Crystallography News

British Crystallographic Association

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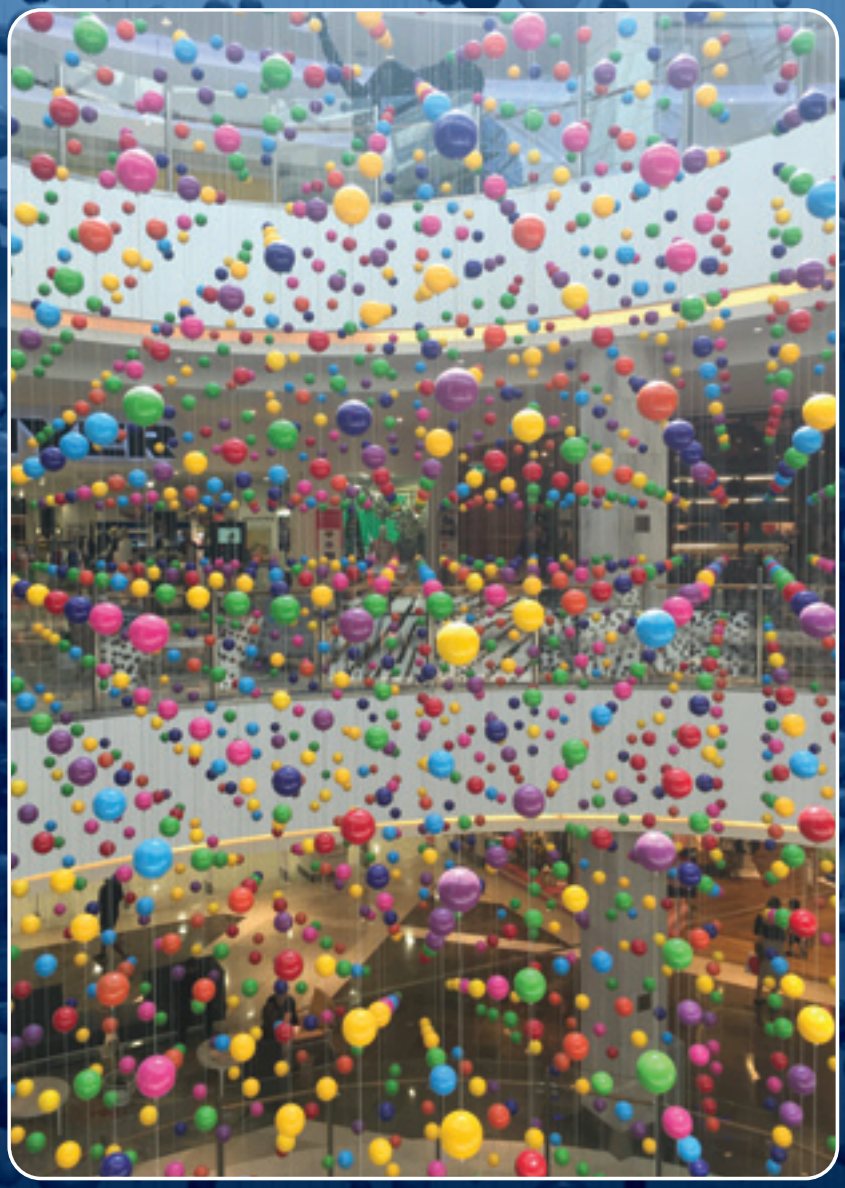

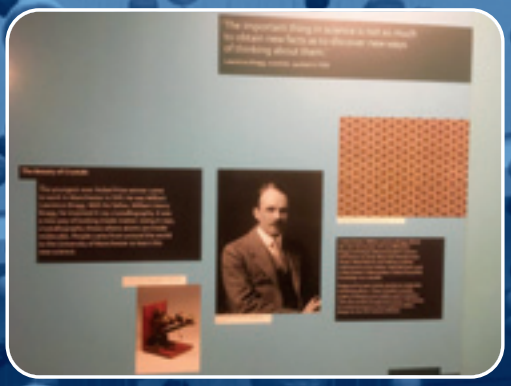

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Particularly in an industrial or applied context relating to the structure and properties of materials?

Then the Industrial Group of the BCA wants to hear from you!

We have spaces available on our committee and seek keen scientists with an interest in the application of crystallography.

For more information please contact Helen Blade – ***Helen.Blade@astrazeneca.com***

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Please ensure that items for inclusion in the March 2020 issue are sent to the Editor to arrive before 25 January 2020.

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This month's cover:

Serendipitous Crystallography Exhibits

From the President

THE recent meeting of the BCA Council was sadly diminished by the absence of Carl Schwalbe as editor of *Crystallography News*, and our purveyor of warmth and good sense. An obituary for Carl, written by John Helliwell, appears elsewhere in this issue. Simon Coles is standing in as editor for the second time, ably assisted by Dave Allan, and once again I would like to extend my thanks to them for their efforts. Council is currently working to establish the longer term future of *Crystallography News* editorial management. Carl will be a hard act to follow.

One of the advantages for me of no longer having a full-time academic post, has been fewer (externally imposed) structured days of meetings, lectures etc. at fixed times. A week before writing this column, I was having a leisurely breakfast at home, listening to BBC Radio 4 at 9.00, and by chance caught an episode of *"In Our Time"* about **Dorothy Hodgkin**, hosted by **Melvyn Bragg**. I used to leave for the lab a full two hours earlier in the past, so tended to miss such gems in the R4 crown. It was an interesting discussion of Dorothy's life with **Judith Howard**, **Patricia Fara** and **Georgina Ferry** (who has also published a nice biography). Dorothy remains the only British woman to win a Nobel Prize for science, but her influence extended far beyond crystallography, into politics, support for women in science and the campaign for nuclear disarmament. I would heartily recommend listening to the programme, which is available as a podcast from BBC Sounds, and is easily located by a Google search. Many readers will already know this, but Melvin Bragg is indeed a relative of our crystallographic heroes, and hails originally from Wigton in Cumbria, as did **William Bragg**.

As a macromolecular crystallographer, I am often impressed by the ever larger and more complex crystal structures solved, with hundreds of thousands of atoms and millions of reflections. These are technological *tours de force*, frequently achieved in spite of high sensitivity of the crystals to radiation damage. A couple of other studies caught my eye recently, however, at the opposite end of the complexity scale, but every bit as technically challenging. Who would have thought, in this Year of the Periodic Table, that we would lack comprehensive data on the crystal structures of the elements. In particular, hydrogen and fluorine had proved problematic.

Hydrogen can adopt a number of solid phases under very high pressures, which are achievable in diamond anvil cells, but crystallographic measurements are difficult, because of the weak signal from such a light molecule, scattering from the heavy materials in the cell, and breakage of the diamond anvils under extreme pressure and X-ray irradiation. Several structures had been determined up to pressures of 190 GPa (1.9×10^6 times atmospheric), but Ji *et al* recently published a report in *Nature* extending this to 245 GPa over five years of painstaking work, using X-ray crystallography to follow the phase transitions of the hexagonally close-packed structure as it is compressed.

The hydrogen atom positions are, however, not resolved in the electron density. When I started out as a small-molecule crystallographer, I was accustomed to seeing the atoms as separate peaks in the density, but then I moved on to proteins, where atoms are not resolved in medium resolution maps, and I got used to needing stereochemical information to help locate them. In the H_2 case, however, high-resolution diffraction is observed, but the atoms have no core electrons so that the only electron density is for the bonding electrons. The molecules therefore appear as single peaks. Believe it or not, atomic positions are harder to find in H_2 crystals than in a protein and the H-H bond distance is not directly measurable.

Fluorine is another case of an element where crystal structure information had been somewhat limited until recently. It has two polymorphs, α and β, that crystallize at 46 and 53 K respectively. Early X-ray studies were again plagued by weak diffraction from the crystals and strong scattering by the copper sample holder. This was further complicated by the tendency of the fluorine and copper to react explosively! The monoclinic α-form was partly solved in 1968, but it was unclear if the space group is C2/c or C2/m. The β-form was found to be in a cubic space group with some disorder. A recent study of the structures has been published by Ivlev *et al* in *Chem. Eur. J.* using neutron powder diffraction and Rietveld refinement, thus avoiding some of the problems of sample holder scattering. C2/c turned out to be the correct space group symmetry for the α-form, while the cubic-β form is in $Pm\bar{3}m$. The α-form structure has finally allowed an accurate crystallographic determination of the F-F bond distance.

Members may be interested to learn that the Royal Society has published a biographical memoir of **Andrew Lang** (1924-2008). Andrew developed the field of X-ray topography, and was a frequent attendee at BCA meetings. The Lang Camera allowed the imaging of individual defects, such as stacking faults, dislocations and domains. Often in our careers we meet major forks in the road, with binary choices that determine our future paths in research. In Andrew Lang's case, in 1953, it was between working with **Linus Pauling** on α-keratin or **Bruce Chalmers** on the growth of metal crystals. He chose the latter, and the rest is history.

The UK has not hosted the IUCr Congress since Glasgow in 1999, and it would seem timely to consider it again. The lead times are very long, however, but a bid could be made for the next realistically available slot in 2029, where the decision would be taken at the 2023 IUCr Congress. The problem with organising such a bid is that none of the current BCA Council members would be in office to see it through, although they could assist in the early stages of bid preparation. The BCA has received proposals from conference centres to host this, so the required professional assistance for organizing such a large event should be available. We would need to supply the overall scientific direction, programme and committees. This is a big conference, with thousands of delegates, so the venue needs to be large enough to cope. Conference centres in London, Harrogate, Birmingham, Manchester etc. would be appropriate. I would call on any BCA member, or members, who might be interested in participating in a bid to organize the 2029 Congress to contact me. I realise this is a big commitment, but nevertheless an exciting one.

I am pleased to report that nominations have been received for the two positions, Treasurer and Ordinary Member, available in the Council membership elections. I would encourage all members to use their votes, having read the candidates' statements in this issue. Electronic voting is easy, and recent political history should teach us all that it is important to register your vote.

Registration is now open for the BCA 2020 Spring Meeting at the University of Leeds, so please get out your pens/keyboards, start writing your abstracts and sign up. In a departure from recent practice, the majority of accommodation this time is off-campus. It is, nevertheless, close by as a result of the university's central location in the city. Universities are increasingly holding their rooms for students in the vacations, and this has partly driven the change in meeting accommodation. The change for the Spring Meeting this time is also in line with some feedback we received from previous meetings. Good rates have been arranged with nearby hotels, and there are, of course, other options such as short-term flat sharing. I look forward to seeing you all there.

Simon Phillips

BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
- 10% discount on exhibition stands at the annual BCA Spring meeting.
- Free insert in the annual Spring Meeting delegate pack.
- Two free non-residential registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly Crystallography News.
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- A copy of Crystallography News every quarter
- Optional E-mail notifications of news items and meeting information
- Influence on the development of crystallography and the BCA

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

From the Editor

SO here I am as interim Editor again – the last three months has passed so quickly! Even though I had more notice this time around, deadlines still managed to creep up on me which makes me much more aware of the fact that this is a job that you always have to keep your eye on! I thank all the contributors for helping me get somewhere close to meeting these targets!

By far the most significant piece in this issue is an obituary marking **Carl Schwalbe**'s work and contributions to the BCA. It is difficult to do these justice but **John Helliwell** has done a truly admirable job. This is the formal BCA obituary in honour of Carl and will remain on the website – John and I also adapted this in writing another for the IUCr Newsletter which marks his international standing. As completing the September issue of *Crystallography News* got struck off my to do list, I found myself filling in for a presentation Carl was to give at an ECM Satellite (Data Science Skills for Publishing, organised by the IUCr Committee on Data, CommDat). It was an honour to present his work, which reflects his community-minded commitment to our discipline – being all about correcting records in the CSD so that others could benefit. I was so lucky to have **Suzanna Ward** from CCDC present the other half of the talk which, as well as some of the work he performed whilst a visiting scientist there, included a wonderful account, in her inimitable style, of Carl's contributions and science through CSD statistics.

Unfortunately, I only attended this satellite meeting and couldn't be at the main ECM conference due to other work and personal commitments. From reading the meeting reports in this issue and personal conversations I have had since, I must admit to being a bit disappointed as it was clearly an excellent conference. Vienna is a very photogenic and lively city – I thoroughly recommend a visit if you weren't there and have snuck in a few of my own photographs here. I wonder how many crystallographers visiting St Stephen's Cathedral pondered / discussed the symmetry exhibited by its stunning and unique roof design…?

I was not the only BCA member to have some crystallography interrupt their travels. I was delighted to receive a surprise email from **Steve Maginn** who happened to be in Valencia on vacation when he stumbled into an exhibition on women in science – where 10% of the examples happened to be crystallographers. Not only this, but there were numerous other crystallography exhibits.

Steve's article got me thinking about serendipitously stumbling across crystallography inspired art and installations – and this was about the same time I was considering what the front cover theme should be for this issue. I am a Twitter user. I find it simultaneously very stimulating in an enlightening way and very stimulating in a frustrating way (particularly with the way UK politics has been playing out over the last three years or so!). I have a kind of 'Marmite experience' every time I open the app, which I have to admit is several times a day – but what else would one do while queueing in the supermarket or walking up the stairs?!

So on the very day when I was looking to address my blank canvass problem, Twitter solved it! @Helen_E_MC (**Helen Maynard-Casely**) posted the most amazing picture of a suspended "lattice" (I have to be very careful when using this term, hence in quotes, or will be publicly pulled up by **@MikeGlazer1** on Twitter!) in the atrium of her local shopping mall, the Macquarie Centre in North Sydney. Almost at the same time **@HelliwellJohn** posted about two exhibits at the Manchester Museum of Science and Industry – one on W.L. Bragg and the other about the Daresbury SRS and protein crystallography. I saw a couple of characteristic red painted supports in the picture which caused a few personal SRS memories to flood back. It really is very gratifying and pleasing to work in a field that has contributed so much which is now being recognised so widely and (seemingly) so spontaneously! So, thank you Twitter (and of course its contributors!) – front cover problem solved…

On a housekeeping matter, you will note that there are Council elections upcoming and in our now formally adopted approach the candidate statements are published here and you will be asked to vote electronically. Please do take the time to read these and consider how you will vote – the candidates are all committed to working hard on your behalf to keep this association going.

As we move into the final stages of the International Year of Crystallography I have two things on my mind. Firstly, I seem to have not ducked quickly enough and with a couple of weeks notice find myself organising a small outreach event associated with RSC's Chemistry Week, where we will be projecting a giant periodic table onto our Life Sciences building. Fingers crossed for good weather, although given its in late November I am not entirely hopeful. Secondly, we are still looking for volunteers to help us fill up our periodic table of crystal structures – see **https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable**/. It's a really good way to get your name associated with a 'novel publication' and you will be acknowledged on the CCDC website (see **https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/contributors/**). We expect to make some teaching activities associated with it, so your contribution will definitely live on well beyond the end of the year!

As I write the group autumn meetings are coming up with the PCG one about to happen and a combined CCG/IG meeting that I am very much looking forward to attending. In fact, I often attend this meeting and for me it always signifies being well over half-way through semester 1. So, I feel I will shortly be looking at the home straight to the Christmas vacation and by the time you are reading this we will pretty much be there. I hope you had a fruitful year and wish you all a restful upcoming break.

Simon Coles

BCA Council 2019

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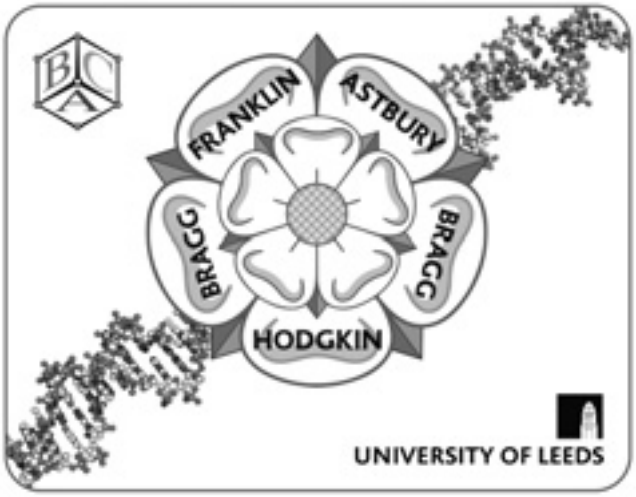
(The dates in parentheses indicate the end of the term of office).

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

BCA Spring Meeting 2020

6th – 9th April 2020, University of Leeds



To register for the BCA Spring Meeting 2020 please go to the website link below:
https://crystallography.org.uk/news/spring-meeting/2019/09/27/registration-bca-2020.html

PLANNING is well underway for the 2020 BCA spring meeting to be held in Leeds so please put the dates in your diaries! Details and titles for sessions are given below to give you time to think ahead to the abstract deadlines in January 2020.

YCG Meeting Monday 6th April – Tuesday 7th April

Monday 6th April:
YCG Meeting

YCG Plenary:
Dr Ehmke Pohl (title to be confirmed)

YCG Research:
(*Chairs:* Natalie Tatum and Tom Roseveare)

The YCG satellite meeting is an opportunity for all early career researchers in the field of crystallography to present their work in a supportive and friendly environment, which will be run by fellow early career scientists. There will be three sessions of talks on Monday, Session 1 chaired by Natalie Tatum/Tom Roseveare; Session 2 chaired by Elliot Carrington/Charlie McMonagle and Session 3 chaired by Aly Abedeldaim/Tom Roseveare, along with posters and flash presentations.

Tuesday 7th April:
YCG Meeting

Parkin Lecture: (to be confirmed)
YCG/IG: A Career in Crystallography: Exploring the Interface of Academia and Industry
(*Chairs:* Natalie Johnson and Rachael Wilkinson)

Crystallography can lead to a wide range of exciting and varied careers. The start of this session will feature research talks exploring both academic and industrial research endeavours. This session will also offers a unique question and answer forum to discuss careers in crystallography via a selected panel of crystallographers who have taken different career paths. This session has been designed to provide greater information about the variety of careers available for young crystallographers, with attendees able to ask any and all questions they have about the careers to the panellists.

YCG Plenary:
Dr **Cheryl Doherty** (title to be confirmed)

Tuesday 7th April:
Main Meeting

Lonsdale Lecture:
Awaiting confirmation by BCA Council (title to be confirmed)
(*Chair:* Aly Abedeldaim)

BSG Plenary: Rosalind Franklin Centenary Lecture
Professor Gabriel Waksman FRS (UCL/Birkbeck)
Mechanism of effector targeting by the Legionella type IV secretion system

BSG:
Structure-based drug design
(*Chair:* Jane Endicott)

Protein structures can assist drug development at all stages of the discovery pipeline, from choosing targets, through identifying hit matter, to supporting iterative medicinal chemistry to enhance potency, pharmacokinetics and pharmacodynamics. Historically, structure-based drug design has addressed well characterised active sites by identifying potential molecular interactions to inform subsequent chemical synthesis. Application of this approach has already contributed to the development of many potent and selective drugs. However, molecular targets with clear disease linkage can be extremely difficult to find, and for this reason more is being asked of structures in drug discovery campaigns. Examples of these new contributions include characterising and capturing biologically

relevant protein conformations to help in the targeting of allosteric sites, and identifying novel classes of target that depend on protein-protein and protein-DNA/RNA/lipid interactions. The keynote lecture will review key advances in the field over the last decade and future possible directions while reflecting on what a drug discovery campaign looks like from the structural biologist's point of view.

Keynote:
Dr. **Pamela Williams** (Astex Pharmaceuticals)
Structure-based drug discovery: how did we get here and where are we going?

CCG:

Advances in Software for Crystallography
(*Chair:* Lucy Saunders)

This session aims to reveal the latest and exciting developments happening in crystallographic software. We encourage abstracts from those in the community working on software for chemical crystallography research. We want to know about the latest tools on offer. This could be in the areas of data processing, structure refinement, property calculation or structure investigation to name a few.

Keynote:
Mairi Haddow (Heriot-Watt) (title to be confirmed)

PCG:

Biominerals & Biomaterials
(*Chair:* Julia Parker)

From the exquisite morphologies of coccoliths and the incredible hierarchical architecture of bone, to the engineering of implants and joint replacements, the structure of biominerals and biomaterials plays an integral role in determining their properties and function. This session will examine the importance of structure in both natural systems and biomedical devices, explore how their composition and assembly controls physical properties and look at how this can be exploited in the development of novel bioinspired materials.

Keynote:
Melinda Duer (Cambridge) (title to be confirmed)

BSG:

Time-resolved crystallography
(*Chair:* Briony Yorke)

Time-resolved crystallography allows the observation of molecular mechanism in real time, providing unique insight into the dynamics that link structure and function. The use of X-ray free electron lasers has pushed the boundaries of time-resolved crystallography, allowing structural changes to be determined with femtosecond time-resolution. The development of serial crystallographic techniques has also initiated a resurgence in synchrotron time-resolved experiments. This session will focus on the exciting developments being made at free-electron laser and synchrotron sources and the science that has been made possible by these developments. Contributions describing these and other structural time-resolved methods are welcomed.

Keynote:
Jasper van Thor (Imperial)
Optical control of protein structural dynamics by ultrafast X-ray crystallography

CCG:

Electron crystallography
(*Chair:* Simon Parsons)

Electron diffraction is one of the mostly rapidly developing and exciting areas of crystallography. The publication of a number of recent papers describing its application in chemical crystallography has led to a great deal of comment and anticipation in the chemical community. The technique enables crystal structures to be obtained from samples with dimensions of the order of the few microns, or even 100s of nanometres. The strength of the interaction between electrons and matter that enables such small crystals to be studied carries with it the problem of multiple scattering, meaning that the kinematical model which has been so successful for X-ray and neutron diffraction no longer applies, and dynamical effects need to be taken into account. This session will give an overview of the most recent advances in the field and progress towards making electron diffraction a more widely used technique in the chemical crystallography community.

Keynote:
Lukas Palatinus (The Czech Academy of Sciences)
Structure refinement from 3D electron diffraction: where are the limits?

PCG:

Entropy & Structure
(*Chair:* Anthony Phillips)

In recent years, entropy has become an explicit target of materials design and synthesis: configurational and magnetic entropy can stabilise materials' structures or form the basis of their functionality. Understanding such disorder requires a variety of experimental and computational techniques drawn from the conventional crystallographic arsenal and beyond. In this session we welcome talks on all aspects of order and disorder: quantifying, designing, and exploiting entropy for materials ranging from high-entropy alloys to calorics.

Keynote:
Xavier Moya (Cambridge)
Giant caloric effects near structural phase transitions

PCG Plenary:

Vaclav Petricek (Czech Academy of Sciences)
The role of crystal structure analysis in investigation of crystals with important physical properties
(*Chair:* Anthony Phillips – QMUL)

continued >>>

Wednesday 8th April
Main Meeting

IG Plenary
Marcus Neumann (Avant Garde Materials Simulation)
Detecting and avoiding disappearing polymorph cases by crystal structure prediction
(*Chair:* Helen Blade)

BSG:
Enzymes
(*Chair:* Wyatt Yue – Oxford)

Metabolic enzymes catalyse the biochemical reactions associated with survival and homeostasis in living organisms while the processes governing the behaviour of cells are mediated by tightly regulated cascades and complexes of cell signalling enzymes. Enzymes that perform various types of chemistry are therefore studied intensively in the fields of biochemistry and molecular cell biology. The essentiality of metabolic enzymes is underscored by various genetic and common disorders associated with their deficiency. Enzymes are also central to the field of biotechnology, where they are engineered to manufacture novel products or act upon novel substrates. This session will include examples of work in which structural biology methods are answering important questions relating to the activity and regulation of enzymes, with a view to understanding their functional, biotechnological and therapeutic applications.

Keynote:
Peter Moody (Leicester)
Using neutron crystallography to watch hydrogens in heme enzymes

PCG:
<3D: Structure and Properties of Low-Dimensional Materials
(*Chair:* Lucy Clark)

There are many examples of crystalline solids whose structures feature quasi-one-dimensional chains or two-dimensional planes of atoms giving rise to low-dimensional interactions. This results in a diverse array of intriguing physical phenomena, from high-temperature superconductivity in, for example, layered iron arsenides to pronounced magnetocaloric effects in one-dimensional framework solids. Furthermore, since the isolation of graphene, there are has been an explosion of activity in the discovery and characterisation of different classes of two-dimensional crystals with remarkable properties that may underpin future advanced technologies. As such, this session is dedicated to showcasing recent developments of crystallography and complementary characterisation methods in the determination of the fascinating structure-property relationships in a variety of low-dimensional solids.

Keynote:
Maria Grazia Francesconi (Hull) (title to be confirmed)

IG (joint with British Association for Crystal Growth):
Pitfalls and challenges in industrial crystallisation
(*Chairs:* Cheryl Doherty and Linda Seton)

The control and prediction of crystallisation processes is a challenge but vital in many areas of industry. This session will cover practical and computational methods that aim to link understanding with the development of control strategies and predictive approaches. Talks from the perspectives of crystallisation, solid form and characterisation will be welcome.

Keynote:
To be confirmed.

Early career prize lectures:
To be confirmed.

BSG:
Computational biophysics
(*Chair:* Matteo Degiacomi)

To successfully carry out their task in an organism, biomolecules must interact with their designated substrates in a controlled manner. The function of a biomolecule thus emerges from its specific atomic structure and associated dynamics. Many computational techniques, as diverse as molecular dynamics simulations, homology modelling and protein-protein/ligand docking, can leverage crystallographic data to characterize molecular structure, dynamics and interactions. This session will focus on the application and development of such techniques.

Keynote:
Franca Fraternali (Kings College London)
Protein-protein interactions in health and disease: the importance of 3D structure

IG joint with CCG:
Control and prediction of crystals
(*Chairs:* Helen Blade and Stuart Kennedy)

This session aims to cover a wide range of research used to control and predict crystals including both experimental and computational tools. We welcome talks on the control and prediction of solid forms, particle and mechanical properties by researchers from a wide range of fields of computational chemistry, informatics, solid state/crystallisation and materials science.

Keynote:
Sten Nilsson-Lill (AstraZeneca) (title to be confirmed)

PCG:
>3D
(*Chair:* Phil Lightfoot)

This session targets crystals and materials that go beyond a conventional description using three dimensional axes and indices. This includes aperiodic crystals, quasicrystals and incommensurately modulated crystals, structures, magnetic structures etc. Examples may include compounds exhibiting compositional, structural or spin disorder at the 3D level, but which is amenable to better description and rationalisation using 4D or higher dimensionality. We are interested in examples where the dimensionality may significantly affect materials' properties, as well as in the fundamental description and understanding of the higher-dimensional crystallography.

Keynote:
Fabio Orlandi (ISIS) (title to be confirmed)

Bragg Lecture:

Richard Henderson
(University of Cambridge)
Title TBC

BCA AGM and conference dinner followed by ceilidh.

Thursday 9th April 2020

CCG Plenary:

Franziksa Emmerling (BAM, Berlin)
Shaken not stirred: enhancing the flavor of mechanochemistry
(*Chair:* Claire Murray)

BSG:

Membrane proteins
(*Chair:* Bonnie Wallace)

Membrane proteins span a wide range of structural and functional types, ranging from multimeric complexes to monomeric or multimeric channels, receptors, and enzymes. They perform very important functions in cells and many are of interest for pharmaceutical development. However, they have proved to be challenging for structural studies due to their amphipathic nature, with both hydrophobic and hydrophilic domains, and the requirement for detergents, amphipols, nanodiscs, and other amphiphiles to solubilise, purify, and stabilise them. This session will include examples of work demonstrating how recent developments in sample preparation and in the complementary techniques of cryo-Electron Microscopy and X-ray crystallography are enabling structural studies of key membrane proteins.

Keynote:
Dr **Amandine Marechal** (UCL)
Respiratory supercomplexes: what can we learn from yeast?

CCG:

Chemistry in extreme conditions
(*Chair:* Hamish Yeung)

Crystallography has traditionally been a major technique with which to understand the structures and reactivity of molecules. This session focuses on how crystallography and other methods can reveal insight into phenomena that occur away from ambient conditions, such as very high or low temperatures, high pressure or electric fields. Think bonding, mechanics, distortions, phase transformations, changes in physical properties etc.—in and ex situ studies allowed!

Keynote:
Colin Pulham (Edinburgh) (title to be confirmed)

PCG (joint with CCG):

Structure Solutions from Powders
(*Chairs:* PCG: Karen Johnston and CCG: Jeremy Cockroft)

This joint session between the CCG and PCG explores structure solution from powders in a variety of organic, inorganic and mixed organic/inorganic systems. Despite considerable advances in the field, structure solution from powder diffraction is by no means routine and, increasingly, complementary methods are being used to aid structure determination. We are interested in recent examples where structure solution has been aided by complementary methods, including in situ and in operando techniques as well as total scattering methods. Examples where the combination of experimental and computational methods has resulted in successful structure solution are also of significant interest.

Keynote:
Kenneth Shankland (Reading)
Accelerating and enhancing the effectiveness of crystal structure determination from powder diffraction data

BSG:

Protein-protein interactions
(*Chair:* Richard Bayliss)

Cellular processes depend entirely upon interactions between proteins, either for the transient or regulated recognition of one molecule by another in interaction networks or the stable assembly of individual proteins into higher order complexes. Specific molecular recognition in protein-protein interaction networks is crucial in cell signalling while protein complexes function in cells as molecular scaffolds, hubs for cell signalling or as molecular machines carrying out concerted functions. This session will include examples of work in which structural biology methods have been used to determine the molecular basis of interaction between proteins and their assembly into multiprotein complexes.

Keynote:
Elton Zeqiraj (Leeds)
Structure and function of ubiquitin signalling complexes

PCG:

Phase Transitions
(*Chair:* Lewis Owen)

Phase transitions are of critical importance to our understanding of a materials structure and its physical and chemical properties. This session will aim to explore a broad range of structural phase transitions; from crystalline solid state transformations to crystalline-amorphous transitions. Particular interest will be placed on novel characterisation including novel experimental set-ups and techniques (e.g. Bragg diffraction, PDF, NMR etc), data-processing methodologies, and structural parameterisation.

Keynote:
Joe Hriljac (Diamond Light Source) (title to be confirmed)

CCG:

Hot and cold structures
(*Chair:* Charlie McMonagle)

In this session we look at how temperature can affect structure in a huge number of interesting and useful ways.

Keynote:
Sven Lidin (Lund) (title to be confirmed)

Obituary

Obituary for Emeritus Professor Dr **Carl Schwalbe** (2nd June 1942 to 1st August 2019)

Carl Schwalbe was an outstanding colleague. At his funeral at Halmer End Methodist Church Staffordshire there were glowing tributes from his sons and from his Aston University academic colleagues. It was clear from these tributes that Carl was a family man. We also learned of Carl's love of classical music and how his wide ranging general knowledge put him in demand for quiz teams. The printed Order of Service remarked above the picture of Carl, reproduced here, *"A man of science", "A man of great integrity"*. My wife Madeleine and I both attended. Carl's former Head of Department of Pharmacy, Emeritus Professor **Malcolm Stevens** OBE FRS, included in his tribute to Carl of how on one occasion a young man was explaining in a seminar how he had *dissolved his crystals in order to measure…* Before he could finish the sentence Carl firmly interrupted *"You did what!?"*.

The BCA President Professor **Lee Brammer** in his December 2017 Crystallography News Column wrote of Carl being admitted as an Honorary Life Member of the BCA as follows *"Prof Carl Schwalbe is recognised not only for his research contributions in crystallography but as a longstanding contributor to the BCA, in particular in his role as editor of Crystallography News over the past decade and for his tireless activity in gathering information from so many sources."* I know that Carl was delighted about this Honour.

In preparing to write this obituary I read through all of Carl's Editorials as Editor of Crystallography News, a role which he commenced in June 2008 and went through to June 2019. I selected just a few items that he shared with us in these about his personal history and also his learned insights as a pharmaceutical science crystallographer. First of all he wrote to introduce himself to the wide readership of Crystallography News *"For those of you who don't know me very well, here is a bit of background. I grew up in Ohio. Unsurprisingly since Ohio is just across Lake Erie from Ontario, some people think my accent is Canadian. I did my PhD research at Harvard with "Colonel" William Lipscomb during which I determined the structures of boron hydrides, those unusual cages where each boron atom seems to make unreasonably many bonds. We admired the Colonel's genius as he made sense of the bonding and won the Nobel Prize in Chemistry. For my postdoctoral research I worked with Wolfram Saenger and Fritz Cramer at the Max Planck Institute for Experimental Medicine in Göttingen, Germany. There I developed my lifelong interest in pharmaceutical crystallography. In 1972 I looked for an academic position back in the U.S.A. but found little because of a round of budget-cutting. I decided to "park" in England for a few years until things got better and therefore took up a lectureship at Aston University. I have been at Aston ever since, receiving a Personal Chair in 2007 and going part-time during the current academic year. One thing that made me decide to stay here permanently is the cordial collaboration I developed with synthetic chemists at Aston, most notably Malcolm Stevens, whose anti-cancer drug temozolomide is approaching "blockbuster" status. Another important factor is the friendship and cooperation I have always received from British crystallographers." In the March 2010 Crystallography News we also learned of Carl that "My grandfather and near namesake Carl Gustav Schwalbe founded the Institute of Cellulose Chemistry at the Technical University in Darmstadt."*

Carl wrote, quite simply, interesting and absorbing Crystallography News editorials. Some years he would attend the BCA, German Crystallographic Association, the ACA and the ECM conferences! So, Carl in his editorials shared with us, for example:- a recipe for the New Orleans' dish Jambalaya in September 2011; the hot weather in Madrid on the occasion of the IUCr Congress where he had some relaxation attired in T shirt and shorts but the Pope, visiting Madrid at the same

time, had of course to wear full Papal attire; and in the September 2012 Crystallography News Carl remarked how the new London Shard reminded him of a crystal of tourmaline and the pictures of each made the front cover of Crystallography News (**https://hg3.co.uk/bca/BCA-News-September-2012.pdf**). In September 2008 Carl remarked *"I am sorry to have missed the meeting of the Slovenian-Croatian Crystallographic Association, charmingly abbreviated "Slo-Cro", in Ptuj, Slovenia. I would have loved to send my friends a postcard from Ptuj."*

The formal details of Carl's impressive academic track record are as follows:-

2010-2019 Emeritus Research Fellow at the CCDC; 1972-2019 Lecturer, Senior Lecturer, Professor, Emeritus Professor in Medicinal Chemistry at Aston University; 1970-72 Research Fellow at the Max Planck Institute for Experimental Medicine (PI, Prof. W. Saenger); 1965-70 PhD, Harvard University (PI, Prof. William N. Lipscomb); 1959-64, Chemistry (summa cum laude) Oberlin College. Carl's depositions in the CCDC ranged from EAMBNO10 first published 1971 to XEZFIU, his most recent, published in 2018. His most cited article (D.Chattopadhyay, S.K.Chattopadhyay, P.R.Lowe, C.H.Schwalbe, S.K.Mazumder, A.Rana and S.Ghosh Journal of the Chemical Society, Dalton Transactions, 1993, 913-916, "Synthesis and Structural Studies of Tetra aqua copper (11) Diaqua bis(malonato) cuprate (11)" with 72 citations) featured the crystal structure PECMIT. In Carl's IUCr World Director of Crystallographers entry he listed his research interests as follows:- chemical crystallography, drug design, hydrogen bonding, molecular modelling, molecular recognition, drugs and MO calculations.

Carl was to have lectured at the IUCr Committee on Data Workshop at the ECM32 in Vienna (**https://www.iucr.org/resources/data/commdat/vienna-workshop**). Instead **Simon Coles** and **Suzanna Ward** presented his latest work and ideas on the challenges of correct tautomer determination. This research was undertaken by Carl as a Cambridge Crystallographic Data Centre Honorary Fellow and which led to questions of how best to remediate those cases held in the CSD as described in his article Schwalbe, C. H. (2018). *Crystallogr. Rev.* **24**, 217-235.

John R Helliwell (Emeritus Professor of Chemistry, University of Manchester).

The definitive online version of this obituary is hosted on the BCA website at:
https://crystallography.org.uk/news/2019/09/22/Carl-Schwalbe-Obituary.html

A modified "IUCr version" with some different material has also been published by **John Helliwell** and **Simon Coles** in the IUCr Newsletter (**https://www.iucr.org/news/newsletter/volume-27/number-3/carl-schwalbe-19422019**).

BCA 2019 AGM Minutes

Draft minutes of the 2019 Annual General Meeting of the British Crystallographic Association, Exchange Building, Jubilee Campus of the University of Nottingham. 18.00, Wednesday 17th April.

1. **Approval of the Agenda**
   The agenda was approved; proposer Mike Glazer, seconded Anthony Phillips.

2. **Apologies**
   Apologies were received from the Treasurer Elizabeth Shotton.

3. **Minutes of the 2018 AGM**
   Minutes of the previous AGM 2018 were published in the December issue of *Crystallography News* and also on the website. No corrections were needed and the minutes were accepted. Proposer Richard Cooper, seconded Simon Parsons.

4. **President's report**
   The President, Simon Phillips, started with the sad report of the loss of two Founder members of the BCA with a few details; Aaron Klug (1926-2018) Nobel Laureate in Chemistry (1982) and President of the Royal Society (1995-2000) and Stephen Wallwork (1925-2019) University of Nottingham (1949-1982) was part of the working group to set up the BCA.

   The President congratulated Elspeth Garman awarded the Sosel Heptares Prize for Biophysics for her outstanding contributions to our understanding of radiation damage, which has contributed to the improvement of X-ray crystallography and structural biology and showed a photo of Elspeth being presented with the prize by Richard Henderson.

   Thanks were given to Emma McCabe, Programme Chair for the current Spring meeting and also to Richard Cooper, Hg3 and their teams for an excellent meeting.

   The 2020 Spring meeting will be held at the University of Leeds, 6-9th April. Thomas (Ed) Edwards was introduced and is the Programme Chair for 2020. Planning for this meeting will start with a brief meeting on Thursday April 18th and main meeting in late May/early June. Members were encouraged to send suggestions for symposia or plenary speakers to their representative from the BSG, CCG, PCG, IG or YCG.

   The President thanked the BCA officers: Richard Cooper, Claire Wilson and Elizabeth Shotton and especially to Richard and Claire who were both retiring from Council after long service. The members of the BCA Council were thanked for their input, enthusiasm and willingness to endure long Council meetings. Thanks were also given to Carl Schwalbe, the editor of *Crystallography News* which is always good and requires a lot of effort, the Education and Outreach Coordinator Simon Coles, Nicola Hardaker and all the team at Hg3 and to all the BCA members for their continued support of the Association.

   The President handed over to the EOC, Simon Coles for an update on education and outreach activities. Simon reiterated that the BCA wanted to change approach away from large events to support members in local smaller scale outreach activities such as department open days, school visits, social events (Pint of Science, Café Scientifique). The aim is to support this through a database of activities that anyone can pick up from the website (**http://learn.crystallography.org.uk/learningresources**). Members were encouraged to consider contributing to resources and help was offered to get these into the correct format. Simon also highlighted that there are grants and bursaries available up to £2500 for internships to develop resources or grants of £300-500 to purchase materials required to develop an activity.

   It is the International Year of the Periodic Table and there is a project involving Claire Murray, Diamond and CCDC filling up a table of crystal structures representing the elements.

5. **Secretary's report**
   There was no report and no questions.

6. **Hg3 Report**
   Current Spring meeting had 205 registrations as of 29/3/19 (218 in 2018); 144 full residential package, 44 day delegate package, 17 exhibitors, 80 delegates at the YCG satellite meeting.

   BCA membership figures 644 on 29/3/19 and the Corporate members were given.

   Crystallography News has the following current advertisers Bruker, Oxford Cryosystems and Rigaku Oxford Diffraction (all issues) and ICDD (June and September). Members were encouraged to put forward companies as potential advertisers.

7. **Report of the Treasurer including presentation of the Accounts for 2018 and Examining Accountant's Report**
   A copy of the account summary was circulated and the meeting was reminded that the accounts cover the period from Jan1st to Dec 31st 2018 and a full breakdown of the accounts is included in the BCA annual accounts available by email or online at the Charity Commission website. Summaries of the income, meeting finances and outgoings (governance and charitable expenditure) were presented. The major difference between 2017 to 2018 is due the CCG school which runs only in odd years. For the last 3 years the Spring meeting has made a small surplus with a small loss forecast for the current meeting which is not problematic. The largest governance expenditure is a slightly higher accounting fee than last year.

In general, the finances are stable and there are no issues of concern. The aim continues to be to try and reduce the governance costs and to maintain a cautious, balanced investment of funds.

Members were urged to encourage colleagues to join the BCA as membership is our lifeline and also to encourage their students to apply for bursaries.

Thanks were given to Hg3, Council members, BCA group treasurers, Charles Stanley Bank and UHY Hacker Young accountants.

8. Acceptance of the Accounts

Moreton Moore queried that the unaudited statements do not include the PCG and it was clarified that their accounts go through the IOP.

The accounts were accepted; proposer John Helliwell, seconded Jeremy Cockcroft.

9. Appointment of the Examining Accountant for 2019

The proposal was to appoint the Young Company with an annual fee of £5400. This was approved; proposer Dave Keen, seconded Simon Coles.

10. Elections to Council

The elections had been carried out by electronic ballot during the period Jan 3rd-Feb 5th 2019 with a total of 259 votes cast (150 in 2018). BCA members were notified by email that voting was opening and provided with a personal link to the voting site. The results were as follows:

Vice President:
Simon Parsons (2019-2022)

Secretary:
Alex Stanley (2019-2022)

BCA Council Ordinary member:
Anna Warren (2019-2022).

It was highlighted that in 2020 there will be elections for Treasurer and an Ordinary member. Candidates are identified by the Nominating Committee or by BCA members and nominations are made to the Secretary, the nomination deadline is 30th September 2019. For 2019-2020 the nominating committee is chaired by Phil Lightfoot with Elspeth Garman, Lee Brammer, Paul Raithby and Chris Frampton.

11. Honorary members

Honorary members are chosen for their contributions to both crystallography and to the BCA. The nomination deadline for 2020 Honorary members was given, August 31st 2019 and nominations should be sent to the BCA President with a brief case for support of not more than 400 words. Nominations will be considered at the September Council meeting and new Honorary members may not be awarded every year and a maximum of two in any calendar year. The President said it was his happy duty to announce two new Honorary members for 2019 as John Helliwell and Sandy Blake and commented that it was impossible to give a full list of their contributions. Both new Honorary members were presented with certificates by the President.

12. Membership, annual subscriptions and subventions

Membership figures were presented showing a high of over 800 members in 2003, a low of less than 400 in 2012 and a slight decline in recent years to 588 members at 31st December 2018. The President encouraged members to encourage colleagues to join.

13. Equality, Diversity and Inclusivity report

The BCA EDI policy was adopted in March 2018 and the President restated the policy on a slide and that the intention is to ensure quality and equality. Programme Committee members for 2020 were also encouraged to be mindful of this and invited feedback to the President. Figures were reported for the membership (estimated) with student members 48% female, Young Crystallographers not including students 47% female and standard members 28% female (128 female, 324 male). Programme committee members and speakers at the current (and previous) Spring meetings were also given; for 2019 the main meeting figures were as follows (YCG in parentheses), percentages given are female; Programme committee 53%, plenary speakers 29 (0)%, keynotes 44%, speakers 38 (36)% and chairs 37 (25)%. It was pointed out that the number of plenary speakers is very small and they are very variable, the contributed talk speakers approximately reflects our membership gender distribution.

14. AOB

Mike Glazer was given the floor to talk about the International Union of Crystallography (IUCr). Mike started with some background about the IUCr, founded in 1948, an explanation of the voting rights of member countries at the General Assembly and programmes organised all over the world, currently with big programmes in Africa and South America including schools, working on behalf of the crystallographic community. He commented that the Newsletter, of which he is the Editor, has recently moved to online publication, allowing dynamic content. The next IUCr congress will be held in Prague in 2020 and they expect more than 2500 participants.

Simon Phillips then raised IUCr nominations to both the Executive Committee and the Commissions. The deadline for nominations by member countries was given as 30th June 2019 and he pointed out there were no UK members currently on the Executive committee. He asked members to send suggestions to the BCA President and Secretary by the end of May.

A final item of other business was that the IUCr congress has not been held in the UK since Glasgow in 1999. The President pointed out that the lead time is very long and a bid would be for the 2029 congress with a decision made in 2023. Given that the current BCA Council members will not be in office but could assist in the early stages. Any venue would need to be suitable for up to 3000 participants. He called on members who would consider leading a bid to contact Council.

Mike Probert queried when a quote had last been obtained for an alternative accountant. Alex Stanley replied that it has been explored and the initial fee to change is likely to be expensive and it was something that could be explored for next year.

The meeting closed at 7pm.

BCA Council Elections 2020

AT the AGM in April 2017, changes to the BCA Statues and Bylaws were approved in order to establish a new procedure for elections to the BCA Council. A Nominating Committee was established and elections will take place by electronic ballot of the membership. Nominations for the following positions on Council were invited from the Nominating Committee and from members of the BCA by the nomination deadline of September 30th:

Treasurer (Elizabeth Shotton, co-opted term comes to an end at the AGM 2019).

Ordinary Member (Hazel Sparkes, co-opted to fill this position due to an Ordinary Member moving abroad and is eligible to be voted for a first full term).

Elections will take place at the start of 2020 with voting by electronic ballot. Details of the voting procedure will be sent to all BCA members by email. The results of the election will be announced and elected members of Council will start their terms at the 2020 AGM.

We encourage all BCA members to participate as the wider participation, beyond those present at the AGM, was one of the motivations for changing the election process as well as providing for a better handover to new members of Council.

The following nominations were received and in subsequent pages statements from each of the candidates are published to enable members to make informed decisions when voting.

Candidates for

Treasurer: Claire Naylor

Ordinary Member: Hazel Sparkes, Matt Cliffe

Claire Naylor

Current position

Marketing Manager and Technical Support, Molecular Dimensions Ltd, 2016-present.

Education and Career

Research fellow and post-doctoral research assistant, Department of Biological Sciences, Birkbeck University, 1997-2016, D. Phil in Biochemistry at the University of Oxford, 1993-1996, BA in Chemistry at Oxford University, 1989-1992.

BCA and other roles

Industrial representative, ECA Council, 2018-present, Biological Structures Group Committee Member 2018-present, Biological Structures Group C-Chair 2019 BCA Spring Meeting.

Statement

Having studied for my undergraduate degree at Dorothy Hodgkin's Oxford college, Somerville, I had already become interested and excited by crystallography by the time I was choosing my Part II Chemistry project. My tutor at the time, Dr Margaret Adams, told me that if I thought Crystallography was good, I should come and work with her in structural biology – because the pictures were much prettier! She was right, and from that time I was captivated. After staying with Margaret for my D. Phil, I moved to Birkbeck College, where I remained for many years, providing crystallographic support on a range of projects and for many supervisors. I was introduced to the BCA while at Oxford, and its meetings have provided a back-drop to my life as a crystallographer, providing regular opportunities to learn about the latest research and catch up with colleagues.

The move to industry, in the form of Molecular Dimensions Ltd 3 years ago, may at first sight appear to be a step away from research. However, Molecular Dimensions has always prided itself on working closely with academics, bringing their techniques and ideas to a wider audience via commercialisation. I have the pleasure of remaining actively involved in crystallography research by working with academics while creating exciting new products from their research. In addition, Molecular Dimensions has always been happy to take an active part in the community: acting as an industrial partner in a number of EU Training Networks and participating in conferences and other events.

For the last few years, it has been my pleasure to be a member of both the ECA and BCA BSG committees. I now have a good understanding of how our association is run and the primary issues it faces. The nomination for Treasurer of the BCA council is an honour, and I would be delighted to have the opportunity to serve the community in this position.

Hazel A Sparkes

Current Position

Research Fellow in X-ray Crystallography, School of Chemistry, University of Bristol.

Education and Career

MChem, University of Bath, Department of Chemistry. PhD in Solid State X-ray Structural Studies, University of Bath, Department of Chemistry. PDRA for Professor Judith Howard, Durham University, Department of Chemistry. Leverhulme Early Career Research Fellowship, Durham University, Department of Chemistry. Chemical Crystallographer, Beamline Scientist on SXD at ISIS, RAL.

Professional Activities

Local organiser (2009 onwards) and tutor (2007 onwards)

biennial BCA/CCG Intensive Teaching School in X-ray Structure Analysis. CCG Committee Ordinary Member (2006-2009), Deputy Chair (2009-2011), Chair (2011-2013). Programme organiser CCG Autumn Meeting (2009 and 2010). BCA Spring Meeting Programme Committee CCG representative (2010 and 2011). Organiser with Professor Judith Howard of the 46th Erice International School 'The Future of Dynamic Structural Science' (2013), Co-organiser with Professor Judith Howard and Professor Siva Umapathy of Faraday Discussion 177 'Temporally and Spatially Resolved Molecular Science' (2015). Ordinary Member BCA Council (2018).

Research Interests

I have been lucky enough, across my scientific career, to work in a number of different areas of small molecule crystallography and gained experience working at both synchrotron and neutron facilities. The areas I have studied have included light induced phenomena such as [2+2] cycloaddition reactions, linkage isomerism and LIESST for spin crossover complexes, temperature induced spin crossover and phase transitions, liquid crystallisation, database analysis and charge density structures of organic and organometallic complexes. In addition, my previous role as a beamline scientist at ISIS and current role that involves running the X-ray facilities at the University of Bristol have allowed me to be involved in various research projects across multiple disciplines including Chemistry, Physics, Biochemistry, Earth Sciences and Geology. My current research is focussed on crystallographic studies to investigate [2+2] cycloaddition reactions and spin crossover.

Statement

I am delighted to be nominated to stand as an ordinary member for the BCA Council, having been co-opted onto the Council in 2018. I have been a member of the BCA since the start of my PhD and have found it to be a very friendly and welcoming community which I very much enjoy being part of. I have regularly attended the meetings and found them invaluable for keeping up to date with developments in instrumentation and research as well as offering opportunities for members at all levels to contribute through posters or talks. I have previously been on the CCG committee, over 7 years serving as an ordinary member, deputy chair and then chair which involved organising speakers for Autumn Meetings, serving on the BCA spring meeting programme committee, inviting speakers and chairing sessions. I am also heavily involved in the biennial BCA/CCG Intensive Teaching School in X-ray Structure Analysis firstly as a tutor in 2007 and since 2009 as a local organiser and tutor arranging sponsorship, handling registrations and local arrangements as well as tutoring. I thoroughly enjoy this role which enables me to interact with students early on in their crystallographic careers and I am very pleased to be able to contribute to the continued running of such a well respected school. I believe that my broad range of crystallographic experience and involvement with BCA activities over the years puts me in a good position to understand the needs of the BCA and its members and I would be delighted to have the opportunity to continue to serve the crystallographic community as a member of the BCA council.

Matt Cliffe

Current Position

Hobday Fellow, School of Chemistry, University of Nottingham (2018-)

Education and Career

Junior Research Fellow; University of Cambridge (Prof. Clare Grey) (2015-18; PhD, University of Oxford (Prof Andrew Goodwin) (2015); BSc/MSci, University of Cambridge (2011).

Research Interests

My research focusses on the physical (magnetic, electronic or mechanical) properties of metal-organic frameworks and coordination polymers, and trying to determine how their structures determine their behaviour. In particular, I am interested in making use of disorder as a tool to not only optimise the properties of MOFs but also to create new disordered states. As a result, crystallographic techniques are naturally a key part of my research: from laboratory single crystal and powder X-ray diffraction to the advanced techniques available at central facilities, such as total scattering, in-situ synthesis and magnetic diffraction. I have also found that using complementary techniques, including physical property measurements, spectroscopy (NMR, neutron, X-ray) and microscopy, can be very valuable in assembling a full picture of complex materials.

Statement

I am delighted to have been nominated for the position of an Ordinary Member on the BCA council. My initiation into the scientific community was the BCA Spring Meeting in 2010 and I have been a regular attendee of the Spring Meeting and the BCA Group meetings, particularly the PCG Winter Meeting, ever since. One thing that was clear immediately and has continued to be the case is how welcoming the BCA community is. This welcome has been, I think, vital to the continuing thriving of crystallography in the UK, both by bringing early career academics into the field, for example via the YCG, and by building bridges with structural scientists who specialise in techniques beyond diffraction. I believe this is particularly important at the current moment, as the recent dramatic advances in instrumentation, e.g. in electron diffraction/microscopy, XFELs and spectroscopy, are opening up new routes to crystallographic information. As an early career researcher with interdisciplinary research interests I believe I would be well-placed to help support BCA community in continuing to be the welcoming group that it is. I would be honoured to serve the UK crystallographic community and play a role in its thriving.

ECM32 Vienna, Austria

ECM32 was held this year in the beautiful city of Vienna, Austria. For me, the meeting started early the day before the main meeting at the satellite meeting for the European Young Crystallographers, GIG-01. This one-day satellite is an opportunity for early career researchers to present their work in a more relaxed environment. This year's format allowed more time to be given over to questions and discussion, a helpful opportunity especially with the variety of topics covered. Dr Ella Schmidt, Germany, opened the meeting with a deep dive into complex world of modelling disorder from single crystal diffuse scattering for a 1-Bromoadamantane Thiourea inclusion compound. This gave a diffuse scattering pattern to strike fear into most crystallographers but with the help of computation modelling this disorder can be rationalised. Anna Gaydamaka, Russia, introduced her high-pressure work on guanine and the future of science at Novosibirsk State University with the building of a 4th generation synchrotron, SKIF Project. The morning session was closed by a fascinating talk from Dr Paolo Pio Mazzeo, Italy, on the controlled release of essential oils from metal-organic framework materials.

The coffee break took place on the roof of the science building giving fantastic views out over the city along with a great selection of cake. After this the middle session of the day was focussed on technique development. I was up first presenting my recent work on reducing the background of data collected at ultra-low temperatures. Having the more time to present and the active discussions that followed I found to be really rewarding as a speaker. Dr **Lucy Saunders**, UK, was up next with a great talk about the work involved in developing an *in situ* applied electric field cell for I19 at Diamond. The voltages used in this cell are frankly terrifying but really cool work. To close the session **Linda Kerkhoff**, Germany, went though some of her methods for crystallising lithium iridate and lithium ruthenates. The furnace-based synthesis using crucibles with ascending steps, much like a spiral staircase, give differing forms of these materials on different steps of the crucible. The place of crystallisation depended on the position of the chemical equilibrium but for me this was a great example of a really elegant experiment.

After the lunch break and successful poster session the meeting reconvened for the last session. This was opened by **Ramokone Malapile**, South Africa, on multicomponent crystals of baclofen with a range of simple acids and bases. Baclofen, a gamma amino acid, is a common muscle relaxant that has found promising use in the treatment of alcohol addiction. Second to last speaker of the day was a trip into the world of nanoclusters with **Stephan Pollitt**, Austria, with a deep dive into the single-crystal structures of Au38 thiolate protected nanoclusters. Obtaining full structural information from nanoclusters is challenging but important to further the understanding of these systems. The final talk of the day was a light-hearted introduction from Dr **Yu-Yuan Hsiao**, Taiwan, on the status of crystallography in Taiwan and the opportunities for young researchers. His open and positive talk was a great way to conclude this year's European Young Crystallographers satellite meeting.

The satellite meeting for the European Young Crystallographers was the perfect start to a very busy ECM. We were immediately brought together as a group of early career scientist to socialise and network for the rest of the week to make the most of the main meeting. The science presented was first class, and the opportunity to ask questions and really open discussions were really refreshing for me. Overall the ECM in Vienna was a fantastic event and one that I came away from really inspired for my work.

Dr Charlie McMonagle
University of Newcastle

MY trip to ECM32 started with a game of spot the crystallographer in the departure lounge of Manchester airport culminating in the satisfaction of seeing my tentative guesses head to the Vienna gate. This was followed by meeting up with some familiar travelling companions on the flight; soon I was on my way to a rewarding and interesting week in the Austrian capital. For those who have not been to Vienna (particularly in August) I would describe it as hot. Vienna is jam packed with impressive architecture and a smattering of green spaces where you can find shade and refreshment to survive the baking sun.

The conference, for me, started a day earlier with the

attendance at the European Young Crystallographers Meeting at TU Wien. I always find these meetings great because of the breadth of topics presented often provides inspiration for synthetic procedures, synthetic targets, new analytical techniques or even science communication ideas. This meeting was no different with work presented on developing new instrumentation for recording data on single crystals at low temperature or under an applied electric field. The use of interface excluders was a cool solution to the challenges of phase purity. The final talk of the day showing how the Taiwan Light Source has made it into popular culture as well as exploring the interface of crystallography and art. These talks were separated by a coffee break on a roof terrace that provided an amazing view of the Vienna skyline. Overall, the satellite was a great start to a week of scientific discussion and a good introduction to the city.

The ECM meeting, itself, was held at the Universität Wien in the main building of the university. This impressive building features an internal courtyard and arcade decorated with busts of famous professors from the university, staircases that would be at home in a piece of work by M C Escher and a Large Ballroom with a ceiling featuring paintings by Gustav Klimt the pictures do not really do it justice (believe me I tried several times). Day 1 started with the a session focusing on Single-Crystal Transformations which featured work on perturbing single-crystals with external stimuli as well as work showing that molecular rearrangements can lead to macroscopic bending, twisting or even jumping of single crystals. Day 1 also featured the Science Slam, an interesting showcase of the different approaches to public engagement. Day 2 expanded my understanding of different *in situ* techniques. On the third day, I was fortunate enough to get a seat in the session Teaching New Dogs Old Tricks, which was standing room only. Later in the day, I learnt that there was a queue outside this session to get in. I am not surprised, with a line-up of speakers who literally wrote the book or software, from whom people were keen to hear their handy tips and tricks. Day 3 also featured the conference dinner at the Orangery of the Schönbrunn Palace. After great food and liberal refreshments in an amazing setting my night concluded with a second skyline view at a roof top bar. The final day of the conference, I was fortunate to speak in the Tuning Crystalline Frameworks session, which, despite technical mishaps, led to interesting discussions to reflect upon. With the conference drawing to a close there was enough time to take a final picture in front of the record breaking crystal structure (with matching shirt of course) and one final evening which was spent at the City Hall Square where we inadvertently attended the City Hall Square Music Film Festival before heading home.

Tom Roseveare
University of Sheffield

Tools for Chemical Bonding (TCB) 2019

THE first Tools for Chemical Bonding software workshop was held in July in the German city of Bremen. Famous for the totem stack 'Town Musicians of Bremen', this week the city hosted over 50 participants in a meeting organised by Prof Dr Simon Grabowsky and his research group from the University of Bremen.

This hands-on workshop introduced various popular software suites for chemical bonding analysis at a beginners' level. It aimed to address the following:

i) Bridge the communities of quantum crystallography and quantum chemistry. In quantum crystallography, experimental electron density measurements are interpreted with respect to chemical-bonding questions, whereas in quantum chemistry theoretical wavefunctions are interpreted with exactly the same aim. Both communities can greatly benefit from adopting strategies and philosophies of the other.

ii) Publication of a new compound or synthesis strategy normally requires both a crystal structure and a geometry optimization, but the wealth of chemical-bonding information in diffraction measurements and wavefunction calculations is rarely exploited beyond the discussion of bond distances and angles.

Participants had a chance to learn about each software and have a go themselves with the experts on hand for live trouble shooting.

Mid-week there was a break in the schedule for a proper tour of Bremen, taken in a historic tram around the old town, out to the university in the north east and ending at a World War II bunker right under the main Bremen train station. To conclude the day, everyone met on the Schlachte to jump aboard the Alexander von Humboldt ship moored along the river Weser for the conference dinner. Attendees enjoyed a beer or two and some good German cooking in the evening sun and with the Heineken factory in view.

From the chair of the organising committee, Prof. Dr. Simon Grabowsky: "The workshop was very well attended with 55 participants and 20 teachers from all over the world. From the organizers' perspective, we were very happy with the engagement of the participants and the mingling of teachers with participants. We hope that this new format will see new editions in the future."

A textbook will follow the successful workshop based on the presented materials in the deGruyter publishing house for university students at graduate level entitled "Complementary Bonding Analysis" available in summer 2020.

Lucy Saunders
(Diamond Light Source)

Puzzle Corner

AFTER a return in September, former Crystallography News Editor Bob Gould is on a roll and has volunteered another Puzzle Corner.

Here are three well known buildings whose shapes represent somewhat unusual polyhedra. Identify the buildings, the point group of their (idealised) symmetry and say whether they could represent a crystal form.

a)

b)

c)

Answers to September Puzzle Corner

IT'S sometimes convenient to use an alternative setting of a space group – which of the following correspond to possible transformations and which do not?

	Standard	Transformed?
1.	Pbca	Pcab
2.	Pbca	Pcba
3.	$Pa\bar{3}$	$Pc\bar{3}7$
4.	$Pa\bar{3}$	$Pb\bar{3}$
5.	C2/c	A2/a
6.	P23	P32
7.	$P\bar{4}2c$	$P\bar{4}c2$
8.	Cmm2	Amm2

Answers: 1,4 and 5 are possible. 2 is not as a b-glide normal to the b-axis is not possible. 3 is not as it would imply three impossible glides. In 6, 7 and 8 two different space groups are represented.

Female Scientists in Valencia

ON a recent visit to Valencia, I was delighted to find a series of around 40 posters celebrating female scientists, displayed in the City of the Arts and Sciences. Four of the posters depict crystallographers; Kathleen Lonsdale, Dorothy Hodgkin, Rosalind Franklin and Ada Yonath. Some pictures of the posters are shown here; apologies for the quality, the weather was unseasonally dark and wet for Valencia! The text is in Spanish, English, and the local Valencian dialect, which is very similar to Catalan.

One of the buildings at the City of the Arts and Sciences (designed by Santiago Calatrava, the same architect as for the Palace and Exhibition of Congresses in Oviedo, the venue for 2018's European Crystallographic Meeting) is an excellent Science Museum. One very impressive space there contains a DNA model around 10m tall, and in the Museum lobby (ground floor, at the eastern end of the building), there is a display showing the highly impressive results of a local schools competition to grow crystals.

I can highly recommend Valencia, not just for the science and the architecture, but also for the food…!

Steve Maginn

Celebrating IYPT through one million crystal structures!

AS you may have read in the last issue of *Crystallography News* we have been asking you to help us celebrate IYPT and CSD one million by highlighting the elements in the Periodic Table and an associated crystal structure. The ultimate goal of this project is to develop a range of community driven educational resources to showcase the amazing science that has been made possible through crystallography and the Periodic Table. Since the last issue we have had some great contributions from you; here are just a few…

Xenon

Quick facts:

- **Chemical symbol:** Xe
- **Atomic number:** 54
- **Discovered by:** William Ramsay and Morris Travers in 1898
- **Group:** Noble gases
- **Melting point:** –111.75°C
- **Boiling point:** –108.099°C

54
Xe
131.29

Thanks to…
Helen Maynard-Casely, Senior Instrument Scientist at the Australian Centre for Neutron Scattering (ANSTO).

Tungsten

Quick facts:

- **Chemical symbol:** W
- **Atomic number:** 74
- **Discovered by:** Juan and Fausto Elhuyar in 1783
- **Group:** 6 (transition metals)
- **Melting point:** 3414°C
- **Boiling point:** 5555°C

74
W
183.84

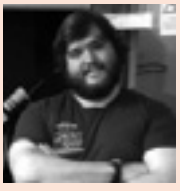
Thanks to…
Ala' Salem, Ph.D. student at the University of Pécs.

Magnesium

Quick facts:

- **Chemical symbol:** Mg
- **Atomic number:** 12
- **Discovered by:** Joseph Black in 1755
- **Group:** 2
- **Melting point:** 650°C
- **Boiling point:** 1090°C

12
Mg
24.31



Thanks to…
Tom Roseveare, Postdoctoral Research Associate at The University of Sheffield.

Nobelium

Quick facts:

- **Chemical symbol:** No
- **Atomic number:** 102
- **Discovered by:** Controversial! Claimed by groups from Sweden, US and the Soviet Union
- **Group:** Actinides
- **Melting point:** 827°C
- **Boiling point:** unknown

102
No
[259]

Thanks to…
Claire Murray, Chemist at Diamond Light Source.

These are just some of the elements available so far on our online interactive Periodic Table! Visit www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/ to view more elements and their crystal structures, to find out about the project, and who else has contributed so far. We would love to get even more of the community involved! If you would like to contribute and help us build this valuable educational resource, email us at hello@ccdc.cam.ac.uk with 'IYPT in Crystals' in the subject line.

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, news@crystallography.org.uk. Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

1-6 December 2019
Advanced Materials Exploration with Neutrons, Boston, MA, USA.
https://mrs.org/fall2019/call-for-papers/call-for-papers-detail?code=MT04

1-8 December 2019
Sixth joint DLS/CCP4 workshop on MX data collection and structure solution, Didcot, UK.
http://www.ccp4.ac.uk/schools/DLS-2019/

2-5 December 2019
BioSAXS 2019 Workshop, Menlo Park, CA, USA.
https://conf.slac.stanford.edu/smbsax2019/

9-12 December 2019
5th MicroED Workshop, Los Angeles, CA, USA.
https://cryoem.ucla.edu/pages/Workshop

9-13 December 2019
American Geophysical Union Fall Meeting, San Francisco, CA, USA.
https://meetings.agu.org/fall-meeting-2019/

11-13 December 2019
BILL2019: "Bilayers at the ILL" Workshop, ILL, Grenoble, France.
https://workshops.ill.fr/event/199/

16-19 December 2019
ANF Diffraction des rayons X appliquée à la cristallogenèse, Grenoble, France.
http://cmdo.cnrs.fr/spip.php?article268

17-20 December 2019
16th Conference of the Asian Crystallographic Association (AsCA2019), National University of Singapore, Singapore.
https://asca2019.org/

7-9 January 2020
CCP4 Study Weekend 2020, Nottingham, UK.
https://tinyurl.com/ccp4sw2020

19-30 January 2020
EMBO Practical course CEM3DIP 2020: **Single particle cryoEM of macromolecular-assemblies and cellular tomography, Kolkata, India.
http://meetings.embo.org/event/20-cem3dip

19-30 January 2020
EMBO Practical course Cryo Electron Microscopy and 3-Dimensional Image Processing (CEM3DIP 2020), IISER, Kolkata, India.
https://www.iiserkol.ac.in/web/en/

21-29 January 2020
SEA COAST – SouthEast Asian Crystallographic Overview and Systematic Training, Bangkok, Thailand.
http://seacoast.kmutt.ac.th

28-30 January 2020
7th BioXFEL International Conference, San Juan, Puerto Rico.
https://www.bioxfel.org/events/details/1218

9-13 February 2020
45th Lorne Conference on Protein Structure and Function, Cumberland, Lorne, Australia.
https://www.lorneproteins.org/

15-19 February 2020
Biophysical Society Annual Meeting, San Diego, USA.
https://www.biophysics.org/2020meeting#/

23-27 February 2020
Joint Polish-German Crystallographic Meeting, Wrocław, Poland.
https://www.dgk-conference.de

26-28 February 2020
Materials Science & Nanotechnology Conference, Sana Malhoa Hotel, Lisbon, Portugal.
https://materialsconference.yuktan.com/

16-20 March 2020
Understanding Biology through Structure, Santa Fe, NM, USA.
https://cvent.me/4kq9P

25-27 March 2020
11th International Workshop on Radiation Damage to Biological Samples, PSI, Villigen, Switzerland.
https://indico.psi.ch/e/rd11

6-9 April 2020
British Crystallographic Association Spring Meeting, University of Leeds, UK.
https://crystallography.org.uk/spring-meetings/#next-meeting

29-6 June 2020
55th Course of the International School of Crystallography (Structural Drug Design), Erice, Italy.
http://www.crystalerice.org

21-26 June 2020
Three-Dimensional Electron Microscopy. Gordon Research Conference, Castelldefels, Spain.
https://www.grc.org/three-dimensional-electron-microscopy-conference/2020/

19-24 July 2020
Gordon Conference on Research at High Pressure, Holderness, NH, USA.
https://www.grc.org/research-at-high-pressure-conference/2020/

22-30 August 2020
Twenty-Fifth Congress and General Assembly of the International Union of Crystallography, Prague, Czech Republic.
http://www.iucr25.org/

24-28 August 2021
Thirty Third European Crystallographic Meeting, Versailles, France.
https://www.ecm33.fr/

S6 JAGUAR

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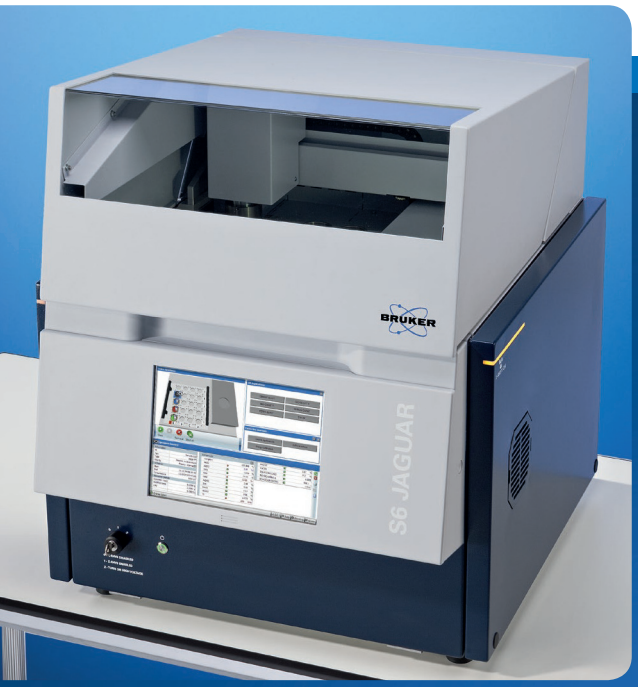

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