most romantic place in the Mediterranean! On the magnificent coast of Istria (Croatia), right below the Lim Fjord, is Rovinj. It began its life on an island, its restricted area resulting in crowded houses, narrow streets and small squares, still untouched by modern urbanism.

Rovinj is accessible from a number of convenient airports. **Pula Airport** is located only 40 kilometres from Rovinj. It is connected via Zagreb with almost all major European capitals. **Zagreb Airport** is located 262 km from Rovinj. Other options include **Ljubljana Airport**, located 205 km from Rovinj, and **Trieste Airport**, 147 km from Rovinj.

The sessions of ECM29 will be held at the AECC – ADRIS Exhibition and Convention Centre (the old tobacco factory of Rovinj), which represents an extraordinary example of the industrial architecture of the late 19th century. It is only a few minutes' walk from a dozen hotels as well as from the majestic old town (all within a circle with a radius of 900 m). The complex includes a modern concert hall and the art gallery, the tobacco museum, and exhibition areas suitable for organization of various events at a large scale.



Abstract submission

The abstract submission deadline is **March 23rd, 2015**. Abstracts should be submitted via the website **http://ecm29.ecanews.org/programme/abstract-submission/**, where the guidelines for the online abstract submission will be available.

The abstract submission is independent of the registration procedure. However, the presenting author **must be registered** at the conference **at the latest by May 23rd, 2015**, in order for his or her abstract to be included into the programme book and book of abstracts. One registered participant can be the presenting author at only one submitted abstract. However, every participant can be a non-presenting co-author on an unlimited number of abstracts.

Registration

ECM29 has six registration fee categories:

- **category 1:** individual members of the European Crystallographic Association,
- **category 2:** delegates who are NOT individual members of the European Crystallographic Association,
- **category 3:** students and retired delegates who are individual members of the European Crystallographic Association,
- **category 4:** students and retired delegates, who are NOT individual members of the European Crystallographic Association,
- **category 5:** accompanying persons, and
- **category 6:** booth crew members at the commercial exhibition.

All participants who want to register by the "early bird" rate must ensure that their payment arrives to the ECM29 account by 23.04.2015 at 11:59 PM, Zagreb time.

Bursary application

A limited number of bursaries are available for PhD students and young scientists (under 35) to enable them to attend the ECM29. The bursary application procedure is as follows:

1. Submit your abstract via regular online abstract submission procedure until 23rd of March, 2015. An applicant should be presenting author of the abstract.
2. Complete the bursary application form and send it, along with the accompanying documents, **no later than 23rd of March, 2015** by e-mail to:

   Bursary Committee ECM29
   E-mail: asantic@irb.hr

Documents required:

- Bursary application form
- Curriculum Vitae containing the list of publications
- Recommendation letter from Supervisor or Head of the Department/Group. The letter should confirm the status of an applicant (PhD student, post-doc etc.)

Please note that only applications containing all the required documentation will be considered for a bursary. A decision about the bursary application will be communicated to all applicants by 7th of April 2015.

If your application is successful, the conference agent will contact you via e-mail regarding organising your registration account. Registrations made through the automated system and paid for will not be refunded, and your bursary application will be made void. After providing the necessary information, the agent will proceed to register you and organise your services according to the bursary agreement, and send you the appropriate documents for payment.

Cat.	Participant	Early bird (EUR)	Regular (EUR)	Late (EUR)
1	ECA IM	450	510	570
2	Non-ECA IM	480	540	600
3	Students & retired, ECA IM	200	260	320
4	Students & retired, non-ECA IM	230	290	350
5	Accompanying persons	180	200	220
6	Exhibitors	300	360	420

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.

2-4 September 2014
Diamond Synchrotron User Meeting, Diamond Light Source, Didcot.
http://www.diamond.ac.uk/Home/Events/2014/SR-User-Meeting-2014.html

7-10 September 2014
ECCB'14. 13th Conference on Computational Biology, Strasbourg, France.
http://www.eccb14.org/

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

8 September 2014
SGK/SSK Annual Meeting, Dübendorf, Switzerland.
http://www.empa.ch/plugin/template/empa/22/147208/---/l=2

8-9 September 2014
IYCr2014@Innsbruck, Austria.
http://biocenter.i-med.ac.at/iycr2014

10-13 September 2014
5th Murnau Conference on Structural Biology, Murnau am Staffelsee, Germany.
http://www.murnauconference.de/2014/index.html

11-12 September 2014
Crossing Frontiers in Life Sciences. Symposium on the 100th birthday of Max F. Perutz, Vienna, Austria.
http://biocenter.i-med.ac.at/iycr2014

11-13 September 2014
Single biomolecules – in silico, in vitro and in vivo, University of Hertfordshire.
http://www.biochemistry.org/Conferences/AllConferences/tabid/379/View/Programme/Filter/2/MeetingNo/SA157/Default.aspx

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/

21-24 September 2014
Minerals at Focal Point, 92nd Annual Meeting of the German Mineralogical Society (DMG), Jena, Germany.
http://www.dmg2014.de

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

12 October 2014
8th International Workshop on Sample Environment at Neutron Scattering Facilities, North Leigh, Oxfordshire.
https://eventbooking.stfc.ac.uk/news-events/se-at-nsf-2014

12-16 October 2014
Computational Structural Biology – from data to structure to function, Cambridge.
http://www.ebi.ac.uk/training/course/ComputationalStructures2015

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

22-23 October 2014
Horace Workshop, ISIS, Didcot.
http://horace.isis.rl.ac.uk/Horace_Workshop

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

29-30 October 2014
Neutron Scattering in Magnetic Fields Above 15 Tesla, Helmholtz-Zentrum, Berlin, Germany.
http://www.helmholtz-berlin.de/events/hfm-workshop/index_de.html

3-7 November 2014
59th Annual Magnetism and Magnetic Materials (MMM) Conference, Honolulu, HI, USA.
www.magnetism.org/

10 November 2014
Advancing Applications of Super-Resolution Imaging, Charles Darwin House, London, UK
http://www.biochemistry.org/Conferences/AllConferences/tabid/379/Filter/2/MeetingNo/HT009/view/Conference/Default.aspx

10-14 November 2014
Fourth Niels Bohr International Academy Meeting on ESS Science, Copenhagen, Denmark.
https://indico.nbi.ku.dk/conferenceDisplay.py?confId=712

17-28 November 2014
Joint ICTP-IAEA School on Novel Experimental Methodologies for Synchrotron Radiation Applications in Nano-Science and Environmental Monitoring, Trieste, Italy.
http://cdsagenda5.ictp.it/full_display.php?email=0&ida=a13226

27-29 November 2014
EMBL Hamburg 40th Anniversary Symposium and Celebrations, EMBL, Hamburg, Germany.
http://www.embl-hamburg.de/training/events/2014/HH-40th-Anniversary/index.html

15-19 December 2014
Structural Biology: Using Synchrotron Radiation to Visualize Biological Molecules, Trieste, Italy.
http://cdsagenda5.ictp.trieste.it/full_display.php?ida=a13194

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

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