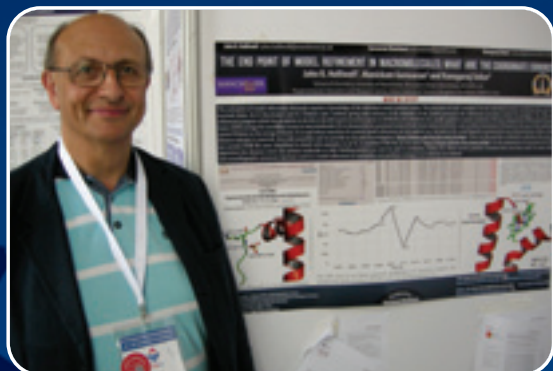


# Crystallography News

## British Crystallographic Association



Issue No. 135 December 2015  
ISSN 1467-2790



◀ **John Helliwell**  
receiving the Perutz  
Prize at the European  
Crystallographic  
Meeting in Rovinj,  
Croatia.

▶ **Judith Howard**  
at her career  
celebration receiving  
flowers, attending a  
surprise symposium  
and dancing.



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## Honouring Two Wonderful JH's

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## ***This month's cover:***

*Rovinj and Durham scenes,  
courtesy of Croatian Association  
of Crystallographers, Horst  
Puschmann, Alex Griffin and  
Joan Schwalbe*





# From the President



**I'M** writing this column from Nanjing, China, where I do a short stint of teaching as part of a joint degree programme The University of Sheffield has with a university here, so I have been teaching a bit of crystallography as part of an introductory solid state chemistry course.

As we approach the end of the year, much of the programme for the 2016 BCA meeting in Nottingham is now in place and can be found at <http://bca2016.crystallography.org.uk/>. At the time of publication of this column, we will only be awaiting your contributions via submitted abstracts to complete what looks to be an excellent and diverse programme. The abstract deadline is 09.00 GMT, Friday 22 January, 2016.

The BCA Council held its biannual meeting on September 16 at Brasenose College, Oxford. I am grateful to my fellow Council members for the contributions to a lively discussion of BCA matters and to our special local contact for the meeting room arrangements (she knows who she is – the arrangement was much appreciated). Our colleagues at Hg3 have been working on finding us a good deal at potential sites for future BCA Spring Meetings and have conducted some site visits to assess the suitability of different venues. Some universities where we may have held meetings in the past are no longer suitable for hosting the BCA meeting, often because accommodation is unavailable at around Easter time when we traditionally hold the meeting. Indeed, The University of York, which I felt was a very good venue for the 2015 meeting, will not be available to us in the future. I am, however, very pleased to announce that the Council has decided to return to University of Lancaster for the 2017 meeting, which will be held from April 10-13. We are also close to securing an arrangement for the 2018 venue and aim to have soon identified a set of venues between which we can rotate meetings on a 4-5 year cycle.

Since writing my last column I attended the ECM in Rovinj, Croatia, which I thought was a very good meeting. There were a number of very good microsymbposia, although the fact that the running order of speakers was changed from the on-line programme to the printed (and operational) programme led to some confusion – I missed a talk I had intended to go to before I realised that the switch had taken place. Although I enjoyed the science very much and there was quite a packed programme of talks of interest to me, I did manage to explore the old town (a very picturesque location) on one of the “quieter” days, and enjoyed the exhibition of Picasso ceramics at a very small museum in town. **Richard Cooper** and I took turns to attend the ECM committee meeting as representatives of the BCA. In addition to reports from SIGs there was an election of new officers, including **Alessia Bacchi** (Parma) as ECA President and re-election of **Georgina Rosair** (Herriot-Watt University), former BCA Secretary, as ECA secretary. Updates were provided on forthcoming ECA meetings: ECM30 (2016) in Basel, ECM31(2018) in Oviedo and ECM32 (2019) in Vienna. The CCDC stand in the exhibition continued their activity of having a novelty Top Gear-style leadership board highlighting the new possibilities to design searches for

interesting (and even obscure) information from the database. On this occasion, participants were ranked according to the aggregate number of different elements in the crystal structures bearing their name in the CSD. Although I was unable to come anywhere near competing with the most prolific crystallographers in our community, I was relieved to at least post a respectable score.

In mid-September, I attended the **Judith Howard** symposium in Durham, organised by her former students and associates to celebrate Judith's distinguished career (to date), and remarkably kept secret from Judith until the last minute. It was a very enjoyable occasion both for Judith and the many participants and attendees. Judith, of course, has had a long and active involvement in the BCA, including terms as BCA President and BCA Secretary, as well as being one of the original signatories at the establishment of the BCA. She has also presented both the Dorothy Hodgkin Prize Lecture (2007) and the Bragg Lecture (2014) at BCA meetings.

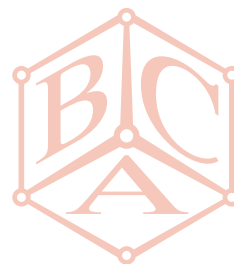


*Speakers and Session chairs with Judith.*

(Picture courtesy of Hazel Sparkes)

In the lead up to writing this column I asked **Simon Coles** to update me on recent BCA Outreach and Education activities that I could bring to the attention of the membership. On page 20 is Simon's update of activities, which as you can see continue to be extensive. I much appreciate the time and effort spent by BCA members in preparing and carrying out these activities and encourage you to get involved. Look out for the Big Bang Fair coming up in March!

**Lee Brammer**



# BCA Council 2015

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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](http://www.crystallography.org.uk)

# From the Editor



**BY** the time this issue reaches you, our exciting November programme of Group Meetings will already have taken place. However, our hardy Biological Structures Group, being receptive to a bit of cryo-cooling, will be meeting this month on the 16th in Manchester. The topic will be “Reactive Macromolecules”.

Furthermore, CCP4 will be holding

its Study Weekend 8-10 January 2016 at Nottingham University with the topic “Protein-Ligand Complexes: Understanding Biological Chemistry”. For all kinds of crystallographers the BCA Spring Meeting is taking shape nicely. Details are given in this issue. Please note that the deadline for submission of abstracts is Friday, 22 January. Crafting a finely polished abstract would be a good way to maintain the brain cells in tip-top condition after a surfeit of turkey. The turn of the year is also a good time to think about taking up or renewing one's BCA membership. The cost has gone up slightly, to a standard rate of £35 and a concessionary rate of £17.50, as agreed at the very well-attended AGM in April. These rates still compare favourably with those of other scientific societies. For those of us who have set up direct debits, renewal will take place automatically; but the stimulating conference programme should make it an “easy sell” to recruit colleagues. Further along in the New Year we have more crystallographic meetings to anticipate: the American meeting 22-26 July in Denver and the European meeting 28 August – 1 September in Basel. Here, too, we have abstract deadlines to bear in mind: 31 March and 6 April respectively. Now it is easier than ever to keep up with European Crystallographic Association events via the new website, online at [www.ecanews.org](http://www.ecanews.org). This site offers information and latest news on ECA activities, meetings, and educational and outreach initiatives. The site also provides a platform to encourage discussions and information exchange among the SIG and GIG members, where all Individual Members can register and take part in the activities.

We can look back to a very interesting, successful and enjoyable European Crystallographic Meeting (ECM29) in Rovinj, Croatia. I am delighted to feature on our cover the honours recently given to our two much-admired JH's.

As the result of a rigorous selection process by a multinational and multidisciplinary committee, **John Helliwell** was awarded the prestigious Perutz Prize at ECM29. This prize included the opportunity to follow the hosts' welcoming remarks with the first scientific lecture of the meeting, at a time when conference delegates were at their keenest and most attentive. John outlined the development of synchrotron radiation sources, detectors and phasing methods to solve previously intractable crystal structures. John was personally involved in these developments; but, typically, he meticulously gave credit to colleagues and members of other research groups. We can be proud of the rapid scientific progress. This was only possible because of the generous way in which developers of new facilities and methods did not seek to retain their competitive advantage but passed their “trade secrets” on to developers

of the next generation around the world. Our cover pictures do not just show John posed in the pomp of the Perutz Prize podium. Instead, I took another picture two days later, showing John putting in a good shift at a hot and crowded poster session just like the rest of us humble presenters. John is also publishing a new book, *Perspectives in Crystallography*, covering a range of topics, from the history of crystal structure analysis to the societal impacts of crystallography in the sustainability of life, and also discussing the future of crystallography for the next century. Details can be found at:

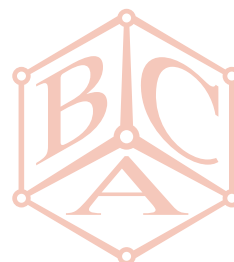
<https://www.crcpress.com/Perspectives-in-Crystallography/Helliwell/9781498732109>.



John Helliwell with Judith Howard.

The honour for **Judith Howard** had an entirely different origin. No formally established committee was involved. Instead, meeting out of respect and love, a group of friends and present and former colleagues put in a lot of effort to organise a colloquium at Durham to celebrate Judith's career. Exciting developments in topics relevant to Judith's research interests were presented by speakers from around the world. Participants also had fun, by way of a ceilidh and a visit to the Beamish Museum of industrial and agricultural history. Although both John and Judith have joined me in the ranks of OAPs, none of us expects our crystallographic interests to subside just yet.

**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.
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- Free insert in the annual Spring Meeting delegate pack.
- Two free full registrations to the annual Spring Meeting.
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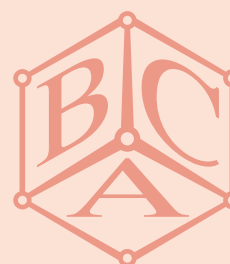
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# Puzzle Corner

**DEVELOP** a seasonal message by replacing each of the numbers below, which refer to a well-known compendium, with the initial letter of the corresponding symbol in whatever notation is appropriate.

H 40 14 4 Y    15 H 155 23 81 196 M 41 82



## Answers to September Puzzle Corner

In Victorian times **Macclesfield** was renowned for the weaving of silk, and indeed the nickname of the football team is the Silkmen. Silk thread is mainly composed of a protein called fibroin. The structure of fibroin from the silkworm *Bombyx mori* was reported by R. E. Marsh, R. B. Corey and L. Pauling in *Acta Cryst.* (1955), 8, 62. Later, Marsh became famous for spotting missed symmetry in other people's papers. However, in this study they *reduced* the space group symmetry to  $P2_1$  from the  $P22_12_1$  claimed by a different author. A complicating factor is that fibroin can assume two distinct solid-state structures, silk I and silk II. Form I gets converted to II by spinning or simply by imposing a macroscopic orientation for diffraction studies.

**Glasgow** developed a major shipbuilding industry in Victorian times, building ships out of steel after 1870. A typical steel contains iron in the form of ferrite, space group  $Im-3m$  (No. 229), and cementite,  $Fe_3C$ , space group  $Pnma$  (No. 62).

**Manchester** got the nickname "Cottonopolis" because of its large number of cotton mills. Cotton fibre is mostly cellulose, which has various polymorphic forms. Cellulose from higher plants such as cotton typically has a small amount of form Ia (space group  $P1$ ) and a larger amount of  $I\beta$  (space group  $P2_1$ ).

# BCA Spring Meeting

## University of Nottingham, 4-7 April 2016



### From the BCA 2016 Programme Committee

**WE** welcome you to attend the 2016 BCA Spring Meeting, which will be held at the Jubilee Campus, University of Nottingham. We have the usual diverse and exciting mix of technical sessions from the four subject groups, in addition to the Young Crystallographers' satellite meeting, commercial exhibition and a 'Crystallisation' workshop. Please consider submitting an abstract: in addition to the technical sessions highlighted here (with space for three contributed talks per session), there will be an 'open' session, and contributions to the workshop are also encouraged. Abstract submission is now open and the deadline is 09.00, 22 January, 2016.

The **Named Lecturers** for 2016 are:

#### Lonsdale Lecture (Tuesday pm)

**Arwen Pearson** (Hamburg)

*Visualising molecules in motion: crystallography as a tool to probe structure and dynamics*

#### BCA Prize Lecture (Wednesday pm)

**Christer Aakeröy** (Kansas State University)

*From molecular sociology to functional materials*

The **Plenary speakers** are:

**BSG: Susan Lea** (University of Oxford)

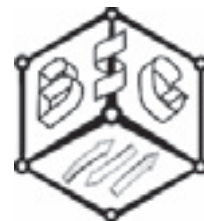
**CCG: Mike Zaworotko** (University of Limerick)

**IG: Rolf Hilfiker** (Solvias AG)

**PCG: Bill David** (Oxford and ISIS)

Session titles and Keynote speakers for all sessions are now in place. For further, up-to-date details please visit the conference website: <http://bca2016.crystallography.org.uk>

### Biological Structures Group (BSG)



The central theme of the 2016 BSG sessions will be **Antimicrobial Resistance (AMR) and Cell Processes**. AMR is an emerging and growing threat to western healthcare providers and the general population. A unique cross council initiative, involving the MRC, BBSRC and EPSRC, has recently been launched to 'jump start' research in this area. The Wellcome Trust also supports research into AMR under the Infectious diseases part of their funding portfolio. Given the importance of this topic we have devised a program that seeks to highlight the role that structural biology can and should be playing in the pursuit of strategies to tackle AMR. This includes understanding the roles that membrane transporters play in giving resistance to current antibiotics and their potential as drug targets themselves. We have also identified a number of recent studies on molecular machines that are also highly relevant to AMR.

Renewed interest and applications of EM, Mass Spectrometry, Small Angle and Wide Angle X-ray scattering to understanding dynamic macromolecular complexes has led to some dramatic advances in our understanding of key cellular processes, such as mitosis and cell division. Another growth area in structural biology is EM tomography, which has the capacity to place atomic structural information into the broader cellular context. To highlight some of these advances we have included a separate session on '**Structural Insights into Cell Processes**' and '**Molecular Machines**' to highlight recent successes from UK based groups.

We hope these topics will highlight some of the world-class structural biology being undertaken in the UK and provide stimulating discussions.

#### BSG Plenary (Wednesday am)

**Susan Lea** (University of Oxford)

*Structural studies in infection and immunity*

*Chair: Simon Newstead (Oxford)*

#### BSG sessions

##### Session 1. Antimicrobial Resistance (Tuesday pm)

*Chair: Ben Luisi (Cambridge)*

Structural biology is playing a key role in the pursuit of novel strategies to tackle Antimicrobial Drug Resistance (AMR). This session highlights exciting new avenues for novel AMR targets.

**Keynote: Changjiang Dong** (UEA)

*Transport lipopolysaccharide from the inner membrane to the outer membrane surface*

**Speaker 1: Dijun Du** (Cambridge)



## Session 2. Developing New Therapeutics (Tuesday pm)

Chair: to be confirmed. Co-chair: Colin Kleanthous (Oxford)

Continuing our theme of AMR, the aim of this session is to showcase the role of structural biology and biophysical methods in developing new protein-based antimicrobial therapeutics.

Keynote: **Colin Kleanthous** (Oxford)  
*Import mechanisms of protein antibiotics*

Speaker 1: **Daniel Walker** (Glasgow)

## Session 3. (joint with PCG) Future of Structural Science (Wednesday am)

Chair: to be confirmed. Co-chair: Xiadong Zhang (Imperial)

Keynote: **Xiadong Zhang** (Imperial)  
*Structures and Mechanisms of Bacterial RNA Polymerase Inhibition and Activation by sigma54 and its AAA activators*

Speaker 1: **Ben Luisi** (Cambridge)

## Session 4. (joint with PCG) Future of Structural Science (Wednesday pm)

See PCG section for details.

## Session 5. Structural insights into Cell Processes (Thursday am)

Chair: to be confirmed. Co-chair: Richard Bayliss (Leicester)

Proteins operate in dynamic networks of interactions and pathways. The aim of this session is to highlight the advances made in understanding dynamic cellular networks, such as phosphorylation and neuronal signalling, using state of the art crystallographic techniques.

Keynote: **Richard Bayliss** (Leicester)  
*Protein Kinases and their On and Off Relationships*

Speaker 1: **Radu Aricescu** (Oxford)

## Session 6. Molecular Machines (Thursday am)

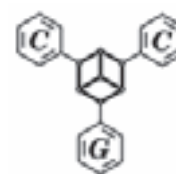
Chair: Susan Lea (Oxford)

In the past couple of years substantial progress has been made in our understanding of how protein dynamics operate at the molecular level. The aim of this session is to highlight recent advances in our understanding of these systems and showcase several important advances from UK laboratories in this field.

Keynote: **Neil Macdonald** (The Francis Crick Institute)  
*Structural insights into growth factor signalling and cell polarity*



## Chemical Crystallography Group (CCG)



### CCG Plenary (Tuesday pm)

Mike Zaworotko (Limerick):  
*Crystal Engineering: Form to Function*  
Chair: Pete Wood (CCDC)

### Session 1. (joint with IG) From Amorphous to Crystal (Tuesday pm)

Chairs: Katherina Fucke (Durham), Ghazala Sadiq (CCDC/Pfizer)

Keynote: **Ivan Marziano** (Pfizer)

This session will cover research into the transitions from amorphous, e.g. solution, glass or gas state, into the crystalline state, the connections between the extremes, and the transition states between them. Special interest is taken in the correlation of these topics with the final crystal structures. This session aims at bridging the fields of pharmaceutical solid-state, organic and inorganic chemistry as well as process engineering, the problems that are encountered in these fields and the solutions that crystallographic methods can offer.

### Session 2. (joint with IG) Interactions and Materials (Tuesday pm)

Chairs: Graham Tizzard (Southampton), Cheryl Doherty (Pfizer)

Keynote: **Robert Docherty** (Pfizer)  
*Towards an Unprecedented Structural Perspective of Drug Product and Process Design*

This session will aim to encompass the flourishing and diverse fields of crystal engineering, the design of structures from first principles by directed assembly, as well as the related areas of polymorphism and co-crystal research. This is a joint session between the CCG and IG that will include broad range of topics of interest to both these communities.

### Session 3. NMR Crystallography (Wednesday am)

Chair: Gareth Lloyd (Heriot-Watt), Co-chair: Paul Hodgkinson (Durham)

Keynote: **Yaroslav Khimyak** (East Anglia)  
*Understanding structure of molecular organic solids: combining crystallography with insights from NMR*

Nuclear Magnetic Resonance (NMR) Crystallography uses the exquisite sensitivity of NMR frequencies to local environment in order to elucidate crystallographic information. DFT-based methods now allow NMR measurements to be directly correlated with molecular packing, and a range of NMR experiments can be used to probe questions of disorder, dynamics, structure and crystallography.

### Session 4. Complementary Techniques (Wednesday pm)

Chairs: Helena Shepherd (Kent), Andrew Stewart (Limerick)

Keynote: **Graeme Day** (Southampton)

There are many techniques that can give complimentary

information to traditional crystallographic approaches. This session will explore the use of techniques including computational studies, electron diffraction and microscopy, spectroscopy and scattering to allow a more complete understanding of the molecules and materials we study.

### Session 5. Tips, Tricks and Trials (Thursday am)

*Chairs:* Mike Probert (Newcastle), Iain Oswald (Strathclyde)

**Keynote: David Allan** (Diamond)

This session will aim to span the crystallisation journeys of various samples through to the measurement of their diffraction patterns, aiming to explain various Tips Tricks and Trials that the speakers have employed under different circumstances.

### Session 6. (Joint with YCG): Would you Publish This? (Thursday am)

*Chairs:* Pascal Parois (Oxford) and Jorge Sotelo (Edinburgh)

**Keynote: Iain Oswald** (Strathclyde)

*Pharmaceuticals... I thought they were meant to make you feel better!?!*

Following last year's success, this interactive session of unusual format is aimed for discussing problematic crystal structures that can be hard to interpret and publish. After an opening talk on the challenge of publishing difficult structures, anyone present can briefly describe one or more structural results that raise the session title question for the audience to discuss, with the aim of constructive rather than negative criticism. Problems might include charge imbalance or other chemical issues, poor resolution or data completeness, complicated disorder, highly restrained models, unexplained residual electron density and other artefacts, etc. A formal abstract is not required, but please contact the session organisers in advance of the meeting (as soon as possible!) if you wish to contribute; we will request 1–3 slides for concatenation into a single session presentation. Contributions from Young Crystallographers are particularly encouraged.



## Industrial Group (IG)

### IG Plenary (Tuesday pm)

**Rolf Hilfiker** (Solvias AG): Title TBA  
*Chair:* Cheryl Doherty (Pfizer)

### Session 1. (joint with CCG) From Amorphous to Crystal (Tuesday pm)

*Chairs:* Katherina Fücke (Durham), Ghazala Sadiq (CCDC/Pfizer)

**Keynote: Ivan Marziano** (Pfizer)

This session will cover research into the transitions from

amorphous, e.g. solution, glass or gas state, into the crystalline state, the connections between the extremes, and the transition states between them. Special interest is taken in the correlation of these topics with the final crystal structures. This session aims at bridging the fields of pharmaceutical solid-state, organic and inorganic chemistry as well as process engineering, the problems that are encountered in these fields and the solutions that crystallographic methods can offer.

### Session 2. (joint with CCG) Interactions and Materials (Tuesday pm)

*Chairs:* Graham Tizzard (Southampton), Cheryl Doherty (Pfizer)

**Keynote: Robert Docherty** (Pfizer)

*Towards an Unprecedented Structural Perspective of Drug Product and Process Design*

This session will aim to encompass the flourishing and diverse fields of crystal engineering, the design of structures from first principles by directed assembly, as well as the related areas of polymorphism and co-crystal research. This is a joint session between the CCG and IG that will include broad range of topics of interest to both these communities.

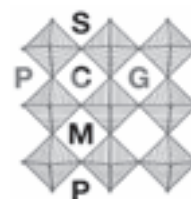
### Session 3. (joint with BACG) Application of Crystallography to Crystal Growth (Wednesday pm)

*Chair:* Neil Feeder (CCDC)

**Keynote: Roger Davey** (Manchester)



## Physical Crystallography Group (PCG)



The final 'Centenary' of the current cycle is perhaps the birth of powder diffraction.

To celebrate this, Prof **Bill David** will give the PCG Plenary, entitled '120 Years of Powder Diffraction'; for the final 20 years, Bill will presumably take out his (poly)crystal ball and invite us to gaze into the future!

### PCG Plenary (Thursday am)

**Bill David** (Oxford and ISIS): 120 Years of Powder Diffraction  
*Chair:* Matt Tucker

### Session 1. Advanced Functional Materials (Tuesday pm)

*Chair:* Matthias Gutmann (ISIS)

**Keynote: Paolo Radaelli** (Oxford)

*Spins and orbitals in multiferroics: from crystals to devices*

The development of advanced functional materials is critical to underpinning the development of modern technologies.





This session covers such materials with current or potential use in cutting-edge applications. This may include magnetic and electronic materials, such as multiferroics, energy related compounds, for use in solar cells or batteries and modern alloys.

## **Session 2. Modelling Crystals and Crystallographic Data (Tuesday pm)**

Chair: Anthony Phillips (QMUL)

Keynote: **Carole Morrison** (Edinburgh)

*Frustrated MOFs: how modelling can help when crystallography can't*

Recent developments in data acquisition, computing power, and our understanding of the fundamental forces at play within crystals have transformed the concept of crystallographic refinement. Among the many "unusual" techniques that are becoming increasingly commonplace are, first, refinement of non-standard parameters: mode amplitudes instead of atomic positions, or thermodynamic properties instead of lattice parameters. Second, refinement against non-standard data is also common: more scattering information than just Bragg intensities, or information from complementary experiments such as NMR or EXAFS, can be incorporated into a crystallographic model. Finally, both empirical and *ab initio* modelling are increasingly necessary to make sense of complex crystallographic information. This session will focus on using modelling techniques such as these to predict, interpret, and generally get the most out of crystallographic data.

## **Session 3. (joint with BSG) Future of Structural Science (Wednesday am)**

See BSG section for details.

## **Session 4. (joint with BSG) Future of Structural Science (Wednesday pm)**

Chair: Mike Glazer (Oxford)

Keynote: **John Spence** (Arizona State)

*Opportunities for structural biology using X-ray lasers*

In the last few years important advances have been made in techniques to investigate the structures of crystals and molecules. In particular the advent of the free electron laser has shown that it is possible to gain structural information on macromolecules without the need to grow large single crystals. Another area of advance is in the field of electron microscopy, where the development of new aberration-free lenses enables individual atoms to be imaged; the use of freezing methods as in CryoEM enable at least protein molecules to be imaged even when not in crystalline form. Alongside the rapid advances in other experimental and computational techniques this raises key questions about the nature of the future of structural science including whether in the future crystals will be needed at all. It is time that crystallographers think about this and consider the impact of these new techniques on their subject.

## **Session 5. Phase Transitions (Thursday am)**

Chair: Christoph Salzmann (UCL)

Keynote: **John Evans** (Durham)

*Phase Transitions and Symmetry Mode Analysis of Functional Materials*

Phase transitions are at the very heart of solid-state chemistry,

crystal engineering and mineralogy. The aim of this session is to cover as many aspects of this important phenomenon as possible including phase transitions between crystalline as well as amorphous materials. Particular emphasis will be put on the real-time and in-situ detection of phase transitions as well as the description and parameterisation of symmetry changes.

## **Session 6. Local Structure-Property Relationships (Thursday am)**

Chair: Matt Tucker

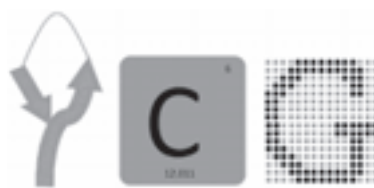
Keynote: **Ian Reaney** (Sheffield)

*Local structure-property relations in perovskite structured ceramics*

The local structure of materials often plays a critical role in determining their properties yet cannot be perceived easily by conventional crystallographic analysis; this is particularly pertinent in amorphous and nanocrystalline systems which lack the requisite long-range order. This session will focus on materials where such understanding of the local structure is vital, discussing results from techniques sensitive to these length-scales, such as Pair Distribution Function (PDF) data, Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy, diffuse electron scattering and computational modelling. Where possible, it will highlight the complementary nature of these techniques and the way in which they can be combined to address difficult problems.



## **YCG Satellite meeting:-**



**Monday pm**

**Plenary speaker 1: Sally Price** (UCL)

*Are polymorphs predictable?*

**Plenary speaker 2: Robin Owen** (Diamond Light Source)

**Tuesday am**

**Special Session: Forgotten Methods in Crystallography**

Three Invited speakers, including: **Mike Glazer** (Oxford), **Paul Raithby** (Bath), and **Bob Eady** (Liverpool)

## **Workshops**

The workshop topic of the 2016 BCA will be **"Crystallisation –**

**Tips and Tricks**". Apart from some invited speakers, we are looking for contributions from delegates. If you have some practical experience and know a few things about the wider area of crystallisation, please consider sharing your expertise during this dedicated workshop session.

Workshop submissions are open until 09.00 GMT, Friday 22 January, 2016.

If you would like to contribute, please enter your Workshop Submission for the BCA Spring Meeting either on the conference registration form, or contact **Horst Puschmann** ([horst.puschmann@gmail.com](mailto:horst.puschmann@gmail.com)) for more information. Any updates to the Workshop Programme will be published on the BCA Spring Meeting 2016 website.

The aim of the Programme Committee is to present the very best in contemporary crystallography, emphasizing the growing significance of the subject to more diverse areas. Please see the Conference website <http://bca2016.crystallography.org.uk> for up-to-date details. Abstract submission is now open and the deadline is 09.00, Friday 22 January, 2016.

#### The BCA 2016 Programme and Organising Committee is:-

**Phil Lightfoot** (Chair)

**Alex Cameron** (BSG)

**Simon Newstead** (BSG)

**Mark Roe** (BSG)

**Pascal Parois** (CCG)

**Lynne Thomas** (CCG)

**Qendresa Osmani** (IG)

**Ghazala Sadiq** (IG)

**Nicholas Funnell** (PCG)

**Paul Saines** (PCG)

**Horst Puschmann** (Workshops)

**Scott McKellar** (YCG)

**Natalie Johnson** (YCG)

**Lee Brammer** (BCA President)

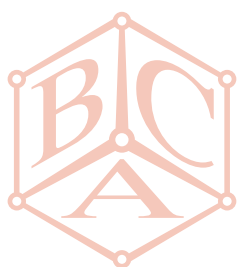
**Richard Cooper** (BCA Vice President)

**Claire Wilson** (BCA Secretary)

**Pamela Williams** (BCA Treasurer)

**Phil Lightfoot**

Chair of BCA 2016 [pl@st-and.ac.uk](mailto:pl@st-and.ac.uk)



*Business School: the venue for sessions*



*Business School: the venue for sessions*



*Exchange building*



*Exchange foyer*



**THERE** was so much going on at the 29th European Crystallographic Meeting in Rovinj, Croatia, that no one person could give a comprehensive account. I am grateful to the BCA bursary recipients for their reports on the sessions that had particular significance for them, reproduced below. British crystallography was very well represented at this meeting. We submitted 96 abstracts, second only to Germany with 107 and well ahead of Russia with 63.

The upbeat, interesting and enjoyable opening ceremony set the tone for the whole meeting. **Aleksandar Višnevac**, the affable Chair of the Organising Committee, welcomed us. Organising such an important meeting had been a bold commitment of human effort and financial resources for a small society like the HUK (Croatian Association of Crystallographers). This commitment was triumphantly rewarded: the attendance of 1069 participants was a record, and 55 younger scientists received bursaries from the IUCr. Support from the Croatian government was an important factor guaranteeing the viability of the meeting and was signified in an address by Professor **Ružica Beljo Lučić**, Assistant Minister of Science, Education and Sport. In how many countries would the holder of such a political post actually have first-hand subject knowledge and the title of Professor? Next, we were treated to mellifluous and characterful singing by Klapa Motovun. Klapa is a UNESCO-recognised Croatian form of unaccompanied multipart male singing that grew out of folk and church music. Nowadays it ranges in sophistication from a bunch of friends in a bar to this group of 9 outstanding singers from the town of Motovun. Joan and I visited Motovun near the end of our stay in Croatia. Situated in a defensive position on top of a steep hill, this walled town offers spectacular views, well-preserved old fortifications, churches and houses, and a profusion of shops selling such things as art works, craft items and truffles.

**Stanko Popović**, President of the HUK, returned us to a scientific agenda with an overview of the history of crystallography in Croatia, which dates back to 19<sup>th</sup> century courses in mineralogy. When Yugoslavia was a united country, preeminent research groups in crystallography were located in Zagreb at the university and the institute named after **Ruđer Bošković** (1711-1783), the Croatian polymath who developed an atomic theory of crystals. After the disintegration of Yugoslavia in 1991, in spite of the resulting chaos and warfare, the HUK was established early the next year. Croatian crystallography has continued to be strong. Stanko finished affectionately by showing us a piece of confectionery, a molecule and a Croatian island, all heart-shaped. Next we were greeted on behalf of the European Crystallographic Association by President **Andreas Roodt**. All this, and another musical interlude, led up to the awarding of the prestigious Max Perutz Prize to our own **John Helliwell**.

John's lecture, entitled "Synchrotron radiation in crystallography instrumentation, methods and applications", began with the state of macromolecular crystallography (MX) in the mid-1970's, making some important breakthroughs but plagued by weak



data and difficulties with the phase problem. At about this time John was asked by **Dorothy Hodgkin** to assess the viability of pioneering MX work at the Stanford synchrotron led by **Keith Hodgson**. Concluding that it was valid, John led the development of SRS PX 7.2 in the UK, the first dedicated synchrotron X-ray source. Using a bending magnet, it produced a beam that was far from ideally shaped, being 0.4 mm high and 14 mm wide! Even so, it achieved 20 times home lab intensity, which became 100 times with the introduction of a vertical focusing mirror. Difficult problems became solvable. Using the tunable synchrotron radiation to measure anomalous dispersion, **Howard Einspahr** was able to distinguish Mn from Ca binding sites on pea lectin. Even though crystals of purine nucleoside phosphorylase had 80% solvent content, **Steve Ealick** and **Charlie Bugg** could determine the structure. **Michael Rossmann** used SRS 7.2 for preliminary work on viruses. The installation of SRS PX 9.6 with its superconducting wiggler provided a big improvement in beam intensity between wavelength limits of 0.6 to 1.5 Å. Now **David Stuart** could advance virus crystallography by collecting data on foot and mouth disease virus, and at the small-molecule end **Marjorie Harding** could determine the structure of piperazine silicate from a very tiny crystal. Complementing the improved X-ray source, films were replaced with a TV detector or image plates. In 1987 the ESRF Foundation Phase Report showed that colossal increases in intensity could be achieved with an undulator, but nobody knew if the samples could withstand it. Collaborating with **Roger Fourme**, John worked out that the beam would raise the temperature of an isolated sample by 20 K per second, but a copper stalk could conduct away this heat. Risk analysis experiments demonstrated feasibility. However, radiation damage leading to splitting of S-S bridges was observed. In parallel with the advances in hardware, phasing methods also advanced: in particular, taking advantage of Se anomalous scattering in SeMet. In the small-molecule context **Madeleine Helliwell** pushed anomalous scattering even further: 11-wavelength measurements on the Zn substituted gallophosphate ZnULM-5 showed the sites and amounts of Ga content. The synchrotron Laue method pioneered with **Keith Moffat** gave speedy data collection that enabled the determination of time-resolved structures, e.g. John applied the Laue method at the ESRF with Dr **Alfonse Haedener** to study a functioning enzyme fed with a pulse of substrate. A final highlight was identification of the cause of colouration in lobster shell ( $\beta$ -crustacyanin with a

carotenoid) that led to much media interest, e.g. “Solution cooked up to red lobster riddle” in the Liverpool Post. John’s talk and slides can be found at this weblink: <http://ecanews.org/mwp/blog/ecm29-opening-ceremony-2/>

Bright and early the next morning, **Carl Henrik Görbitz** gave a keynote lecture about amino acid structures, for which it was well worth setting one’s alarm clock. Along with the 20 standard amino acids, 366 more compounds can reasonably be called amino acids; some of these occur in nature. At first glance their protonation states and modes of packing seem bewildering. Considering  $\alpha$ -amino acids, Carl Henrik devised a classification scheme which imparted clarity. Each amino acid in the CSD is given a label  $x(N)$ , where  $x$  describes the protonation state ( $a$  = anionic,  $z$  = zwitterionic,  $c$  = cationic) and  $N$  the charge. The most numerous state in the CSD, with 206 distinct entries, is  $z(0)$  with  $NH_3^+$  and  $COO^-$  groups; several of which have been redetermined under varied conditions of temperature and pressure. Not all feasible states for an amino acid have yielded crystals. Next, Carl Henrik addressed the issue of hydrogen bonding patterns. When the side chain  $R$  has a strong hydrogen bond donor or acceptor, each structure is unique and there are no polymorphs. However, when  $R$  is hydrophobic, a small number of patterns recur, providing a hydrophobic region and paired hydrophilic sheets. Only 5 patterns of hydrogen bonds occur in the sheets, and one of these is rare. Crystals of racemates either have alternating sheets of  $D$  and  $L$  enantiomers or a layer of paired  $DL$  sheets. In either case the two sheets constituting a hydrophilic layer are antiparallel. With enantiomeric samples such an arrangement is impossible; a relative rotation of ca.  $\pm 60^\circ$  is needed to make the hydrogen bond donors and acceptors match up. If anions are present, they are most commonly halides. Interchanging  $Cl^-$  and  $Br^-$  gives crystals that are isostructural in 12 cases but not in 4 others. Amino acids display a rich variety of metal binding modes from monodentate to tetradentate. Bidentate through  $O$  and  $N$  atoms is the most common. Two and a half centuries ago the great Swedish scientist **Carl Linnaeus** established a rational classification scheme for life forms (and also attempted to classify crystals by shape!). Now another Scandinavian Carl has done the same for amino acid structures. Readers wishing for more detail can find it in *Crystallography Reviews* (2015) 21, 160-212.

A microsposium which particularly attracted my interest was MS9, “Pharmaceutical crystallography and drug design”. **Rod Hubbard** introduced us to “Current perspectives in fragment-based ligand discovery”. Whereas typical values of molar mass are 250-500 for entire molecules giving hits in high-throughput screening tests, 110-250 is customary for fragments, allowing scope for subsequent attachment to a scaffold. Rod uses a fragment library with about 1500 compounds of average molar mass 190. Suitable fragments for a given target are usually subjected to a competitive NMR screen. This needs a lot of protein but verifies that the protein remains folded and the fragment remains in solution. X-ray crystallography can be used at this stage if necessary but may give false negative results if the fragment fails to soak in. Once hits have been found, a binding model is constructed and optimised, and at this stage X-ray data are very valuable. Systems studied include the bacterial defense protein TolB as well as enzymes processing  $o$ -GlcNAC, where a non-competitive fragment which binds adjacent to the active site was unexpectedly found to enhance activity, presumably by stabilising the transition state.

**Jim Kiefer** was “At play in the briar patch of epigenetics”. DNA and histone proteins may be chemically modified, altering

transcription. Suites of enzymes add or remove chemical “marks”, which are “read” by other enzymes. Marks may be made by phosphorylation, ubiquitination or methylation/demethylation; Jim specifically discussed the latter. Lysine demethylases (KDMs) have a catalytic core that is conserved; but with 1000-1800 amino acids there are plenty of other domains and surfaces. Study of the KDM5 family has been useful. Drug resistance in tumours arises from a subpopulation of drug-tolerant cells prior to treatment. Knocking down KDM5a reduces or eliminates this resistance. A model for nucleosome binding has been developed; despite unusual features, it looks plausible.

**Puja Pathuri** continued with “Identification of novel allosteric inhibitors through Fragment-Based Drug Discovery and X-ray crystallography”. Using a library with about 1600 entries, screening detects fragments binding away from known binding sites in about 60 % of cases. Such sites are often more druggable, offering more potential for selectivity. An example of a target is soluble adenylylase (SolAC), which is activated by bicarbonate and involved in  $CO_2/HCO_3^-$  pH sensing. The human apoenzyme is a dimer, on which an allosteric site binds  $HCO_3^-$ . 46 hits led to 12 crystal structures showing 3 binding sites.

**Franziska Huschmann** gave a presentation on “Crystallographic fragment-screening – Results from the HZB-Marburg collaboration”. High throughput methods, high diffraction quality of the target protein and a well-chosen fragment library are essential for the success of drug discovery by fragment screening. To this end, the project “Frag2xtal”, funded by the German government, features a 1000-compound library, and a fully automated beamline optimised for fragment screening is being established at the BESSY II storage ring. Validation studies against two target proteins, endothiapepsin and human prolidase, identified binding partners at a hit rate of about 10%.

**Sabine Schneider** concluded the session with “Inhibition of human Aldehyde Dehydrogenase1 by the anti-tumor agent Duocarmycin”. Instead of increasing activity by adding fragments, this study aimed to reduce side effects by removing functionality. It began with a natural product, duocarmycin, that is a powerful anti-cancer agent but unfortunately is also extremely cytotoxic. It has two modes of action: alkylation of DNA and binding to aldehyde dehydrogenase 1A1 (ALDH1A1). The former mode appears responsible for the general toxicity. Removal of the moiety responsible for DNA binding left a drug with activity against ALDH1A1, which is over-expressed in human lung cancer cells.

The main cultural event was an evening of folk-tinged classical Croatian music presented by clarinetist **Bruno Philipp** and the **Rucner Quartet** in the fine baroque Church of the Franciscan Monastery, shown on our cover. South European baroque church architecture usually does not appeal to me, putting me in mind of an excessively sweet and rich dessert; but this church was different. In its simple dignity it could have been English. Such was the love of music among European crystallographers, the church was packed. After a hot sunny day and in the presence of so many warm bodies, it was also very hot. I was lucky to arrive too late to get one of the seats provided. I had to sit on a stone bench with my back against a stone pillar – not very comfortable, but keeping my bottom and back wonderfully cool. The music, nearly all by composers we had never heard of, was ingratiatingly tuneful.

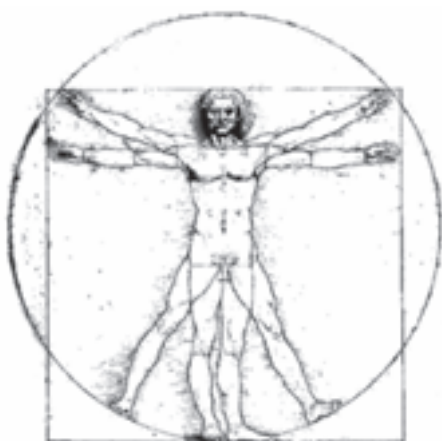
**Carl Schwalbe**

## Putting up a poster at ECM29

**SINCE** I intended to display this poster at both the ACA meeting and the ECM, I printed it on fabric. That way, I didn't have to carry a tube past suspicious agents of the Department of Homeland Security, who might think I was carrying enough rocket power to obliterate a medium-sized American city, nor to persuade airline staff to let me carry it on board. Displaying the poster in historic Philadelphia posed no problem whatsoever. We used the same method by which **Benjamin Franklin** would have attached a poster about lightning: drawing pins on board.

Matters were much more complicated in high-tech Croatia. The poster boards were white and beautifully glossy. Sticking pins into them would probably have resulted in arrest and detention. Instead, we were provided with double-sided sticky tape bearing one of the most powerful adhesives known to science. Unfortunately, the order of adhesion from strongest to weakest was (1) tape to backing paper, (2) tape to board, (3) tape to poster. When I tried attaching a piece of tape to the board, removing the paper and leaving the tape *in situ* to receive the poster, I discovered that the board was covered with film. Pulling on the backing paper pulled the tape away from the board, taking a ragged piece of film with it. Fortunately, the resulting hole was subsequently covered by the poster. The tape fell to the floor. As my movements came to resemble those of a very agitated bee, I forgot where it was and stepped on it. I discovered that its adhesion to shoe soles far exceeded the previous top two (chewing gum and dog muck). The attached illustration (Vitruvian Man) is an approximate representation of me working on that poster. Eventually, two lovely ladies from the conference organisers came along with even stickier tape and better fingernails than mine, and we got the poster up with sufficient adhesion that it stayed proudly in place.

**Carl Schwalbe**



*Vitruvian Man, which might just be Leonardo da Vinci's anticipation of a man trying to get a fabric poster to stick to a glossy board (reproduced from the website <http://leonardodavinci.stanford.edu/submissions/clabaugh/images/vm/leonardo.jpg>).*

## ECM29 Bursary Recipients' Reports

**AFTER** setting off very early on a damp and rainy morning from Leeds, I landed in sunny Pula airport on my way to the ECM29. A short drive took us to Rovinj, a small, picturesque town in northern Croatia, with crystal clear waters and rocky beaches. This was the magnificent setting of this year's vibrant European Crystallographic Meeting, attended by hundreds of crystallographers sharing their science through a variety of talks and posters, represented by the 200+ abstracts circulated.

The meeting started with a lecture from Professor **John R. Helliwell** (University of Manchester), recipient of the 8<sup>th</sup> Max Perutz Prize, with an overview of his exceptional work in developing X-ray diffraction methods. The two plenary lectures of the meeting were delivered by Prof. **Henry Chapman** (DESY/Universität Hamburg) on the latest developments in X-ray free electron laser science and its application in solving some of the most complex biological questions, and Prof. **Andrea Ferrari** (University of Cambridge), on the discovery and applications of graphene, an extremely versatile material that may, one day, underpin some of the greatest technological advances of the 21<sup>st</sup> century.

The 4 days of the conference were split into 50 microsymposia, covering a wide range of topics, from macromolecular and small molecule crystallography to the history and teaching of crystallography. With so many sessions running in parallel, I focused on lectures concerning macromolecular crystallography. Some of the talks gave fantastic tours of how to solve complex Others taught me more about the latest software developments, with case studies on how to implement them, practical aspects regarding crystal growth and handling approaches, as well as instructing me on the newest available facilities at synchrotrons.



*Microsymposium 5: structure and function of enzymes. From left to right: Diana Monteiro, Ute Krengel, Petra Fromme, Adrian Goldman, Andrew Wang, Joel Sussman and Miroslaw Cygler.*

I was very fortunate to be able to present my work on new chemical tools for time-resolved structural studies during the Structure and Function of Enzymes microsymposium. The two invited speakers in this session, Prof. **Petra Fromme** and Prof. **Adrian Goldman**, presented some of their latest work in visualising and understanding the structural changes that are coupled with protein activity using XFELs and synchrotron radiation respectively.

continued ➤



The conference provided ample opportunities for networking, including island parties hosted by Bruker and Rigaku/Oxford Diffraction, a Young Crystallographers mixer evening and a conference dinner. The lunch breaks allowed for extensive discussions in the sunshine followed by vibrant poster sessions, which showcased a lot of exciting work from early research career crystallographers. The ECM29 was an exciting meeting immersed in the sunny and beautiful coastal town of Rovinj.

**Diana Monteiro**  
University of Leeds

**THE** European Crystallographic Meeting was perfectly located on the Mediterranean coast by the picturesque old town of Rovinj in Croatia.



The conference welcome session began in the evening of Sunday 23 August and ended with the award of the 8th Max Perutz Prize to **John Helliwell** for his inspiring work on synchrotron crystallography. Drinks and food were served afterwards, giving a chance for the crystallographers to meet and mingle!

The next four days were filled with 6 parallel sessions, covering topics from protein crystallography to magnetic structures, and techniques from electron diffraction to femtosecond X-ray diffraction collection. Many structures were investigated using diffraction under non-ambient conditions, such as low temperature, light irradiation, gas absorption and high pressure.

I was particularly fascinated by work from **Tomislav Friščić** and **Helena Shepherd** on their highly-responsive crystals which bend in response to light irradiation following processes such as cis-trans isomerisation and spin crossover. There were highlights regarding porous framework materials, such as the pressure-induced polymerisation of small molecules within zeolites by **Julian Haines**, and the rich phase behaviour and structural flexibility of the linker orientation in metal-organic frameworks when exposed to high gas pressures by **Jorge Sotelo** and **Michael Wharmby**. As one person remarked, the results highlighted that these materials "are far from being dead". We also discovered that there existed naturally-occurring metal-organic framework (specially designed by nature) from **Igor Huskić**. From an oxide ceramic perspective there were many impressive talks on magnetism and multiferroicity; an approach taken by **Ana Sanchez** to study the dynamic polar nanoregions using transmission electron microscopy was particularly interesting. From the biological perspective,

**Henry Chapman** impressed us all with his structural models of complex proteins, solved using X-ray free-electron laser diffraction collected in the femtosecond timescale: the trick is to obtain diffraction before destruction.

During the conference, there were many opportunities to discuss with other crystallographers: over the poster sessions, coffee and lunch breaks, and perhaps less formally during the Young Crystallographers Mixer party and the various boat rides from the hotel to the conference center (yes, many of the hotels were located on islands!).

The closing ceremony included a showcase for the forthcoming exciting events: the third European Crystallographic School to be held in very scenic Bol, on the island (!) of Brač in Croatia, and the next European Crystallographic Meeting in the European Alps country, in Basel, Switzerland! In summary, it was a very successful conference in a relaxed and sunny atmosphere.

**Ines Collings**  
University of Bayreuth

**JUST** as I stepped out of the transport in the city of Rovinj, I luckily witnessed the annual summer festival fireworks; and whilst staring in awe, I was getting the feeling that this was going to be a memorable conference. As I headed out for my first pre-conference session, the light of dawn revealed a breathtakingly picturesque scene. Daylight reflected a completely colourful and vibrant coastal city, with houses splashed in pink, yellow and stone white; definitely a beautiful place worth getting lost in. It was quite difficult to resist staring at the turquoise blue sea whilst walking down the cobbled streets to the conference venue.

The Young Crystallographers' Satellite Meeting had a range of fascinating talks, including beamline tips and tricks, protein structural and high-pressure crystallographic studies. The evening continued with the opening ceremony of the 29<sup>th</sup> European Crystallographic Meeting, which kick-started with lively Croatian A Cappella music and an amazing talk on synchrotron radiation in crystallography by Professor **John Helliwell**, winner of the 8<sup>th</sup> Max Perutz Prize.

The welcome reception party was a great success of a social with a never ending buffet of canapés and Istrian wine. Also, there was a bar right outside the hall in the conference centre to try out some very good Ožujsko!

The 'How to?' session the next day helped me personally gain a deeper insight into working in both industry and academia. Luncheon seminars included a crystallographic software fayre, where new developments in software were presented. Posters were set up according to the participants' focus areas, helping to create a flow of new ideas and form new networks. The exhibition was enjoyable and impressive, with lots of activities and a great showcase of in-house diffractometers and crystallisation screen optimisers. One thing I forgot to pack for Rovinj was sunglasses but that too was being handed out by Rigaku!

The four-day scientific programme was filled with a diverse collection of crystallographic sessions, from crystalline processes at ambient and non-ambient conditions to

molecular machines and motors. Professor **Titia Sixma**'s keynote on trapping a transient state in DNA mismatch repair was very awe-inspiring. As a DNA crystallography student, the microsymposium on nucleic acids and their complexes was of the best interest for me, although truth be told, I was equally inspired by every session I attended. Two particular highlights for me out of my research area were the works presented as plenary lectures by Professor **Henry Chapman** on serial crystallography with X-ray free-electron laser pulses, and Professor **Andrea Ferrari** on graphene as the future's emerging technology.

Social events were scheduled for every evening throughout the conference, including an open air mixer for young crystallographers, a concert and a conference dinner with live music; providing ample time for networking. The meeting came to an end with an award ceremony of 20 poster prizes! To conclude, the conference was definitely one to remember. Not only did it have everything you could wish for in an international conference: great weather, beautiful location, amazing food and a very engaging programme but it also provided an ideal opportunity to explore, learn and share new concepts within the strong and enthusiastic crystallographic community.

**Sarah Gurung**  
University of Reading

**THE 29<sup>th</sup> ECM was held on the 23<sup>rd</sup>-29<sup>th</sup> of August in the beautiful town of Rovinj, Croatia. I was extremely excited to attend my first international conference with the opportunity to present my own work.**

My conference began two days before the main meeting at the 'Metadata for raw data from X-ray diffraction and other structural techniques' satellite meeting, where I had been invited to speak. The meeting was organized by the IUCr's Diffraction Data Deposition Working Group, which aims to work on the practicalities that would lead to the routine deposition of raw diffraction images alongside structure factor and CIF files. It was a packed two day programme of informative presentations and, at times, lively discussion. Giving my first academic talk at the meeting was initially a daunting prospect but I am grateful to have had this experience in the first year of my PhD. Arriving early also meant that I caught the tail end of 'Rovinj's Night', a yearly festival which included musical performances throughout the town and culminated in a spectacular fireworks show over the harbour.

There was no rest after the satellite meeting, as that evening ECM29 was officially opened and we were treated to performances of traditional Croatian A capella singing and the Max Perutz Award lecture, given by **John Helliwell**.

Over the 4 days at the main meeting I attended many interesting sessions. Being a young crystallographer, I found the "How to?" microsymposium extremely useful: **Rachel Macmaster**, **Alessia Bacchi** and **Mathias Meyer** detailed how to they began careers in industry, while **Simon Coles** and **Sine Larsen** described their careers in academia, all imparting invaluable tips and advice on subjects such as interviews, CVs and desirable soft skills to younger members of the audience.

As my research is mainly focussed on the improvement of charge density data refinements, the 'Charge Density

Studies' microsymposium was an excellent opportunity to find out about recent advances in the field. In particular, **Emmanuel Wenger**'s presentation about the XPAD hybrid pixel detector and **Krzysztof Wozniak**'s talk on the improvement of single crystal structural refinements were both very engaging and relevant to my own research.

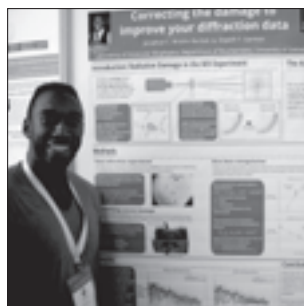
I also had my first experience of presenting a poster at a conference. Thankfully, it was less terrifying than giving a talk, and provided a great chance to explain my research to people, which prompted many helpful and interesting conversations.

Alongside the fantastic presentations, the ECM provided me with the opportunity to discuss ideas in less formal settings. I was excited to meet many other young crystallographers as well as getting the chance to have conversations with exhibitors about their products, some of which I use in my research. I even managed to sneak some sightseeing in, exploring Rovinj's old town and braving the climb to the top of the church tower to get some spectacular views of the city.

And then it was over, the closing ceremony held and poster prizes distributed – I was honoured to be awarded one of the CCDC Poster Prizes for Younger Scientists. All in all, I thoroughly enjoyed ECM29 and I am extremely grateful for bursaries awarded by the ABBF, RSC and IUCr, which enabled me to attend the meeting.

**Natalie Johnson**  
University of Newcastle

## BCA Members at ECM29



*Jonathan Brooks-Bartlett at his poster*

(Pictures courtesy of Carl Schwalbe)



*Elspeth Garman introducing Plenary Lecturer Henry Chapman*

(Pictures courtesy of HUK)



*Rovinj harbour looking towards the conference centre*

(Pictures courtesy of Joan Schwalbe)

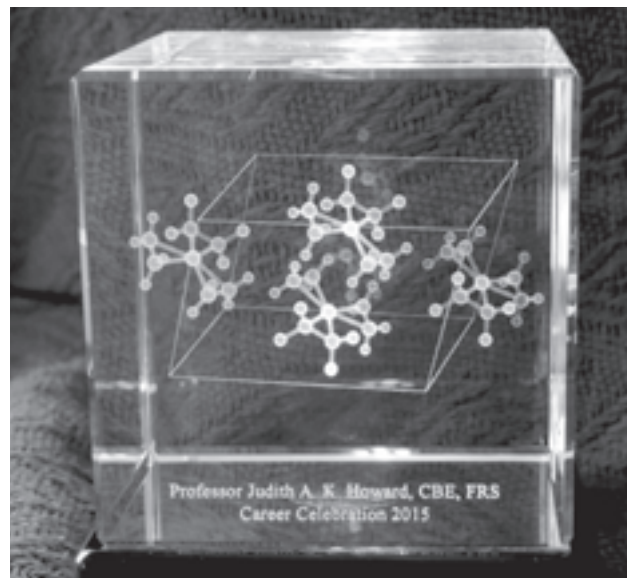
# Career Celebration – Professor Judith A. K. Howard

A surprise career celebration was organised for Judith in Durham over the 17th-18th of September 2015. Whilst Judith was informed that a small meeting was occurring, to keep the dates free in her busy diary, the full details of the events and participants were kept secret thanks to the efforts of the invitees. Indeed in one University this included attendees being surprised to find their departmental colleagues were also attending and in another case on the day one participant was shoved into a room to avoid meeting Judith in the corridor before the event started! Consequently Judith was very pleasantly surprised on the day by the many friends and colleagues, including a large number from outside the UK, who had gathered to celebrate her many achievements.



*Judith in the audience*

A fascinating range of talks were presented during the day crossing from chemical crystallography through biological studies, instrumentation developments and into spectroscopy. The talks were given by collaborators as well as former PhD students and PDRA's and highlighted the wide ranging contributions that Judith has made and is continuing to make within crystallography and through the formation of cross-disciplinary links: **Simon Parsons** highlighted the benefit of employing energy calculations to provide understanding of crystal structures and not focussing solely on hydrogen bonds; **Elsbeth Garman** discussed the benefits of low temperature crystallography in biological studies noting Judith's contribution to the development of various pieces of low temperature equipment; **David Albesa-Jové** a former PDRA acknowledged Judith's support in helping him move from small molecule to protein crystallography and discussed the enzymatic activity of a GT-8 glycosyltransferase at a membrane interface; **Siva Umapathy** discussed the potential for using spectroscopy to aid with diagnosis particularly for some types of tumour which will hopefully help surgeons target patient treatment; **Michael Probert** highlighted some of the low temperature and high pressure research that has been carried out on the XIPHOS instruments he helped to develop whilst working in Judith's group; **Helena Shepherd** gave an interesting talk on spin-crossover Fe complexes she has studied which included a nice video that showed a spin-transition propagating across a crystal; **Horst Puschmann** discussed recent developments in Olex2 and additional plug-ins that are being released



alongside a new OlexSys product LabSafe; **Masaki Takata** presented some of his studies using a MaxEnt charge density methods and the interesting results that can be obtained; **Jane Endicott** provided the final biological talk of the day discussing the regulation of CDKs in relation to inhibitor design and **Jason Cole** discussed how he got involved with the CCDC initially as part of Judith's group and looked at some of the research arising from the Cambridge Structural Database and recent software developments.

In the middle of the day there were brief talks from **Tony Watts** (University of Oxford) on Judith's contribution to the British Biophysical Society and **David Parker** (Durham University) on Judith's contribution to Durham Chemistry and more widely. These were followed by a small presentation to commemorate the event which was made to Judith and comprised of some flowers and a laser etched glass block. The laser etched glass block contained a representation of bis(ethylene)(tetrafluoroethylene) platinum (Howard, J.A.K., Spencer, J.L and Mason, S. A. (1983) *Proc. R. Soc. London*,



*Elevating the glass model of her early crystal structure*





Ser. A., **386**, 145-161) a structure that arose from some challenging work that Judith had done early in her career for which she had 'worked in a cold room dressed in hat, gloves etc to mount the crystals and slow the decomposition'. It was lovely that both of her co-authors on that paper, **John Spencer** and **Sax Mason**, were able to attend the symposium and also chair sessions along with our other two session chairs **Ehmke Pohl** and **Philippe Guionneau**.

During the day there were plenty of chances to socialise over coffee at registration, lunch and an afternoon wine/soft drink reception that followed the presentation; these breaks also provided an opportunity for attendees to study photos collated onto four posters from throughout Judith's career. The evening saw a number of friends from outside chemistry join the celebration to enjoy a hearty hot buffet followed by a ceilidh. The ceilidh provided a great deal of fun as people tried to remember the various steps in the right order to master the dances and many including Judith barely left the dance floor throughout the evening. The following day saw a smaller group of participants, including many who had travelled quite long distances to attend the event, taking a coach trip to Beamish Museum to experience life from the 1800-1940s; this provided a nice relaxed follow-on from the previous day's celebrations.

Throughout the two day event, alongside the recognition of Judith's significant research contributions, there were also numerous recollections of her generosity and grateful acknowledgment of the help and support that she had provided to many participants which had helped them to progress within their career. Indeed, I along with many other former members of her group fondly remember our time working in Judith's group with freedom to test and develop



research ideas, the supportive 'family' atmosphere she creates within the group and her continued efforts to help us progress in our careers in whatever direction we choose are much appreciated.

I would like to thank **Horst Puschmann** and **Alex Griffin** who took a large number of photos during the career celebration enabling us to put together a photobook reminder of the two days for Judith after the event. Finally, thank you to my co-organisers **Irene Harries** (Durham University), **Ehmke Pohl** (Durham University) and **Michael Probert** (Newcastle University) for all of their help coordinating the event.

**Hazel Sparkes** (University of Bristol)



# Symposium Celebrating the Career of Judith Howard

**INVITED** in great secrecy by the “Team of Conspirators” (Hazel Sparkes, University of Bristol; Irene Harries, Durham University; Ehmke Pohl, Durham University; Michael Probert, Newcastle University) friends and colleagues of Judith from around the world gathered in Durham on September 17 for a symposium that would do credit to any scientific society meeting.

**Simon Parsons** (University of Edinburgh) started the proceedings with a powerful message, “How focussing on hydrogen bonds can miss the big picture”. Comparing two recent papers about phase transitions in glycine, he categorised the “Desiraju approach” looking at specific interactions such as hydrogen bonding and  $\pi$  stacking, and the “Dunitz approach” using energy calculations. Calculations with the PIXEL methodology correctly showed that  $\gamma$ -glycine should be most stable under normal conditions. At 40 GPa a sluggish change to layered  $\epsilon$ -glycine occurs. This layered structure has N-H...O hydrogen bonds supported by C-H...O interactions. However, according to energy calculations, 6 out of 14 of the latter are repulsive. Full interaction maps are also instructive: there is one mismatch between found and expected oxygen atom positions in the  $\epsilon$  form, which may explain its lesser stability under ambient conditions. Simon’s conclusion was that the synthon approach is an excellent guide to synthesis but not to stability.

**Elspeth Garman** (University of Oxford) discussed “Low temperatures: links between small and biological cryocrystallography”. For small molecules low temperature has the advantage of lower displacements, less thermal diffuse scattering and reduced radiation damage. Such high-quality data may support charge density studies. Interesting phase transitions may occur. Judith’s group at Durham has made major advances in low-temperature apparatus design. Their Fddd diffractometer is able to get down to 9 K, and XIPHOS at Durham holds the record for a home lab: 2 K for the structure of *m*-nitroaniline. For macromolecules by far the greatest benefit is diminution of radiation damage. Primary radiation damage is unavoidable; but secondary damage, e.g. by the products of water radiolysis, can be reduced to about 1/70 by cooling from room temperature to 100 K.

**David Albessa-Jové** (University of the Basque Country) showed us how “Secondary structure reshuffling modulates the enzymatic activity of a GT-8 glycosyltransferase at the membrane interface”. The mycobacterial cell envelope contains unique glycolipids and carbohydrates. Glycosyltransferases and acyltransferases are involved in the PIM biosynthetic pathway. PimA initiates the biosynthesis. The catalytic centre is near a fissure. Substrate binding appears to start with GDP-Man. Differential scanning calorimetry shows changes in melting temperature that indicate substrate-induced conformation changes. PimA in solution was visualised by SAXS.

**Siva Umapathy** (Bangalore University) took us firmly into the field of spectroscopy with “Laser spectroscopy applications to biology and medicine”. He pointed out that Judith was always willing to cross disciplines; and spectroscopists, like crystallographers, are interested in bonds. Lasers have the advantages of a small focal spot and fast pulses. A single bond vibrates in 5–8 fs, and a laser can match this. While a living cell gives complex spectra, a Raman microscope can resolve them analytically and monitor tissue distribution. In the

case of glioblastoma, spatial markers of different types aid location of tumour margins and staging, thereby facilitating appropriate treatment. In a mouse model of liver injury from paracetamol, a Raman shift gives the earliest indication of damage. Monitoring of neonates’ blood circulation to the brain, now done with near-infrared, may work better with Raman spectroscopy.

After lunch **Michael Probert** (University of Newcastle) began by describing his interview with Judith for a PhD studentship, which included the opera and dinner as well as lots of discussion about science. His talk, “From low points to high times: crystallographic extremes”, gave us more details about the record-breaking XIPHOS-1 diffractometer. X-rays came from a 5.4 kW rotating anode source with Helios focusing optics. Since the crystal could not be aligned optically, least-squares analysis of area detector positional data had to be employed. Cooling a crystal of *m*-nitroaniline to 2 K reduced thermal parameters by ca. 50% compared with 100 K. Overlap with diffraction from the container caused trouble, but re-measurement at a different distance resolved the peaks since they had different origins.

**Helena Shepherd** (University of Kent) told us about “Understanding structure and exploiting properties in functional molecular materials”. Certain Fe(II) complexes display spin crossover (SCO) as temperature or pressure are changed. Since the high-spin (HS) state has longer and weaker metal-ligand bonds than low-spin (LS), SCO results in volume changes that may be useable in actuators. As a single crystal of Fe(babpby)(NCS)<sub>2</sub> is heated, transitions from HS with  $Z' = 0.5$  to an intermediate phase with commensurate modulation to low-spin with non-merohedral twinning are observed. In Fe(dppz)<sub>2</sub>(NCS)<sub>2</sub>.Py at low temperature and ambient pressure the aromatic ring “scissors” have a wider opening in HS than in LS; raising the pressure encourages opening and delays closing. A flat crystal attached to a passive support bends impressively as SCO occurs. Dispersion in a polymer may work for other morphologies of SCO material.

**Horst Puschmann** (OlexSys) led us into “Adventures with Olex2”. He acknowledged the importance of Judith’s support in the development of this fully-featured package for small-molecule crystallography that is free and open source. Because 97% of small-molecule refinements are done with SHELXL, this software has been incorporated into Olex2. Olex2 is user-friendly enough that it enables interested chemists to perform their own structure determinations. Horst gave an impressive demonstration of solving and refining a disordered structure. In the question period afterwards, he was asked if Olex would eventually be expanded to encompass incommensurate structures. He replied that the JANA group does this outstandingly well, and there is no need to duplicate this work.

The next two talks had a strong focus on Judith herself. **Tony Watts** (University of Oxford), in a “Brief summary of Judith’s connections to the BBS”, described how, when he took over the chair of the British Biophysical Society (BBS) in 2009, he was concerned about future prospects for this long-established but small society. Consulting with Judith, he received two pieces of advice: (1) get recognised, and increase the society’s appeal to young researchers via the Young BBS awards; (2) link up with other groups such as the Royal Society of Chemistry (RSC) and the Institute of Physics (IoP). This approach is bearing fruit in the form of the World Biophysics Congress in 2017 being organised by the BBS and IoP. **David Parker**, a professorial colleague of Judith at Durham, gave a “Brief summary of some aspects of Judith’s career (to date)”. Durham

had a Chair of Crystallography in the 1970s, but this was lost in the cuts of the 1980s. When this chair was re-activated in 1991, Judith was the preferred candidate and was persuaded to come. She can trace her scientific ancestry by way of Dorothy Hodgkin, J D Bernal, W H Bragg... all the way to Isaac Newton. David reminded us that, along with everything she had done for Durham, as Scientific Chair she worked closely with Local Organiser Chris Gilmore for the very successful IUCr Congress in Glasgow in 1999.

The talks resumed after a very enjoyable reception with wine, soft drinks and snacks. **Masaki Takata** (Tohoku University), in his talk entitled "Progress, challenge and perspective of the MaxEnt charge density study on smart crystallography", blew away some more of our prejudices. I had thought that one needed a single crystal of exceptional quality to carry out a charge density study. However, Masaki was able to calculate charge densities from synchrotron powder diffraction data recorded at SPring8 on a large Debye-Scherrer camera designed to minimise absorption and extinction. Use of the maximum entropy method treats the imperfections in the data. Si from NIST yielded a set of high-quality powder data at a wavelength of 0.4 Å in an exposure time of just 20 minutes. Studies carried out by this method include finding metals encapsulated in a fullerene molecule, oxygen physisorption by a MOF and hydrogen-nanopore interactions. After the lecture a questioner asked whether the charge densities were really as good as those from a single crystal. A test of powder *versus* single-crystal data at SPring8 actually came out in favour of the powder data.

**Jane Endicott** (University of Newcastle) told us about "regulating CDKs – lessons for inhibitor design". CDK complexes control the eukaryotic cell cycle. The CDKs themselves do not change concentration; but their regulators, cyclins, do. Although the CDKs have some overlapping functions, they are still distinct. They are deregulated differently in different cancers. While the residues within the CDK active site are conserved, there are a few notable differences. The compound NU6300 is an irreversible inhibitor of CDK2, and some cancer cells appear "addicted to CDK2". Inhibition of CDK2 is not life-threatening: knockout mice without CDK2 are viable though infertile.

In his lecture "From structures to knowledge: the application of crystal structural data to molecular modelling" **Jason Cole** (CCDC) began by recalling his early days as one of Judith's first PhD students at Durham, also getting valuable guidance from Frank Allen. Displays of Judith's largest and smallest structures, space groups represented and co-authors clearly illustrated the collaborative mindset and breadth of interests in Judith's group. Jason went on to illustrate the value of the database for the design of molecules. (1) Affinity and conformation: locking a torsion angle by methylation at the right value to fit a receptor can improve affinity. (2) Scaffold replacement: overlays of active structures can define a pharmacophore; searching for this group in the Cambridge Structural Database (CSD) can find it attached to new scaffolds. (3) Solubility by design: *t*-butyl groups have specific packing patterns and rings tend to stack; changing to isopropyl esters and making central rings less planar may destabilise the crystal and increase solubility. The CSD is being adapted to meet modelling needs by providing web-based tools.

**Carl Schwalbe**



## Next ACA Meeting

**THE** 66th Annual Meeting of the American Crystallographic Association (ACA) will be held in Denver, Colorado, July 22 – 26. The transactions symposium will highlight Structural Dynamics across the disciplines represented by the ACA. The rest of the meeting will continue to reflect the wide reach of crystallographic research with sessions on sources, methods, and results. These include Opportunities from new and improved instrumentation, single/multiple crystal, powder and solution methods, and hot structural results. There will be sessions highlighting those results requiring complementary techniques

including cryo-electromicroscopy. Invited speakers include this year's honorees, **Jason Benedict** (SUNY Buffalo), **Axel Brunger** (Stanford University), **Elsbeth Garman** (University of Oxford), and **Benno Schoenborn** (Los Alamos National Laboratory).

The meeting will include a strong educational component for early career scientists with specific talks designed to introduce research areas in addition to presenting results. Related evening sessions include a mixer, career development, and diversity in the laboratory. The conference will end with a closing banquet and the award of poster prizes for the best presentations.



# Outreach Activities

**BCA** members are livelier than ever these days when it comes to Public Engagement and Outreach and activities can range from schools visits to science fairs by individuals or large groups. We should not only note these great contributions, but also use them to inspire others, so from summer 2015 here is the first of what I intend to be a regular biannual roundup of activities. This is undoubtedly not comprehensive as it's difficult to keep up with everything (especially if I don't know about it!), so please do get in touch with me ([s.j.coles@soton.ac.uk](mailto:s.j.coles@soton.ac.uk)) and provide summaries of your own updates and I will incorporate them into upcoming roundups. Even better, brief news pieces can be made available on the BCA Education website, 'What's in a Crystal?', – check out <http://learn.crystallography.org.uk/> for more detailed accounts of items in my summary below...

The most significant event of the summer was the Cheltenham Science Festival – and **Pam Thomas** led a large presence from Warwick University that had a significant crystallography component. The highlights from the Warwick 'What If' tent were the Crown Jewels on display (!) – these were grown by D Prabakharan, a Crystallography Ideas Café and a Family Day incorporating many of our 'The Structure of Stuff is Sweet' activities. **Jonny Brooks-Bartlett** and the inimitable **Mike Glazer** played a big part in the crystallography activities, in fact Mike's contributions to outreach are far too numerous for me to summarise here, but fortunately he provides plenty of information himself – I suggest you follow him on Twitter (@MikeGlazer1)!



*A montage of activities at the Cheltenham Science Festival.*  
(Pictures courtesy of Mike Glazer)

The prize for furthest afield in the UK goes to **Michael Wharmby** of Diamond Light Source who spent a week putting on no less than 5 events up at the 25th Orkney International Science Festival in September! "First, I organised and ran an exhibition at the Nautical School in Stromness, showcasing Diamond Light Source – "Diamond Light Source: Light for Science", explaining what Diamond is, how the machine works and highlighted some science done there, specifically

*the Foot & Mouth Disease Virus vaccine. To complement the exhibition and as part of the International Year of Light, I gave a talk at Stromness Library, "Brought to Light – The History & Future of Earth's Greatest Resource". I then gave a talk in the art department at Orkney College, Kirkwall, which was a review of what crystals are, how they're studied and where we find them. Furthermore I went to a couple of local schools (P7 pupils at Dounby Primary School and P5, P6 and P7 at Stenness Primary School) to give talks on tilings, which included making Escher tiles and this was then linked back to crystals. I also took one of Diamond's Lego Beamlines and the pupils had the chance to collect their own diffraction patterns."*

**Lynne Thomas** took part in Soapbox Science in July – an event designed to raise the profile of female scientists which involved standing on a soapbox in central Bristol for an hour talking to the passing general public. It was a scorching day, which encouraged (unintentionally) some polymorph conversion in chocolate, but also provided plenty of opportunities to talk about the wonders of ice! She has also been busy with colleagues in Bath, developing a Chemistry of your Smartphone exhibit funded by the Royal Society of Chemistry. It features the crystallography of the production of silicon and the workings of lithium ion batteries and she took this to the Big Bang Fair South West and a Family Science day in Dorchester.

At YorNight (European Researchers' Night, York – 25 September), **Michael Wharmby** ran a hands-on exhibit on light and Diamond. This included posters and videos, demonstrations of the properties of light, making crystals from marshmallows & cocktail sticks, one of Diamond's Lego Beamlines and a 3d printed model of the outside shell of foot & mouth disease. The Kings Manor venue had about 1000 visitors over the course of the evening.

Finally, I have been managing to get out and about a bit myself, with the highlight of my summer definitely being an invite to open the inaugural Sardinian 'Pint of Science' public debate event in July – held at an artisan brewery 20 miles outside of Cagliari!

We are continuing in the coming year (March 16-19) to attend the Big Bang Science Fair. This is by far and away our biggest showcase and a tremendous event – so I hope this update of great recent contributions inspires you to sign up and help out when the request is circulated!

**Simon Coles, Education and Outreach Coordinator.**



# News from the Cambridge Crystallographic Data Centre



## The CCDC Celebrates the 800,000th Structure in the Cambridge Structural Database

Essential resource for scientists worldwide hits another record

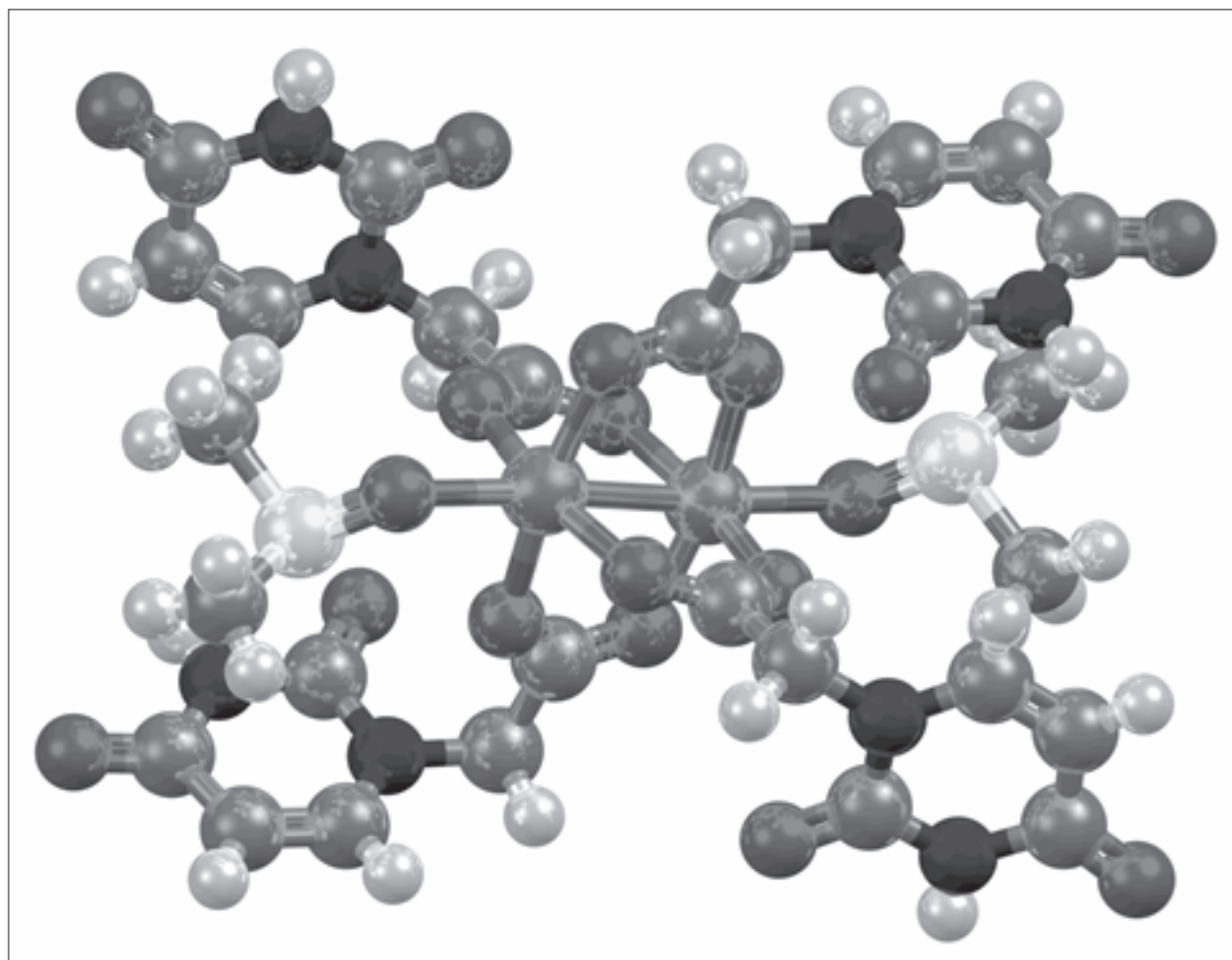
**THE** Cambridge Crystallographic Data Centre (CCDC) announces that the Cambridge Structural Database (CSD) has passed the milestone of 800,000 expert-curated

experimental crystal structures with the addition of a novel metal-organic paddle-wheel structure from researchers in Spain.

The CSD's 800,000th entry is a metal organic copper structure (CSD refcode: TUWMOP), published by **Khaled Hassanein, Oscar Castillo, Carlos J. Gómez-García, Félix Zamora** and **Pilar Amo-Ochoa** in *Crystal Growth and Design*. Knowledge of this structure, coupled with the wealth of structures in the CSD, will inform the design of new materials, and will be used to predict new crystal structures and validate X-ray data.

Pilar Amo-Ochoa, from the Instituto de Ciencia Molecular (ICMol), Spain, said, "We are delighted that our structure, *tetrakis(μ-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)acetato)-bis(dimethyl sulfoxide)-di-copper(ii) dimethyl sulfoxide solvate*, is the 800,000th entry in the database. We use the CSD in order to know the number of structures containing paddle-wheel type copper(ii) units with ligands of biological interest. Being able to have access to and share the very latest novel

continued ➤



metal organic structures with the world is fundamental to our understanding of these frameworks and complexes."

"The remarkable growth of the CSD is testament to the ongoing commitment of the crystallographic community to share their results to benefit scientists everywhere," commented **Colin Groom**, Executive Director of the CCDC. "Fifty years on from the first crystal structure collection we are reaping the benefit of this unique data resource by learning more and more about the wonderful interplay between molecular conformation and molecular interactions."

**Robin Rogers**, Editor, Crystal Growth & Design added, "I have always been a big fan of the power of the CSD and what it brings to the scientific community, and indeed was very pleased when my own structure was celebrated in 1999 as the 200,000th structure in the CSD. One of my primary goals in founding Crystal Growth & Design with the ACS has been to forge strong collaborations with the CCDC. I am delighted that one of our papers contains the CSD's 800,000th entry and I will continue to work for seamless cooperation between our authors, reviewers, and readers and the invaluable services provided by the CCDC."

The Manager of the Cambridge Structural Database, **Suzanna Ward** commented, "It is exciting that the 800,000th entry has been shared through the CSD so soon after we hit ¾ million entries. This demonstrates both the sheer number of crystal structures published annually in scientific articles as well as the growth in otherwise unpublished structures being shared through the CSD as Private Communications."

The CSD's 800,000th structure can easily be viewed online at <http://dx.doi.org/10.5517/cc1jj92f>

Ref: Khaled Hassanein, Oscar Castillo, Carlos J. Gómez-García, Félix Zamora, Pilar Amo-Ochoa, Crystal Growth and Design, 2015, DOI: [10.1021/acs.cgd.5b01110](https://doi.org/10.1021/acs.cgd.5b01110)

### About the 800,000th structure

This particular structure is a di-copper paddle wheel with four bridging uracil-1-methylcarboxylato ligands and two dimethyl sulfoxide molecules occupying the apical positions. These dimeric entities are able to involve the entire uracil residue in base pairing interactions to provide supramolecular sheets. Di-copper paddles have been used since ancient times as pigments and fungicides and are today used in organic syntheses as catalysts or oxidizing agents. A simpler copper paddle wheel structure, namely copper acetate monohydrate, was critical in the development of modern theories for antiferromagnetic coupling. Uracil is one of the four nucleobases in the nucleic acid of RNA and it was originally discovered by Alberto Ascoli in 1900.

all of the test systems, which included the complexities of polymorphs, salts and hydrates, were generated by one or more methods. In addition, a number of the target experimental structures were predicted to be the most stable form.

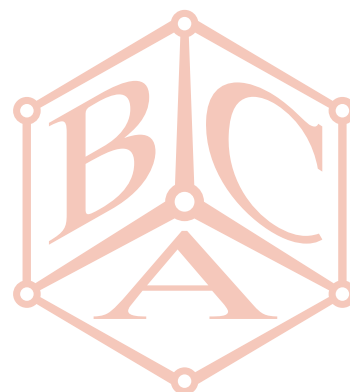
Participants in the blind test were invited to predict the full three-dimensional crystal structures of five previously unpublished compounds, starting solely from the chemical diagram and basic crystallization conditions. The participants came from a record number of 25 different groups, spread over 14 countries (Argentina, Austria, Canada, China, Germany, India, Italy, Japan, The Netherlands, Poland, Russia, UAE, UK, and USA).

The subjects of the test included a co-crystal, a large flexible molecule, a salt hydrate, and a drug molecule with five known but unpublished polymorphs; the drug molecule was released by a major pharmaceutical company especially for the blind test. The inclusion of the polymorphic drug molecule for the first time highlighted the value of crystal structure prediction-derived knowledge for identifying polymorph issues and opportunities for molecules of commercial importance. The salt hydrate is the first three-component system in the blind test, and potentially one of the hardest to predict, to date.

"Overall the target structures in this blind test were significantly harder than for previous tests," commented **Colin Groom**, Executive Director of the CCDC. "So the results this year are especially impressive. The increased participation and breadth of methods adopted underline the importance of crystal structure prediction methods, in particular for pharmaceutical R&D."

Professor **Richard Cooper**, Oxford University, who selected the target systems for the blind test added, "These targets were not model systems but were selected to represent real-life challenges. The remarkable results of this blind test demonstrate the huge potential of crystal structure prediction methods for informing experimental solid-state chemistry."

A paper detailing the full results of the blind test will be published as part of a special issue on organic crystal structure prediction of the International Union of Crystallography journal, *Acta Cryst. B*.



## CCDC Blind Test Showcases Major Advance in Crystal Structure Prediction Methods

**THE** Cambridge Crystallographic Data Centre (CCDC) announces that the results of its 6th blind test of crystal structure prediction methods demonstrate significant advancement in crystal structure prediction methods in comparison with previous tests. This year, structures of



## Eric James William Whittaker (1921–2015)

**Eric James William Whittaker, distinguished crystallographer, mineralogist and geochemist, died on Thursday 2 July 2015 in Kidlington, Oxfordshire, after a short illness. Born on 1 November 1921, he attended Stockport Grammar School and Derby School, where he showed an early aptitude for mathematics and science, and then took his BA degree (1943) in Chemistry at Magdalen College Oxford during the Second World War. The circumstances of the time were to influence his undergraduate research project since much university work was naturally directed towards the war effort. Using X-ray methods he investigated the structure of phases within the charcoal used in gas masks – an unusual but good experience in helping establish his crystallographic interests and expertise.**



On leaving Oxford, Eric joined the research team at the brake-lining manufacturer Ferodo UK (based in Derbyshire and a subsidiary of Turner & Newall, the asbestos manufacturing company) and started his long and successful research career into the structure of amphiboles and related minerals. An early ground-breaking achievement was solving the difficult problem, using X-ray diffraction, of the true nature of chrysotile fibres, a mineral of much importance to the industry. He revealed that their structure is based on silicate curved layers rather than chains. Indeed, chrysotile was to remain one of his favourite topics over many years, with its varieties and the nature of its cylindrical lattice. Many other seminal papers on mineral structure, especially for the asbestiform amphiboles and serpentines, were to follow, with several in association with other crystallographers including Jack Zussman.

Eric was a natural researcher but success within Ferodo led inevitably to promotion (1963) and to an increasing managerial role – as head of the Mechanical and Physical Sciences unit – and away from his favoured vocation. Within two years he had resigned to take up (1965) the lectureship in geochemistry at the Department of Geology, University of Oxford. But his time at Ferodo had given him exceptional experience in structural crystallography, established his reputation as a world authority on the structure of asbestiform minerals and had earned him a doctorate (1957) from the University of London. Oxford refreshingly gave him opportunities to work with new colleagues, students and methods, as well as to develop the postgraduate course for the Diploma in Geochemistry. Within two years he became Reader in Mineralogy (on the departure of Jack Zussman to the Professorship of Geology at Manchester University) until his retirement in 1983. This was a very fruitful period. Amphiboles were to remain his principal

focus, working with colleagues including Barbara Cressey and John Hutchison, on important topics such as the accommodation of defects and disturbances, the termination of lamellae, and the role of twinning within their structures. He also brought innovative approaches to other subjects such as silicate liquid structures and the application of ionic radii for use in geochemistry. Twice (1977 and 1978) he and his co-author Fred Wicks, received the annual Hawley medal of the Mineralogical Association of Canada for the best paper in their journal, on serpentine structures and textures.

Eric was indeed admired for his systematic and logical approach to all aspects of his work (the words ‘systematically explored’ often occur in his own publications). His clarity of thought could be daunting when in discussion with him about a research topic but it was always tempered by his gentle humour and infectious laugh. Not surprisingly, his text book with its purposeful title *Crystallography: An Introduction for Earth Science (and other Solid State) Students*, published in 1981, has a special elegance through its logical emphasis on the repeating pattern of atoms. His style and expertise also made him a valuable member over several years of the International Mineralogical Association’s committee on the nomenclature of amphiboles and his renown led to the amphibole Whittakerite being named after him.


Oxford also gave Eric a special role in his College – St Cross – where he was an official fellow from 1967 and Vice-Master for three years (1979–1982). He made a substantial and appreciated contribution during a phase of expansion and change especially with the College’s move to its new site in St Giles.

For many years Eric enjoyed the pastime of painting, in addition to his interest in ancient cultures and hieroglyphics. Later in his career he became interested in more theoretical aspects of crystallography, especially involving higher dimensions. He published his *An Atlas of Hyperstereograms of the Four-Dimensional Crystal Classes* (OUP, 1985) and became fascinated by Penrose patterns as soon as he learned of them and understood their relationship to higher dimensional lattices. He was delighted to be made an Honorary Life Fellow of the Mineralogical Society in 2010 in recognition of his considerable achievements.

He is survived by his two sons Anthony and Roger. His wife, Dorothy, whom he married soon after joining Ferodo, predeceased him. He is remembered with considerable affection by many colleagues and students especially for his invaluable help, encouragement and genuine interest.

**Paul Henderson**

*Reproduced with permission from an obituary by Paul Henderson, published in Mineralogical Magazine (2015), 79, 809–810.*



## 30<sup>th</sup> Meeting of the European Crystallographic Association

28 August – 1 September 2016

Congress Center Basel, Switzerland

<http://ecm30.ecanews.org>

**ECM-30** will be a four-day vibrant and intensive scientific meeting held between **August 28 and September 1, 2016 in Basel, Switzerland** and will provide many learning opportunities in every current aspect of crystallography.

In addition, there will be a Young Crystallographers meeting, workshops and user meetings, lunch meetings, and a social program, which will allow scientists from all over Europe and the world to meet, connect and exchange. Besides the satellite meetings, a visit to the free electron laser SwissFEL is planned.



Basel is a welcoming, active and enterprising city of open minded citizens who excel in business as well as in the arts. The famous Basel mathematicians Bernoulli and Euler are of course known to many of you. In addition to the architecturally interesting campuses of some leading pharmaceutical and chemical enterprises, world-renowned museums, like the Beyeler, the Vitra Design or the Tinguely museum with its modern architecture, are ready to welcome you.

The conference is located close to the Basel exhibition area, in the triangle between Switzerland, France and Germany. Within a 30 minute ride on public transportation, more than 1000 hotel rooms are available in Basel, St. Louis (France) or Weil am Rhein (Germany). It is well connected to Europe by car, by plane (Basel-Mulhouse-Freiburg Euroairport hosts many low cost carriers) and has frequent train connections to Germany, France, Italy and Austria.

We look forward to welcoming you to Basel in 2016!



Katharina M. Fromm  
University of Fribourg

Jürg Schefer  
Paul Scherrer Institute



# 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](mailto:c.h.schwalbe@hotmail.com). Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

## 9-10 December 2015

**New synchrotron radiation and optical techniques for nanoscale microscopy of biological systems: from single molecules to cells, Trieste, Italy.**  
<http://www.elettra.eu/Conferences/2015/NMBS/>

## 11 December 2015

Tender X-rays in Macromolecular Crystallography, Berlin, Germany.  
<http://hz-b.de/xraysmx>

## 14 December 2015

NMR Crystallography, Institute of Physics, London.  
[www.iop.org/activity/groups/subject/brsg](http://www.iop.org/activity/groups/subject/brsg)

## 16 December 2015

BCA Biological Structures Group Winter Meeting, Manchester.

## 8-10 January 2016

CCP4 Study Weekend, Nottingham.  
[http://www.ccp4.ac.uk/events/CCP4\\_2016/](http://www.ccp4.ac.uk/events/CCP4_2016/)

## 13-15 January 2016

Bio-XFEL STC 3rd Annual International Conference, San Juan, Puerto Rico.  
<https://www.bioxfel.org/events/details/64>

## 22 February – 4 March 2016

47th IFF Spring School : Memristive Phenomena From Fundamental Physics to Neuromorphic Computing, Jülich, Germany.  
[http://www.fz-juelich.de/pgi/EN/Leistungen/SchoolsAndCourses/SpringSchool/\\_node.html](http://www.fz-juelich.de/pgi/EN/Leistungen/SchoolsAndCourses/SpringSchool/_node.html)

## 25 February – 4 March 2016

36th Berlin School on Neutron Scattering, Berlin, Germany.  
<http://www.helmholtz-berlin.de/events/neutronschool/>

## 27 February – 2 March 2016

Biophysical Society Annual Meeting, Los Angeles, CA, USA.  
<http://www.biophysics.org/2016meeting/GeneralInfo/Overview/tabid/6242/Default.aspx>

## 27 February – 2 March 2016

Biophysical Society Cryo-EM Subgroup Symposium, Los Angeles, CA, USA.  
<http://www.biophysics.org/2016meeting/Program/Subgroups/CryoEM/tabid/6635/Default.aspx>

## 9-11 March 2016

9th International Workshop on X-ray Radiation Damage to Biological Crystalline Samples, Lund, Sweden.  
<http://indico.maxlab.lu.se/event/67/>

## 14-17 March 2016

24th Annual Meeting of the German Crystallographic Society (DGK), Stuttgart, Germany.  
<http://www.dgk-conference.de/>

## 29 March – 29 April 2016

HERCULES 2016 - European School. 26 Years of Neutron & Synchrotron Radiation Science, Grenoble, France.  
<http://Hercules-school.eu>

## 30 March – 2 April 2016

2nd International Conference on Image Analysis in Three-dimensional Cryo-EM, Lake Tahoe, CA, USA.  
<http://ncmi.bcm.edu/cryoem-software-2016>

## 4-7 April 2016

BCA Spring Meeting, Nottingham.  
<http://www.crystallography.org.uk/bca-spring-meeting-2016/>

## 10-14 April 2016

Powder Diffraction and Rietveld Refinement School, Durham.  
Contact [ivana.radosavljevic@durham.ac.uk](mailto:ivana.radosavljevic@durham.ac.uk)

## 11-12 April 2016

Understanding Complex Macromolecular Systems from Sparse Data: The Astbury Conversation, Leeds.  
<http://www.astburyconversation.leeds.ac.uk/>

## 11-15 April 2016

SCTE: 20th International Conference on Solid Compounds of Transition Elements, Zaragoza, Spain.  
<http://scte2016.unizar.es/>

## 24-29 April 2016

RapiData 2016. 18th Annual Course, Stanford, CA, USA.  
Contact [ana@slac.stanford.edu](mailto:ana@slac.stanford.edu)

## 29 April – 1 May 2016

Protein Structure, Dynamics and Function, Providence, RI, USA.  
<http://www.brown.edu/conference/sailing-the-protein-seas/>

## 27 May – 5 June 2016

High-Pressure Crystallography: Status Artis and Emerging Opportunities. 49th Erice Course, Erice, Sicily, Italy.  
<http://www.crystallrice.org/2016/>

## 6-9 June 2016

IWPCPS-17: International Workshop for Physical Characterization of Pharmaceutical Solids, Winter Park, FL, USA.  
<http://www.assainternational.com/workshops/iwpcps-17/>



**12-15 June 2016**

15th European Powder Diffraction Conference (EPDIC15), Bari, Italy.

<http://www.ba.ic.cnr.it/epdic15/>

**19-22 June 2016**

74th Device Research Conference (DRC 2016), Newark, DE, USA.

<http://www.mrs.org/drc-2016/>

**22-24 June 2016**

58th Electronic Materials Conference, Newark, DE, USA.

<http://www.mrs.org/58th-emc/>

**27 June – 3 July 2016**

International School on Fundamental Crystallography with Applications to Electron Crystallography, Antwerp, Belgium.

<http://www.crystallography.fr/mathcryst/antwerp2016.php>

**3-8 July 2016**

ICCBM-16. 16th International Conference on the Crystallization of Biological Macromolecules, Prague, Czech Republic.

<http://www.iccbm16.org/>

**4-8 July 2016**

3rd International School on Aperiodic Crystals, Antwerp, Belgium.

<https://www.uantwerpen.be/en/summer-schools/aperiodic-crystals/>

**6-8 July 2016**

British Biophysical Society Biennial Conference, Liverpool.

[www.bbs2016.co.uk](http://www.bbs2016.co.uk)

**10-14 July 2016**

American Conference on Neutron Scattering, Long Beach, CA, USA.

<http://www.mrs.org/acns-2016/>

**10-15 July 2016**

18th International Conference on Metal Organic Vapor Phase Epitaxy (ICMOVPE-XVIII), San Diego, CA, USA.

<http://www.mrs.org/icmovpe-xviii/>

**22-26 July 2016**

American Crystallographic Association Annual Meeting, Denver, CO, USA.

<http://www.americalcrystalassocn.org/content/pages/main-annual-meetings>

**1-5 August 2016**

Denver X-ray Conference. 65th Annual Conference on Applications of X-ray Analysis, Rosemont, IL, USA.

<http://www.dxcicdd.com/>

**21-24 August 2016**

12th International Conference on Biology and Synchrotron Radiation (BSR), SLAC National Accelerator Laboratory, CA, USA.

<https://conf-slac.stanford.edu/bsr-2016/>

**28 August – 1 September 2016**

European Crystallographic Association Meeting, Basel, Switzerland.

<http://ecm30.ecanews.org/ecm2016/home.html>

**4-9 September 2016**

The 54th European High Pressure Research Group (EHPRG) International Meeting on High Pressure Science and Technology, Bayreuth, Germany.

<http://www.ehprg2016.org/>

**11-15 September 2016**

5th International Conference on Metal-Organic Frameworks & Open Framework Compounds (MOF 2016), Long Beach, CA, USA.

<http://www.mrs.org/mof-2016/>

**25 September - 2 October 2016**

3rd European Crystallography School (ECS3), Bol, Croatia.

<http://3rdEuropeancrystallographyschool.weebly.com/>

**2-7 October 2016**

MEDSI2016. Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation, Barcelona, Spain.

<https://indico.cells.es/indico/event/42/>

**2-7 October 2016**

International Workshop on Nitride Semiconductors (IWN 2016), Lake Buena Vista (Orlando), FL, USA.

<http://www.mrs.org/iwn-2016/>



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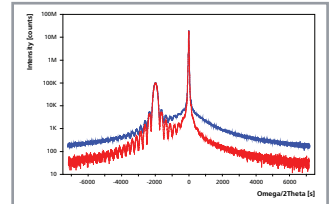
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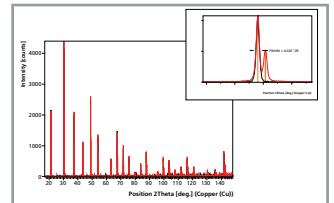
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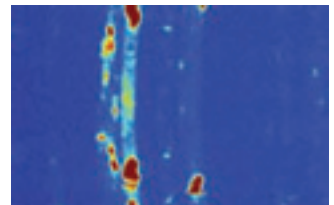
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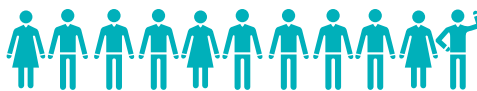
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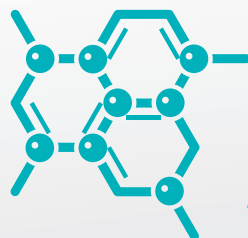
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