Crystallography News

British Crystallographic Association

Issue No. 159 December 2021
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BCA Spring Meeting 11th - 14th April 2022

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British Crystallographic Association

Conference Bursaries 2022

Bursaries are available for BCA members to attend national/international crystallographic meetings in 2022.

Local meetings and virtual meetings (with no travel) are supported. Eligible members may apply every year.

Apply early for in person attendance at international meetings. Successful local/virtual meeting bursary winners are still eligible.

Further information on the eligibility criteria and the application portal is available here:
https://crystallography.org.uk/prizes/bursaries

Additional carers grants are also available to BCA members at any career stage:
https://industrial.crystallography.org.uk/bursaries-and-awards/

BCAIG

Contents

Erratum:
On page 10 of September's Crystallography News, the dates of James Watson's and Francis Crick's Nobel Prizes were incorrectly stated. Both were awarded the prize in 1962.

This month's cover:

Leeds – where we shall be meeting in the Spring

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by North Wolds, York. Text should preferably be sent electronically as MSword documents (any version - .docx, .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.
Please ensure that items for inclusion in the March 2022 issue are sent to the Editor to arrive before 25 January 2022.

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From the President

WELCOME to the December issue of *Crystallography News*. As we reach the end of 2021 there is still a great deal of uncertainty in the unfolding pandemic and associated restrictions which impact decisions around meeting planning, travel and teaching. While we may get used to dealing with unexpected last-minute changes in our daily lives, the organisation of events and meetings is still fraught with balancing complicated risks and finances. Therefore, I would like to express gratitude to individual and corporate members for continuing to strongly support the BCA. Remember that the cost of individual BCA membership works out at £3.33/month (less if you are a student), which is a mere third of the cost of an online film streaming subscription, and about the same as a takeaway cup of coffee (around here at least). I would encourage you to recruit new members or even re-recruit lapsed members where you can. Student members and those without travel funds can access bursaries to attend crystallographic meetings, including, but not limited to the BCA.

My thanks are directed to the BCA Nominating Committee for securing several nominations for upcoming BCA Council elections (details below). The committee is now in its fifth year of operation and has been successful in increasing the number and balance of candidates for Council elections each year. I would like to acknowledge the current members for their recent endeavours: **Chris Frampton**, **Elspeth Garman**, **Chick Wilson**, **Paz Vaqueiro**, and **Lee Brammer**. Lee and Chick are both retiring from the committee at the end of this cycle and new members will be appointed at the next Council meeting. Statements from the candidates for Vice-president, Secretary and one Ordinary member of Council are included in this issue. As in recent years, the elections are entirely online and in advance of the AGM – which enables all members to vote and has a side effect of speeding up the admin. at the AGM – so keep an eye out for the email during December. If you think you've been missed, please contact **bca@hg3.co.uk** before voting closes at the end of January to ensure you can exercise your democratic rights.

In the coming months, we will circulate a short survey to all members to help feed into discussions on Council. We would like to gather opinions about a range of areas across the organisation including membership options, ways of meeting our charitable aims, and the frequency, content and format of scientific meetings, especially now that online options have been forced into the mainstream. We will report a summary of the results in a future *Crystallography News*, and any proposals arising from the survey will be brought to the AGM for discussion in the usual way. Please look out for the survey in your email in the next couple of months and take a few moments to complete it.

The last column went to press before the delayed IUCr 2020, even though it didn't appear until the September issue. The meeting was held in hybrid mode in Prague. I'm not aware of any UK delegates attending in person – if you did, please let me know how it was. As a remote delegate in a hybrid meeting, we could glimpse friends and colleagues during the Q&A sessions, and though it was a sensible arrangement given the circumstances, it was a reminder of how enjoyable it would be on a purely personal level to be able to gather for discussions and coffee at international meetings. I endured an unstable rural internet connection during the IUCr meeting itself, so was very grateful to be able to catch up once I was back home by viewing recordings of lectures that I had missed, which were available for a few weeks afterwards.

The BCA is the national adhering body to the IUCr, and so we sent a virtual delegation to the General Assembly meeting during the Congress. We were disappointed not to get a UK candidate elected to the IUCr Executive Committee, but in a nail-biting series of online votes we made it to the very last round against a large field of outstanding candidates who I am certain will serve the IUCr well over its next cycle. Thank you to all of the UK delegates and backup delegates who took time out from their evenings to attend the GA meetings and vote, especially **John Helliwell** for facilitating discussions to reach consensus for the key votes and for writing up the process for *Crystallography News* readers.

If you keep an eye on the BCA website, you will have seen that a short film was released recently as part of the *BBC Ideas* collection of short videos. These cover a broad range of general interest topics and issues. This film was made in partnership with the Royal Society, and featuring **Judith Howard** and **Georgina Ferry**, it tells an inspiring story of scientific success despite established societal and academic conventions. Link: **https://bit.ly/dorothy-hodgkin**.

At the time of writing I am looking forward to the online CCG group Autumn meeting on the theme of Crystals out of Equilibrium, though it will have already taken place by the time of publication. Nominations are open for the annual CCDC Chemical Crystallography Prize for Younger Scientists – please see the CCG website for details. Keep an eye on the BCA and group websites for details of other upcoming meetings and prize nominations.

The BCA website and social media accounts are at your disposal (within reason!) for promoting studentships, job vacancies and events. Please send requests, preferably with a link to a website containing the full information to **web@crystallography.org.uk** (**Claire Hobday**) and it will be distributed on the appropriate channels.

I am delighted to announce that based on nominations from the membership, Council has decided to award Honorary BCA membership to Professors **Paul Raithby** and **Chick Wilson**. These awards have been made in recognition of significant contributions by the recipients, to crystallographic science and to the work of the BCA. Nominations including a short case for support of not more than 400 words can be sent to **president@crystallography.org.uk** at any time and will be considered by Council at the end of August each year.

Finally, we were saddened in September to hear of the passing of Professor **Jack Dunitz**, BCA Founder Member and Honorary Member. Professor **Judith Howard** has provided an obituary and personal reminiscences of Jack in this issue which includes links to an interview with Jack and other biographies in this issue and online.

Richard Cooper

BCA Council 2021

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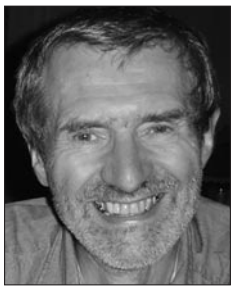
(The dates in parentheses indicate the end of the term of office).

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

From the Editor



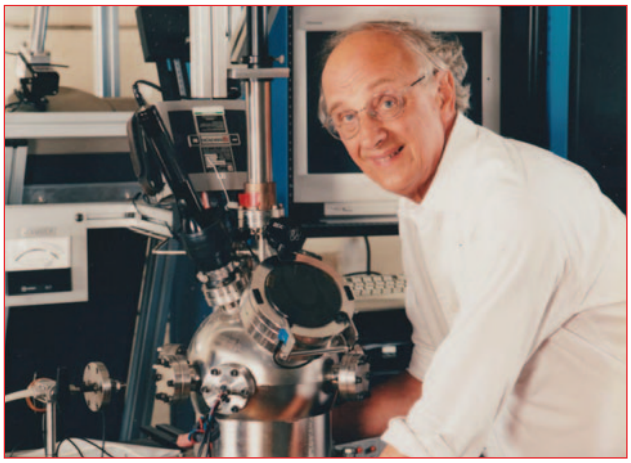
IN contrast to the – perhaps experimental – September issue that focussed on one of the greats of 20th century crystallography, this issue is more back to normal. In it you will find reports of sessions at a number of crystallographic meetings including IUCrXXV and the 71st Annual Meeting of the ACA. Also, as is usual for December, there's a preview of the 2022 Spring Meeting – where hopefully the UK crystallographic community can get together in person in Leeds – and the election statements of candidates for BCA Council. In addition, we have an account of the ambitious Endeavour development programme for the UK's pulsed spallation neutron source ISIS which will open up new opportunities to structural science. We also sadly say farewell and thank you to another great crystallographer, Jack Dunitz.

Returning to the September issue – which from the responses I've had seems to have been appreciated (not least by the IUCr Newsletter which has 'reprinted' the Bernal articles) – space limitations meant that an article on Bernal's ideas on 'generalised crystallography' had to be dropped. These ideas were of particular interest to me as a young lecturer some 50 years ago in the Birkbeck department trying to get to grips with understanding the structures of liquids. Because of the absence of a lattice, the standard crystallographic armoury doesn't help us very much: the best we could do with diffraction techniques was to obtain the radial distribution function (rdf) – the distribution of pair distances in the liquid.

This function has a formal relationship with the Patterson function then used extensively in solving the phase problem. I therefore thought it opportune, half way across the Pacific Ocean in the summer of 1972 returning on an ACA chartered flight from the 1972 IUCr Congress in Kyoto, to get into conversation at the (free!) bar with **Dave Harker** who had worked with Patterson and was responsible for the Harker section of the Patterson function that crystallographers were finding particularly useful. What an opportunity! To discuss the problems of liquid structure determination with him, in the hope that his insight into the development and use of the Patterson function would suggest how we might move forward to try to obtain data on liquid structures that could be comparable in detail to that obtainable on crystals.

Although having no clear ideas at the time as to how the problem of the absence of a lattice could be overcome, I argued with Harker that there must be some way of extracting more information than the rdf, and ultimately obtain detailed structural information on those relatively complex liquids that are of biological and chemical importance – for example in obtaining information on the mechanisms of protein association and enzyme-ligand binding in solution. I thought that making significant progress in this direction would be my scientific career well spent. He very patiently listened, though he made it pretty clear that he thought I was on a wild goose chase.

The subsequent 50 years – my scientific lifetime – has proved Dave wrong, thanks to the pioneering work of another great scientist, **John Enderby**, who sadly died last August. Although John would not have regarded himself as a crystallographer,



Picture courtesy of Mark Simmons Photography.

his contribution to the structural science of non-crystalline systems has revolutionised the field. Although I wasn't aware of his early work when I was talking to Harker, this revolution began with his 1966 landmark paper[i] with **Peter Egelstaff** and **D.M. North**. Though the title *"The Partial Structure Factors of Liquid Cu-Sn"* may sound obscure, this paper laid the foundations of an experimental technique that has incredibly wide applications. Taking advantage of the fact that, unlike X-rays, neutrons interact differently with different isotopes of many elements, John solved this difficult problem, enabling us at last to determine the structures of non-crystalline systems.

Thus John gave us a remarkable tool for understanding processes in Physics, Chemistry, Geology and Biology. His research has thrown new light on structures and processes in alloys, liquid semiconductors, molten salts, ionic liquids, electrolytes, and aqueous solutions, systems central to many physical and biological phenomena, and crucial to many technological applications. Consequently, he has given us a fuller understanding of – among many other things – the hydration of ions, and the relationship between chemical bonding and electrical properties.

But that was only a start. Unselfishly encouraged and helped by John, many others have built on what he has made possible. Consequently, we can now see how water molecules interact with chemical and biological molecules more generally, and begin to understand how these interactions facilitate chemical and biological processes. Thanks to John, we have begun to understand better the molecular-level interactions that facilitate life itself.

By making possible what I call *liquid state crystallography*, John's work really has revolutionised our ability to understand structure and function in a vast range of liquid systems. He made a huge scientific advance. Nobel prizes have been awarded for less.

Scientists are remembered for the science they have done themselves. Great scientists are lauded also for the doors they have opened for others to build on their groundbreaking work.

John was one of those giants, on whose shoulders we others stand.

John Finney

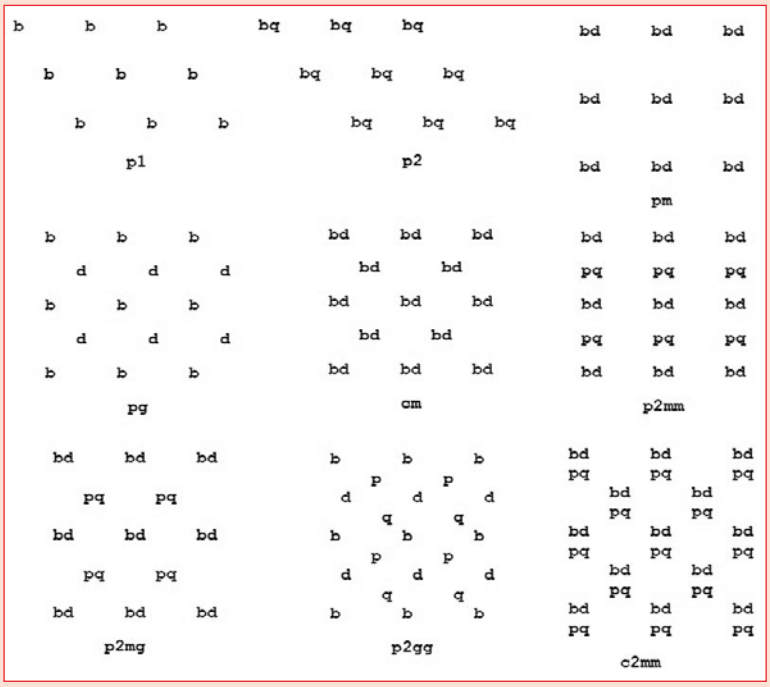
Reference:

i J.E. Enderby, D.M. North and P.A. Egelstaff. *Phil. Mag.* **14**, 961 (1966).

Puzzle Corner

IN poker, four of a kind (e.g. four kings) is worth more than a "full house" – three of one kind and two of another (e.g. three kings and two queens). Show that for a deal of five cards this rating is sensible.

Answer to September's puzzle



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.
- Two free registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly Crystallography News.
- Corporate Members will be listed in every Crystallography News and on the BCA website with clickable links to your organisation's website.

Corporate Membership is currently **£800** for one year.

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Benefits of Individual BCA Membership:

- The professional organisation for crystallographers in the UK
- A broad range of meetings organised by the BCA and its subject groups
- Preferential members' rates for such meetings
- Eligibility of students and postdocs for an Arnold Beevers Bursary award
- A copy of Crystallography News every quarter
- Optional E-mail notifications of news items and meeting information
- Influence on the development of crystallography and the BCA

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

BCA Spring Meeting 2022

PLANNING is well under way for the 2022 BCA Spring meeting to be held – in person (cheers!) 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 of the abstract deadline of January 21st 2022.

To register for the meeting, please go to https://registrations.hg3conferences.co.uk/bca2022

YCG EARLY CAREER SATELLITE MEETING

Monday 11th April, 2022

University of Leeds

Session Details

Young Crystallographers Group (YCG)

13:00 – 21:00

The YCG satellite meeting is an opportunity for all early career researchers in the field of crystallography, from across the BSG, CCG, PCG and IG, to present their work in a supportive and friendly environment, which will be run by fellow early career scientists.

13:00 – 13:30

YCG Opening Plenary

Session Chair: **Tom Roseveare** *(University of Sheffield)*
Speaker: **Dr Claire Hobday** *(University of Edinburgh)*

Pressure driven phase transitions – a look to the future of solid-state refrigeration

13:30 – 17:15

YCG Research Sessions

Contributed talks from the YCG community.

Session 1 Chair: **Tom Roseveare** *(University of Sheffield)*
Session 2 Chair: **Dr Natalie Pridmore** *(University of Bristol)*
Session 3 Chair: **Aly Abdeldaim** *(ISIS Neutron and Muon Source/University of Birmingham)*

17:15 – 17:45

YCG Annual General Meeting

18.30 – 21.00

Flash Poster Presentations

Session Chairs: **Dashnor Beqiri** *(University of Warwick)* & **Lee Birchall** *(University of Kent)*

Researchers have an opportunity to present an overview of their poster in 30 seconds with one PowerPoint slide. A poster session (with buffet and wine) follows.

BCA 2021 MAIN MEETING PROGRAMME

Tuesday 12th April, 2022

09:00 – 09:30

Parkin Lecture

Session Chair: **Dr Rachel Wilkinson** *(Swansea University)*
Speaker: **TBC**

09:30 – 10:30

YCG Research Sessions

Contributed talks from the YCG community.

Session 4 Chair: **Dr Charlie McMonagle** *(European Synchrotron Radiation Facility)*

10:30 – 11:00

YCG Closing Plenary

Session Chair: **Dr Charlie McMonagle** *(European Synchrotron Radiation Facility)*
Speaker: **Dr Sam Horrell** *(Diamond Light Source)*

10ish things your beamline scientists wish you knew

MAIN MEETING

11.30 – 12.15

Lonsdale Lecture

Session Chair: **Tom Roseveare** *(University of Sheffield)*
Speaker: **Prof. Andrew Goodwin** *(University of Oxford)*

Disorder by design: from form to function

13:00 – 13:45

PCG Plenary

Session Chair: **Dr Alex Gibbs** *(University of St Andrews)*
Speaker: **Prof. Xiaodong Zou** *(Stockholm University)*

Electron crystallography: past, present and future

14:15 – 15:45 Parallel Sessions

PCG: Porous Materials

Session Chair: **Aly Abdeldaim** *(ISIS Neutron and Muon Source/University of Birmingham)*
Keynote: **Dr Sam Chong** *(University of Liverpool)*

The importance of cooperativity in understanding porous molecular crystals

The diverse functionality associated with the versatility of porous materials allows for the discovery and realization of properties that are crucial for advances in next generation applications. Specifically, their broad structural-property adaptability explains the enduring appeal of their research, as porous materials find diverse applications ranging across, among others, energy storage, drug delivery, and nanotechnology. As such, this session will focus on exploring the ongoing trends in this field, delving into their synthetic complexity, structural-property relationships, and their relation to *ab initio* techniques.

BSG: RNA-Protein Interactions

Session Chair: **Prof. Phil Evans** *(University of Cambridge)*
Keynote: **TBC**

CCG: Crystallography Under Extreme Conditions

Session Chair: **Dr Charlie McMonagle** *(European Synchrotron Radiation Facility)*
Keynote: **Dr Christine Beavers** *(Diamond Light Source)*

Extreme Conditions for All: Expanding the Exploration of Phase Space in a Multitude of Materials

Crystallography under extreme conditions comes with its own associated challenges. In this session we explore the advances in technique development and data analysis under non-ambient regimes that inform on interesting chemistry. Extreme conditions can provide critical insight into the structures, reactivity, and behaviour of molecules and materials. This session will cover scientific, technological, and methodological developments across a wide range of extreme experimental conditions including high magnetic fields, electric fields, high and low temperatures, high pressure.

16:30 – 18:00 Parallel Sessions

PCG: Structure-Property Relationships in Energy Storage

Session Chair: **Dr Karen Johnston** *(University of Durham)*
Keynote: **Prof. Laurence Croguennec** *(Institut de Chimie de la Matière Condensée de Bordeaux)*

Developing an in-depth understanding of new materials to optimise cathodes in metal-ion batteries

As we strive to achieve net zero emissions it is increasingly clear that energy storage will play a crucial role in addressing this global challenge, driving areas such as the electrification of transport and large-scale storage of renewable energy. Rechargeable Li- and Na-ion batteries will be key in delivering future energy storage demands. This session explores battery materials, their complex structure-property relationships and the methods used to characterise them. We are interested in new battery materials and technologies (beyond Li-ion). Examples where the combination of experimental and computational methods has resulted in significant structural understanding are also of interest.

BSG: Correlated Tomography

Session Chair: **Dr Maria Harkiolaki** *(Diamond Light Source)*
Keynote: **TBC**

CCG: Nucleation & Phase Changes

Session Chair: **Dr Katharina Edkins** *(University of Manchester)*
Keynote: **Prof. Gérard Coquerel** *(Université de Rouen, Normandie)*

Polymorphic transitions in the organic solid state: two complex cases with simple molecules

The phase transitions between liquid and solid, or indeed between two solid phases, can have an immense impact on the manufacture and stability of organic materials. Most phase transitions include a nucleation step, while nucleation is best known as the first step in the generation of a crystalline material from solution or the melt. In this session, we will be looking at the impact and the underpinning fundamental science of phase transitions and their related nucleation in organic or organo-metallic materials for the application in pharmaceuticals, agrochemicals or fine chemicals, sensors and energy materials non-exclusively.

18:15 – 19:00

CCG Plenary

Session Chair: **Dr Michael Probert** *(University of Newcastle)*
Keynote: **Prof. Michaele Hardie** *(University of Leeds)*

Supramolecular cages and networks with pyramidal ligands

Wednesday 13th April, 2022

08:45 – 09:30

IG Plenary

Session Chair: **Dr Helen Blade** *(AstraZeneca)*
Keynote: **Dr Colin Small** *(Swansea Materials Research & Testing)*

10:15 – 11:45 Parallel Sessions

PCG/CCG: Advances in Complementary Techniques and *In Situ* Crystallography

Chair: **Dr Hamish Yeung** *(University of Birmingham)*
Keynote: **Prof. Fiona Meldrum** *(University of Leeds)*

In Situ Imaging of Crystallization Processes

Advanced complementary techniques offer fantastic potential to improve our understanding of structure, mechanisms and processes far beyond what is possible using conventional crystallography. X-ray tomography, coherent diffraction imaging, NMR crystallography and electron diffraction are just four examples of emerging methods that give a wealth of information

beyond long-range ordered structure and are all the more powerful when performed *in situ* or *in operando*. Such techniques push the boundaries of possibility with existing instruments and methodology, leading to advances across many diverse scientific disciplines including biological crystallisation, energy storage, catalysis and advanced materials.

BSG: Electron Diffraction

Session Chair: **Dr Peijun Zhang** *(Diamond Light Source)*
Keynote: **Dr Tim Gruene** *(University of Vienna)*

Electron crystallography for X-ray crystallographers

The field of electron diffraction of micro/nanocrystals (microED) is emerging. A growing number of structures were determined by microED and several protocols and workflows for data collection and structure determination have been established. This session will be focused on advances in software/hardware for microED, results obtained and discussions of future development.

IG: Metallurgical Crystallography

Session Chairs: **Dr Judith Shackleton** & **Dr Helen Blade** *(AstraZeneca)*
Keynote: **Dr Will Bodel** *(University of Manchester)*

Premature ageing of British nuclear reactor cores

12:15 – 12:45
BSG Annual General Meeting
PCG Annual General Meeting

12:45 – 13:15
CCG Annual General Meeting

13:15 –14:45
Early Career Prize Lectures

Biological Structures Group Early Career Prize

The BSG will award a prize to someone who has had an impact in the field of Structural Biology (with an emphasis on crystallography) and recently obtained a personal fellowship, a lectureship or equivalent position.

CCDC Chemical Crystallography Group Prize for Younger Scientists

The CCG and CCDC will award a prize to a younger scientist who has performed original research in the field of chemical crystallography or the application of crystallographic information to structural chemistry.

Physical Crystallography Group Prize

The PCG Physical Crystallography Prize is awarded for the best recently published work by a person in the early stages of their career, working in the field of Physical Crystallography, whose research is expected to make a significant impact in the field.

15:30 – 17:00 Parallel Sessions

YCG+ Careers Session

Session Chairs: **Dr Natalie Pridmore** *(University of Bristol)* & **Tom Roseveare** *(University of Sheffield)*
Panellists: **Prof. Andrew Goodwin** *(PCG, University of Oxford)*; **Dr Claire Hobday** *(CCG, University of Edinburgh)*; **Dr Sam Horrell** *(BSG, Diamond Light Source)*; **Dr Helen Blade** *(IG, AstraZeneca)*

An opportunity to hear from, and pose questions to, the panellists about their jobs and career paths in various fields of crystallography.

BSG: Membrane Proteins

Session Chair: **Dr Julien Bergeron** *(King's College London)*
Keynote: **TBC**

IG: *In Situ* Crystallography – Looking Inside the Black Box

Session Chair: **Dr Helen Blade** *(AstraZeneca)*
Keynote: **TBC**

17:10 – 18:00
Hodgkin Lecture

Session Chair: **Prof. Richard Cooper** *(University of Oxford)*
Keynote: **Prof. Elspeth Garman** *(University of Oxford)*

Macromolecular Crystallography in 112 AD (After Dorothy)

18:00 – 19:00
BCA Annual General Meeting

19:30 – 01:00
Conference Dinner

Thursday 14th April, 2022

08:45 – 09:30
BSG Plenary

Session Chair: **Dr Katherine Brown** *(University of Cambridge)*
Speaker: **Prof. Randy Read** *(MRC, Cambridge)*

Discussing the Implications of AlphaFold2

10:15 – 11:45 Parallel Sessions

PCG: Extracting information from disordered and poorly crystalline solids

Session Chair: **Dr Arianna Minelli** *(University of Oxford)*
Keynote: **Dr Kirsten Jensen** *(University of Copenhagen)*

Materials on the nanoscale: Total scattering analysis for nanoparticle chemistry

Increasingly, materials with structural disorder are studied with diffraction techniques, which were considered for many years only able to show perfectly periodic arrangements. In reality, this perfect periodicity simply describes an average reconstruction of the structure and the disorder adds a supplementary signal, normally found as diffuse scattering. This session looks at all degrees of complexity in disordered materials; from correlated disorder in a single crystal to poorly crystalline materials and all the way to amorphous phases.

BSG: Room Temperature Data Collection

Session Chair: **Dr Allen Orville** *(Diamond Light Source)*
Keynote: **TBC**

CCG: Tricks of the Trade – From Crystallisation to Publication

Session Chair: **Dr Claire Wilson** *(University of Glasgow)*
Keynote: **Prof. Ton Spek** *(Utrecht University)*

PLATON tools to help with resolving cryptic checkCIF ALERTS

This session is an opportunity to share tricks of the trade, to highlight tools or methods of interest to many in the chemical crystallography community but which are not currently as widely used as they could and should be. These could be software, practical or analytical tools or methods which have been newly developed or older ones which have fallen out of use and been rediscovered or repurposed to provide a valuable option for current chemical crystallographers at any stage from crystallisation to publication.

12:00 – 13:30 Parallel Sessions

PCG: Functional Materials

Session Chair: **Dr Paul Saines** *(University of Kent)*
Keynote: **Dr Josh Makepeace** *(University of Birmingham)*

The role of compositional flexibility in energy storage applications of lithium imide-based materials

Functional materials are critical to underpinning the technologies needed for modern society, including, for example, clean energy generation, medical sensing and quantum technologies. This session will focus on understanding the structure-property relationships in functional materials and how this enables materials to be optimised for application. Studies using experimental approaches that extend conventional approaches, including those combining computational methods, are of particular interest for this session.

BSG: Covid Drug Discovery

Session Chair: **Dr Daren Fearon** *(Diamond Light Source)*
Keynote: **Dr Ivan Ahel** *(William Dunn School of Pathology, University of Oxford)*

The outbreak of Covid-19 has inspired international efforts to develop novel antiviral agents to help address both the current pandemic and any future pandemics caused by coronaviruses. Fragment-based drug discovery and structure-based drug design have made significant contributions to the development of these much needed antivirals with over 1500 X-ray crystal structures deposited in the PDB to date. This session will focus on structural methods used to identify ligands which bind to coronavirus proteins and how these methods have been applied to further develop these ligands into promising leads and drugs.

CCG/BSG: Understanding Crystallization Through Diffraction and Complementary Methods

Session Chair: **Prof. Joop ter Horst** *(University of Rouen)*
Keynote: **Prof. Sven L.M. Schroeder** *(University of Leeds)*

Deeper Insight into the Mechanisms of Organic Molecule Nucleation from Advanced X-ray Analytical Methods

Crystallization is the process of forming crystal solid particles, preferably of a certain structure, size, shape, and purity. This process is governed by the sub-processes of, among others, crystal nucleation and growth which are still not completely understood. This session will discuss innovative diffraction and complementary methods that deliver breakthroughs both in the understanding as well as control of crystallization processes of all types of solids.

CLOSE OF CONFERENCE

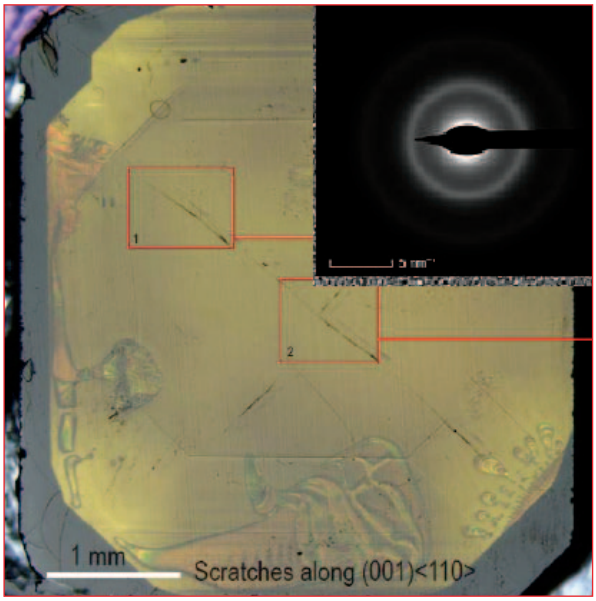
What happens when you compress Buckyballs?

WE all know that diamond gets its hardness from its 3D network of sp^3 carbons – as against its soft sp^2 bonded allotrope graphite. Much work has been done over more than 30 years exploring the possibility of a non-crystalline arrangement of sp^3 carbons, and to find out what its (useful?) properties might be.

Recently published work[i] that has caught my eye recently compresses buckyballs to 25GPa under increasing temperature. As the temperature increases, the fraction of sp^3 carbons increases until at 1,200C the authors reckon that 94% of the carbons are sp^3. This apparently largely non-crystalline network of carbon atoms (see the X-ray pattern inset in the figure) is so hard it can scratch diamond (see the figure) and is of similar compressive strength.

But unlike diamond – an insulator – the material is a semiconductor. With a band gap similar to that of silicon, it could be very useful in e.g. solar cells and other interesting applications.

John Finney
UCL



(Image: Copyright © 2021, Oxford University Press)

Reference:

i S. Zhang *et al, Nat. Sci. Rev.* (2021). http://dx.doi.org/10.1093/nsr/nwab140

BCA Council Elections 2022

Candidate Statements

NOMINATIONS for BCA Vice President, Secretary and Ordinary Member of Council have been received. Elections will be held by electronic ballot of the BCA membership. The short CVs and statements produced by the candidates are given below; the order in which they are given for each post is random.

Vice President Candidates:

Simon Coles

Current Position:
Professor of Structural Chemistry; Director of the U.K. National Crystallography Service and Director of the U.K. Physical Sciences Data-science Service, School of Chemistry, University of Southampton.

Education and Career:
2012-2016 Associate Professor, University of Southampton; 2010-2012 Lecturer, University of Southampton; 1998-2010 Manager, National Crystallography Service, University of Southampton; 1996-1997 PDRA Royal Institution of Great Britain and CLRC Laboratory (Daresbury); 1992-1996 Research Assistant, National Crystallography Service, University of Wales, Cardiff; 1989-1992 B.Sc. (Hons), University of Wales, Cardiff.

Professional Activities:
I am Director of an M.Sc., Sustainability Champion, Library Liaison and PostDoc. Champion in my department and represent my faculty on university Open Research Group and ED&I committees. I help run the RSC Local Section and am FRSC and Senior Fellow of the HEA. Internationally, I serve on the IUCr Committee on Data and IUPAC FAIR Data Taskforce and on Editorial/Advisory boards of Crystallography Reviews, Cryst. Eng. Comm. and Supramolecular Chemistry.

BCA positions held:
2019-2020 Crystallography News Editor; 2015-2021 BCA Education and Outreach Coordinator; 2011-2015 Vice Chair and Chair CCG; 2009-2010 Spring Meeting Programme Chair; 2006-2008, YCG Chair; 2000-2003 Ordinary Member, CCG; 1995 Spring Meeting Local Organising Committee.

Research Interests:
I have been at the leading edge of service crystallography for three decades (*ca* 1000 publications, H-Index = 57, >15000 citations). However, my research interests are much broader – I lead a national facility devoted to chemical and physical sciences data and have run projects on CT Imaging, SHG Laser Spectroscopy, Dynamic Light Scatting, Computational Modelling, Additive Manufacturing, Formulation, eLearning, Data Management, Artificial Intelligence and Chemical Informatics. Structural chemistry research interests include crystal sponges, solid-state reactions/transformations, structural systematics, quantum crystallography, structure-property relationships and crystal growth.

Statement:
I am very familiar with the operation of the BCA, having served in numerous committee positions and attended every Spring Meeting since 1992! I have served on BCA Council in a number of different roles and having worked through different levels of the CCG and helping get the YCG established, I understand the roles and operation of our groups.

I am passionate about enhancing chemistry and crystallography education at all levels and I will continue to help ensure education and outreach is supported throughout all aspects of the BCA. Science is global and I feel it is vital that the BCA is not only represented at this level, but that it is internationally leading. While helping organise the Pan-African Conference on Crystallography I realised the value of promoting British crystallography as a way to help developing nations and as a very active member of the IUCr Committee on Data, the ECA and the ACA, I will help to keep the BCA globally recognised.

I believe I have considerable experience to bring to this position and relish the opportunity to be fundamentally involved in operating the BCA.

Suzanna Ward

Current Position:
Head of Data and Community, The Cambridge Crystallographic Data Centre (CCDC), Cambridge, U.K.

Education and Career:
M.Chem., University of Southampton, Department of Chemistry, including a placement in crystallography with Professor Mike Hursthouse based in Southampton and at the pharmaceutical company Rhône-Poulenc. In 2006 I joined the CCDC as a Scientific Editor and now lead the team responsible for the creation of the Cambridge Structural Database (CSD) and the education and outreach activities of the centre.

Research Interests:
After realising how powerful a technique crystallography is in my time at Southampton, I began my career at the Cambridge Crystallographic Data Centre (CCDC) as a Scientific Editor

where I worked to curate and enrich crystal structures into the CSD. This led to work to improve the efficiency of data curation and in 2013 I took on responsibility for managing the team that creates the database. Since 2019 I have been working as Head of Data and Community for the CCDC and as such I now also lead the education and outreach activities for the centre. As well as helping the centre spread the wonders of crystallography, I have presented and chaired sessions at many international conferences, and hosted training workshops for the CCDC and crystallographic schools.

Statement:
I am passionate about our wonderful world of structural science, but perhaps what I value most is our supportive community of crystallographers. The importance of this has been clear to me since attending my first Durham School and BCA meeting back in 2003. The value of bringing the community together, learning from each other, and the importance of welcoming new members and helping to train future generations has been reinforced in every conference, school, and event I have attended since. The BCA holds a key role in this ecosystem. Our community is crucial for the future of structural science, and I feel proud to be part of such an active crystallographic association.

Working for the CCDC has given me a tremendous opportunity to see first-hand how our field is evolving, and the impact crystallography has across science and beyond. I have also been privileged to attend many local, regional, and international conferences in crystallography and learn from these experiences and the people I have met.

How we connect with each other is changing, and it is more important than ever that we establish links outside of our field and grow and diversify our society. As a discipline we are also seeing new techniques and research areas emerge which will undoubtedly bring new and exciting opportunities, and perhaps some challenges too. I would be honoured to support our association as Vice President of the BCA and would relish the opportunity to help organise our annual meetings and to help our society engage more widely in the scientific community and beyond.

Secretary Candidates:

Lauren Hatcher

Current position:
Royal Society University Research Fellow in the School of Chemistry, Cardiff University, 2020-present.

Education and career:
Postdoctoral Research Associate in Crystallisation Science for Manufacturing, Future Continuous Manufacturing and Advanced Crystallisation (CMAC), Research Hub at the University of Bath, 2018-2020. Postdoctoral Research Associate in the Metastable Materials Group, Department of Chemistry, University of Bath, 2014-2018. Ph.D. in Chemistry at the University of Bath, 2010-2014. B.Sc. in Natural Sciences with Industrial Placement at the University of Bath, 2006-2010.

BCA activities:
YCG IG representative, 2010-2012; YCG Committee Secretary/Treasurer, 2012- 2014; CCG Committee Ordinary Member 2016-2019; CCG Committee Vice Chair 2020-present; Programme Organiser CCG Autumn Meeting (2018 and 2021); tutor at the biennial BCA/CCG Intensive Teaching School in X-ray Structure Analysis (2015, 2017).

Statement:
Being lucky enough to find myself in a Department with a strong solid-state chemistry community, my interest in crystallography was sparked early in my Undergraduate studies. I found myself drawn to not only the beautiful structures and patterns that we deal with daily, but it also spoke particularly to my problem-solving mind!

I attended my first BCA Spring meeting as an Undergraduate in 2009 and was immediately absorbed by the welcoming and supportive environment that our association excels in providing. One of the stand-out features of the BCA is the fantastic opportunities offered for early career researchers by the YCG and I was lucky enough to be an active member of this community as part of the YCG Committee throughout my Ph.D. Undoubtedly, the opportunities provided at YCG satellite meetings, and later main BCA meetings, to hone my presenting skills, to make friends and to build networks within our community have particularly guided and shaped my research career to-date. In particular my time as Secretary/Treasurer of the YCG, as well as my current role as Vice Chair of the CCG, have helped me to understand much more about how the BCA is run, our values and goals, as well as the challenges we face as a professional society. I believe this background now prepares me well to stand for this role on Council and I am honoured to have been nominated to stand as Secretary.

Samantha Chong

Current position:
Lecturer, Department of Chemistry and Materials Innovation Factory, University of Liverpool.

Education and career:
Research Coordinator and PDRA, University of Liverpool (Prof. Andy Cooper, Prof. Matt Rosseinsky); Software developer, RM Education, Abingdon; PDRA and Ph.D., University of Birmingham (Dr M. Tremayne); M.Sci. Chemistry, University of Birmingham.

Professional activities:
Diamond Light Source Peer Review Panel member (2018-2021); Tutor for BCA/CCG Intensive Teaching School in X-ray Structure Analysis (2021); Member of Organising Group for Recent Appointees in Materials Science (2019); Scientific Committee for the RSC Solid State Chemistry Group Christmas Meeting (2019); Diamond Light Source User Committee member (2015-2017).

Research interests:
The broad motivation for my research is to understand how structure affects the functional properties of crystals, as this is a fundamental step towards the rational design of materials for targeted applications. I have worked on the characterisation of a broad range of materials using powder diffraction methods, and with a specific interest in the responsive behaviour of porous organic and metal-organic crystals probed by *in situ* crystallographic measurements, benefitting greatly from access to large-scale facilities such as Diamond Light Source and from close collaborations with computational chemistry colleagues, whose simulations of materials' structures and

functions are vital to our work. My group also works on the development of computational methods to analyse powder diffraction data, and we are currently working on integrating structural characterisation into laboratory workflows that include automated and autonomous robotics.

Statement:
I am delighted to be nominated for the position of Secretary of the BCA Council. The BCA Spring Meeting was the first conference that I attended as a first year Ph.D. student, having made the journey directly down from Durham from a week at the Intensive Teaching School in X-ray Structure Analysis. I could not have imagined that it was the start of an almost 20-year (so far) journey that would see me teaching undergraduate chemists, computer scientists and robots about powder diffraction.

I have benefitted from attending many BCA and BCA-related events over the years, and from the existence of a community that supports and promotes the importance of crystallography to such broad areas of science. For students and early career researchers, in particular, being able to attend the Spring Meeting and take part in other activities is both inspiring and invaluable to supporting their development. Earlier this year, I had the honour of tutoring at the Durham School, and I hope that the nomination for this position will provide another opportunity for me to give back to the BCA and the wider community, in order that it can continue support our future scientists.

Ordinary Member Candidates:

Briony Yorke

Current Position:
Lecturer in Structural Biology, University of Bradford (2020 – present).

Education and Career:
Sir Henry Wellcome Post-Doctoral Fellow, School of Chemistry, University of Bath (Prof. Paul Raithby) and Institute for Nanostructure and Solid State Physics, Universität Hamburg (Prof. Dr Arwen Pearson) (2016-2020); Research Fellow, Hamburg Centre for Ultrafast Imaging, Universität Hamburg (2014-16); Wellcome Trust 4-year Ph.D. Scholar, Astbury Centre for Structural Molecular Biology, University of Leeds (Prof. Dr Arwen Pearson) (2014); M.Chem., School of Chemistry, University of Leeds (2009).

BCA Related Activities:
2021 – BCA/BACG Online Spring Meeting: Chair BSG: Time-resolved Crystallography. 2020 – BSG Early Career Prize. 2017 – YCG Parkin Lecture Prize.

Research Interests:
I am particularly interested in understanding the relationship between structure, function, and dynamics. For this reason, my research focuses on applying time-resolved techniques to X-ray crystallography and combining this with complementary spectroscopic methods. In this way it is possible to build a more complete description of molecular function and provide greater insight into the molecular origins of life. I have developed new approaches to time-resolved experimental design, including Hadamard Time-Resolved Crystallography (HATRX) and am currently involved in projects at Diamond Light Source, UK, EMBL@PetraIII, Hamburg and ELI-Beamlines, Czechia. My favourite beamlines are I24 and T-REXX and my favourite space group is $P6_122$.

Statement:
I am very excited to have been nominated for the position of Ordinary Member on the BCA Council. Ever since my first BCA Spring Meeting in 2010 I have felt proud to be a member of the crystallographic community. I have been inspired by my crystallographer mentors and peers to overcome adversity and be ambitious in my career. Mentorship from senior crystallographers has been transformative to my approach to not only science but to life and I am grateful for the opportunities that have been provided to me through the BCA community. In 2017 I was awarded the Parkin Lecture Prize by the YCG and in 2020 I was awarded the BSG early career prize. This provided me with an opportunity to present both research and teaching activities which I consider of equal importance. I believe that it is my duty to give back to the community that has given me so much. I will use this opportunity to reach out to the next generation of crystallographers and to serve the members of the BCA.

Steve Hull

Current Position:
Head, Crystallography Group, The ISIS Facility (since 2012).

Education and Career:
B.Sc. and Ph.D. in Physics, Reading University. Joint PDRA between the Clarendon Laboratory, Oxford and UKAEA Harwell, investigating the high temperature properties of nuclear fission oxide fuels and their structural analogues. Instrument Scientist for the Polaris neutron powder diffractometer at the ISIS Facility. Visiting Professor in Neutron Scattering, Department of Materials Science and Engineering, University of Sheffield.

Research Interests:
My research interests focus on the relationships between crystal structure and the properties of materials, specifically probing the ionic diffusion processes within solids possessing high ionic conductivities. This includes both 'model' superionic compounds and more technologically important materials with potential applications in fuel cells and solid state batteries. These studies exploit a number of complementary techniques, including neutron and X-ray diffraction, impedance spectroscopy and computer simulation methods. Many have been supported by joint Ph.D. studentships between ISIS and university collaborators and have included the development of novel techniques. Examples include the development of new *in situ* devices which allow neutron diffraction studies to be performed under conditions which closely mimic those found in technological applications. These include *in situ* electrochemical cells to investigate the structural changes within battery materials under charge-discharge cycling, and form part of my role within the Faraday Institution funded FutureCat consortium (led by University of Sheffield) to develop new cathode materials for electric vehicle applications.

Statement:
I am delighted to have been approached by the Nominating Committee to be considered for the position of Ordinary Member on the BCA Council. I was first introduced to crystallography in 1988, when I joined the ISIS Facility as an

Instrument Scientist on the Polaris powder diffractometer. I attended my first BCA Spring Meeting in 1990 (I think!) at the University of Exeter and have regularly attended meetings ever since, including being awarded the PCG Philips Prize in Newcastle in 1994 and presenting the results of my research work outlined above. In 2012 I became head of the ISIS Crystallography Group. In that role, I have prioritised the career development of junior members of staff by, for example, encouraging supervision of Ph.D. and Industrial Placement students. If fortunate to become a member of the BCA Council, I would aim to use this experience to help younger scientists within the field of crystallography to develop their research activities. I have also been a strong supporter of the BCA by, for example, providing significant funding and organisational support to the PCG Winter Crystallography Meeting – which has seen a steady increase in attendance in recent years. Most recently, the meeting has been arranged in collaboration with the Crystallography Group at Diamond and, together with colleagues from our central facilities, I would work as an Ordinary Member of the BCA Council to ensure effective two-way communication with our all-important user communities. In the case of ISIS, this is essential to guarantee that the needs of the UK's research community in crystallography are fed into plans for future instrumentation.

Lucy K. Saunders

Current position:
Beamline Scientist on High Resolution Powder Diffraction Beamline, I11, at Diamond Light Source (2021–present).

Education and Career:
M.Chem. University of Bath, Department of Chemistry (2007–2011); Ph.D. in Physical Chemistry, University of Bath (2012–2016); Postdoctoral Research Associate on Small Molecule Diffraction Beamline I19, Diamond Light source (2017–2021).

Professional Activities:
Member of British Crystallographic Association; Young Crystallographers committee member 2014–2016; Chemical Crystallography Group Ordinary Member (2018–2019) and Vice Chair (2019–2021). Member of Programme Committee for the 2015, 2019 and 2021 BCA Spring Meetings. Co-organiser of Chemical Crystallography Group Autumn Meeting 2020.

Research Interests:
I am a small molecule crystallographer with many years' experience on synchrotron beamlines. My research activities centre around solid-state proton transfer in hydrogen bonded systems, a topic I began investigating during my Ph.D. with Prof. Chick Wilson at the University of Bath. I design and study new proton transfer systems, exploring how to engineer them in the solid-state and what associated properties they have once formed (such as colour change or a switchability). I use a combination of crystallographic techniques to probe the proton transfer behaviour including synchrotron X-ray (single and powder) and neutron diffraction or where my samples have begun to contribute to the work of others, via X-ray photoelectron spectroscopy and first-principle calculations. My investigations also extend beyond the static, offering the opportunity to study this transfer behaviour by performing *in situ* crystallography, initially as a function of temperature and later, during the application of electric fields to identify new switchable materials.

Statement:
I am very proud to be nominated for the position of Ordinary Member on the BCA Council, to have made an impression already in the British crystallographic community. My involvement in the BCA started during my Ph.D. with a pounding heart as I raised my hand to ask my first ever question at a Young Crystallographer's satellite meeting. Since then, I have totted up over 8 years' service to BCA activities including attending various Spring and Autumn meetings, being on the YCG Committee as an ordinary member, the CCG Committee as an ordinary member and then in a Vice Chair role. In all roles, I have been involved in the organisation of various Spring and Autumn meetings and have really enjoyed thinking of session ideas to highlight emerging and progressing areas of crystallography. As I came to the end of my postdoc. on I19 at Diamond, one thing that really stood out to me was that I wanted to remain a part of this brilliant and friendly crystallographic community. In my new position at Diamond, I'm so pleased that I can keep meeting and interacting with all the different faces of the community, to continue to promote BCA activities and learn from its members. I therefore believe that I have a lot to offer to the Ordinary Member role on the BCA Council and would be very pleased to have this next opportunity to contribute to the BCA community.

The "2021" Winter Crystallography Meeting

February 14th-15th 2022

Milton Hill House Hotel
Steventon, Abingdon, Oxfordshire, UK

This year's Winter Crystallography Meeting has been delayed until February 2022 to enable us to meet in person for the first time since November 2019!

The meeting brings together ISIS & Diamond users with members of the BCA Physical Crystallography Group in a two-day celebration of structural science.

As always we hope to put together a diverse and exciting programme. Students and early career researchers are particularly encouraged to apply to give a talk or present a poster.

More information will be posted on **www.pcg-scmp.org** in due course. Please email **Helen Playford** (**helen.playford@stfc.ac.uk**) with any questions or comments.

25th Congress and General Assembly of the International Union of Crystallography

From the left: Ivana Kutá Smatanová (IPC Chair), Radomír Kužel (Congress Chair), Martin Haloun (PCO Auletris) and Pavlína Řezáčová (Chair of the Local Organising Committee). (Image: IUCr.)

THE XXV IUCr Congress took place in Prague 14-22 August 2021. It was a hybrid meeting, with physical delegates assembling at the Prague Congress Centre, joined by participants world-wide using a virtual platform. Several BCA members took part in the proceedings, some of which are reported here.

Microsymposium 7

High throughput vs careful planning: How to get the best data?

*Session chairs **John Helliwell** and **Selina Storm**. (Image: IUCr.)*

In times of highly brilliant beamlines and fast detectors, data collections only take seconds – but what is the way to get best data? **Aina Cohen** presented SSRL's efforts to enable more specialized experiments such as experiments at room temperature, controlled dehydration experiments or light triggered experiments remotely, making specialized experiments possible in times of crises. **Danny Axford**, senior beamline scientist at Diamond's beamline I24 exploits their brilliant microfocus beam in multiple crystal approaches and serial crystallography, pushing the limits of fast data collections and highest quality data. **Peter Zwart** from LBNL demonstrated that the use of Gaussian process regression in high throughput infrared spectromicroscopy reduces the amount of measurements and significantly speeds them up. **Marcus Müller** from Dectris first remembered his colleague **Andreas Förster**, who was a highly valued member of the community and who has sadly passed away. He then presented the best strategies of collecting data with hybrid photon counting detectors, ranging from fine slicing to strategies for phasing strategies at room temperature. In the next talk **Amy Thompson** from the University of Queensland introduced her approach of automatic analysis for elastically flexible crystals called CX-ASAP, reducing the processing time significantly. **Martin Maly** from the Czech Technical University then reported a new approach to assess the optimal resolution cut-off with PAIREF.

Can we answer the question whether the best data are obtained via high throughput or careful planning? As the late and great **Michael Rossmann** indicated, it all depends on the challenge you are facing. For his pioneering work with highly radiation sensitive virus crystals there is but one option: "shoot first and ask questions later" *(Rossmann and Ericson 1983 J. Appl. Cryst.)*. Since that time the development of incredible detector and beamline capabilities has expanded the possibility to the researcher to 'just open the shutter'. Furthermore, the huge amount of data which can be obtained within a short time creates new challenges, which require new solutions such as presented in this session.

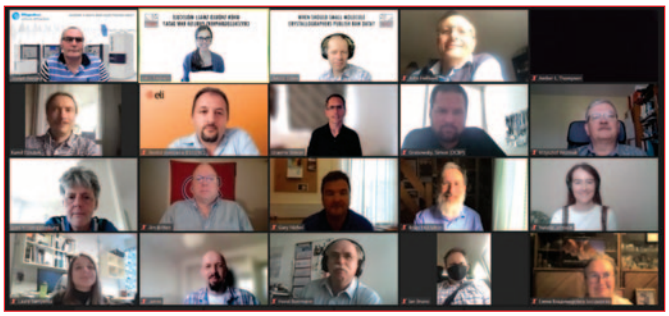
How to get the best data depends on what your objectives are for your measurements, which should certainly be carefully planned. This is a similar overall conclusion to the individual conclusions of the speakers in this session that spanned a quite vast array of topics.

John Helliwell, University of Manchester
Selina Storm, EMBL Hamburg

This article was also published in the IUCr Newsletter and is published here by permission.

IUCr Workshop

When should small molecule crystallographers publish raw diffraction data?



(Image: Amy Sarjeant)

Nearly two years ago, we undertook a survey of the chemical crystallography community in order to better understand current practices and ideas around raw data management, archival and sharing. In early 2020 we presented a summary of the responses of nearly 200 survey participants in an IUCr Newsletter article (**https://www.iucr.org/news/newsletter/**

volume-28/number-1/raw-data-availability-the-small-molecule-crystallography-perspective). To keep momentum building in the hopes of defining a set of community best practices, we began organising a workshop to run alongside the 2020 IUCr Congress in Prague. While our original workshop was delayed by a year due to the coronavirus pandemic, this additional time allowed us to engage more members of the chemical crystallography community, which ultimately resulted in a richly rewarding workshop for all involved. For those who could not attend, we present the following summary of the two-day virtual event.

Originally planned as an in-person, day-long workshop featuring invited presentations and a panel session from crystallographers at the leading edge of raw data usage and management practices, we adjusted both the schedule and platform to allow for as many international colleagues to attend as possible. The meeting was held via Zoom over two half-day sessions – we make a special thanks to our generous colleagues at Rigaku who provided this platform and helped with coordination. The workshop website (https://www.iucr.org/resources/data/commdat/prague-workshop-cx) shows the schedule and provides links to the presentations that were delivered.

Each day's session began with a short summary of the survey results. On the first day, **Amy Sarjeant** presented an overview of survey respondents' demographics as well as their thoughts surrounding what uses a store of raw crystallographic data could have. This was followed by contributions from **Michal Dusek**, **Kamil Dziubek**, and **Amber Thomson**. Michal's talk focused on the economic factors surrounding raw data archival, specifically in the field of modulated or incommensurate structures. He also gave a compelling case study of how a 1990s dataset was revisited three different times over 20 years and drastically improved (R-factor going from 19% to 9%) along the way, thus becoming publishable, as new data processing and refinement software became available. Kamil highlighted efforts from the high pressure crystallography community to establish standards on metadata to accompany raw data archives. This is an activity that is well underway and we hope to see new CIF standards specifically supporting high pressure crystallography emerging as a result. Amber shared several accounts underscoring the need for returning to original raw data files in order to solve complex structural problems and also raised the truly fundamental question – in the case of service crystallography, who really 'owns' the data?

After a coffee break, the session resumed with a presentation from **Simon Grabowsky** and **Krzysztof Wozniak**, highlighting the utility of raw data to validate assertions about electronic structure and properties in the field of quantum crystallography. This is an emergent aspect of crystallography that raises some major questions around what raw data actually is – if you are calculating a wavefunction based on a particular set of diffraction data, is that considered raw data? A further problem is where and how to store such a thing, as they are rather large for a CIF and there are no standard ways to describe them. **Jim Britten** provided a real-world application of raw diffraction data by demonstrating his 3D diffraction space visualizer, MAX3D. He showed so many beautiful examples that were a stark reminder that we don't spend enough time looking at our raw diffraction data these days – and that if you do, you can often answer structural questions at some level or other despite how 'bad' the data might appear! The session concluded with **Joe Ferrara** who provided a vendor perspective on what can be done to help the community adopt raw data management best practices and touched on the ideas of an archive of data processing software and conversion of formats.

The second day of the workshop focused more on community standards. **Simon Coles** started the session with an overview from the survey looking at current raw data management practices. **Graeme Winter** brought a massive amount of experience and insight from his work supporting raw data management across Diamond Light Source facilities, pulling out important points such as whether to use generic *vs* specific repositories and when, or 'who pays?' **Loes Kroon Battenberg** pointed out that most service crystallographers don't have any infrastructure to properly help them with raw data management. She also touched on the reusability of the raw data currently publicly available – just because you put it online doesn't mean that others can actually use it! Finally she touched on the importance of the concept of a 'CheckCIF for images', which would enable proper understanding and reusability of our raw data. **Teodor Ivanoaica** spoke about current data policies at the EU's Extreme Light Infrastructure. Their volumes and rates of data generation are considerably greater than lab-based crystallography – however, from about 150TB of data collected, generally only 20TB is useful, which raises the question what to keep and what not to keep! The final speaker was **Natalie Johnson** from the CCDC who spoke about challenges in curating and maintaining a raw diffraction database, how it should be related to results data and how both of these interface to established ways of publishing. The workshop concluded with a group discussion of the various challenges highlighted throughout the previous talks. This was very vibrant and went on for three times the allocated slot – definitely a bonus of having such meetings online and not having to rush out to the next event at an in-person conference?

We left the workshop understanding several primary challenges facing widespread adoption of raw diffraction data. These mainly encompass the costs involved in maintaining an arguably huge data store, deciding which data should be archived if storing everything is cost-prohibitive, agreeing on what metadata to store and how best to record it, understanding what and how to 'publish', and finally, how to promote this within the community in order to effect widespread culture change. Though the challenges are many, the promise remains great.

Simon Coles, Southampton University
Amy Sarjeant, Bristol-Myers Squibb

The IUCr25 General Assembly

The International Union of Crystallography (IUCr) is a community driven, globally focussed organisation for crystallographers and crystallography and allied subjects. The IUCr website carries the formal and more detailed description:-

'The IUCr is a scientific union adhering to the International Science Council (ISC). Its objectives are to promote international cooperation in crystallography and to contribute to all aspects of crystallography, to promote international publication of crystallographic research, to facilitate standardization of methods, units, nomenclatures and symbols, and to form a focus for the relations of crystallography to other sciences.

The IUCr fulfils these objectives by publishing in print and electronically primary scientific journals through Crystallography Journals Online, the series of reference

volumes International Tables for Crystallography, distributing the quarterly IUCr Newsletter, maintaining the online World Directory/Database of Crystallographers, awarding the Ewald Prize and the W.H. and W.L. Bragg Prize, implementing outreach initiatives and organising the triennial Congress and General Assembly.'

Every three years there is a General Assembly (GA) of the adhering bodies *i.e.* the national crystallographic associations. Each Congress includes three evening sessions of the GA, which approves the policies of the Union. There are different numbers of votes for each adhering body. The UK delegation is one which has the maximum number of votes, which is five. The five UK voting delegates at IUCr25 comprised myself, **Alex Stanley** (Secretary of the BCA), **Claire Naylor** (Treasurer of the BCA), **Christine Beavers** and **Gary Nichol**. Matters for voting by us were of course discussed with the BCA President, **Richard Cooper**. To allow for the possibility of unavailability on any one of the three GA sessions there were alternate UK delegates appointed by the BCA namely **Lee Brammer**, **Mike Glazer**, **Simon Parsons**, **Georgina Rosair**, **Hazel Sparkes** and **Anna Warren**. As all the UK Delegates were virtual registration attendees, our discussions on particular GA agenda items were done by email.

The complete agenda for the three GA sessions for IUCr25 can be found here
https://www.iucr.org/__data/assets/pdf_file/0019/151606/Prague-GA-agenda.pdf

At the first session (GA1) the following items were to be voted on.

On the first three we voted 'yes' to each motion and each motion was carried:-

- Agenda item 1 Approval of Agenda
- Agenda item 3 Application by the United Arab Emirates to become an adhering country of the IUCr
- Agenda item 3 Application by Guatemala to become an adhering country of the IUCr

The next two items involved deciding either to freeze or recommend withdrawal of adhering countries for which two:

- Item 4a Status of membership of Ireland
- Item 4b Status of membership of Morocco

were to be considered. The IUCr provided the following explanatory note to Delegates:

'Freeze. Will not incur further dues but existing dues will need to be paid before reactivation – can reactivate immediately on payment of dues.
Withdraw. Debts will be cancelled but can only be readmitted by formal application to General Assembly.'

The decision on each case was to 'Freeze', which was the way we voted.

There then followed approval of requests to make changes re the Adhering Body for Albania and Kosovo to become the Ivodent Academy (formerly Polytechnic University of Tirana). Then, for the AsCA Regional Committee, this specifically was:

'The Adhering Body for the Regional Committee of Crystallographers from Indonesia, Malaysia, Thailand and Vietnam will change to the Regional Committee of Crystallographers from Cambodia, Indonesia, Malaysia, Sri Lanka, Thailand and Vietnam.'

These two requests were both approved.

We also had to formally approve the Minutes of 24th General Assembly held in Hyderabad which were indeed so approved without amendment. [N.B. They had been previously circulated to delegations and then published in *Acta Cryst. A*, so this really was a formality. This was a last chance, as it were, for Delegates to suggest changes.] These minutes can be found at **https://journals.iucr.org/a/issues/2020/02/00/es5013/index.html**.

At GA2 there are the reports of the Committees of the IUCr, then the non-publishing Commissions, the regional and other associates of the IUCr (i.e. ACA, AsCA, ECA, LACA, wwPDB, ICDD and the IOCG) and as well as of the Representatives at the various international science bodies to which the IUCr is affiliated. I am actively involved with three of these (Chair of the Committee on Data, IUCr Representative to the ISC's Committee on Data 'CODATA' and Chair of the IUCr OUP Book Series Committee). These are all usually matters of noting the reports and this was the case at this GA; I did not therefore have to excuse myself from a discussion of my three Reports!

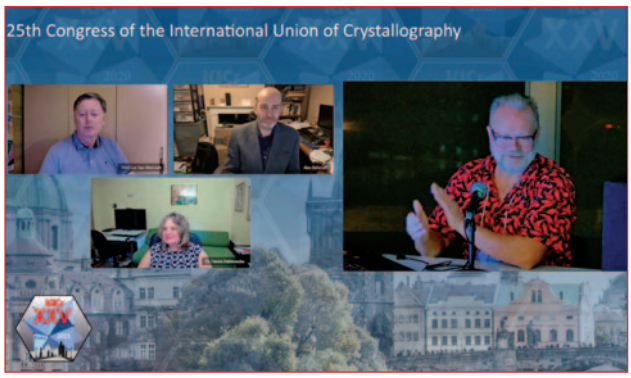
There were reports on behalf of the Executive Committee by the President, **Sven Lidin**, and the Financial Report by the Treasurer **Luc van Meervelt**. Sven heartily commended the marvellous work of the Prague IUCr25 Congress led by **Radek Kuzel** in such extraordinary circumstance that Covid-19 had presented. **Luc van Meervelt** gave 'an overall positive report in challenging financial times for the IUCr's activities and on which all IUCr's good works for the community rests'.

The IUCr is advised by a Finance Committee (FC), introduced in the early 1980s when there was a financial crisis for the Union. The FC is chaired by a Convenor, so far from the UK, namely **Michael Woolfson**, **Bob Diamond** and **Malcolm Cooper**. The IUCr Journals have provided the bulk of the monies for the Union's activities. The publishing scene, as we all know as researchers at the coal face, is transitioning to open access. The IUCr's eleven journals includes already three fully open access journals; *IUCrJ*, *Acta Cryst. E* and *IUCrData*. From January 2022 the *Journal of Synchrotron Radiation* will transition to fully open access. As a documentation of the IUCr's extensive outreach and community support activities around the globe, **Michele Zema** presented the Outreach and Education Report at Item 14.

Items 16 and 17 were also extensive reports by the IUCr Journals' Editor in Chief **Andrew Allen** on behalf of the Commission on Journals, now comprising more than 200 Editors and Coeditors, and on the Commission on International Tables by **Carol Brock**. At Item 21 we were called on to vote on the Gender Equity and Diversity Committee's new Code of Conduct. This can be found at **https://www.iucr.org/iucr/governance/advisory-committees/gedc**. This was approved by the Delegates, including by ourselves for the UK.

There were reports summarised by the President on the *IUCr Newsletter*, edited by **Mike Glazer**, the Africa Initiative Committee chaired by **Claude Lecomte**, the Committee on Data and the IUCr OUP Book Series Committee, both of which are chaired by me. At item 27 there were required votes on (small) adjustments on the number of members of some of the Commissions. These were approved by the Delegates.

We then had a presentation from the Canadian National Committee and the American Crystallographic Association of the one bid for IUCr27 to be held in 2026 in Calgary, Alberta. We found this to be a highly professional and very impressive bid. The vote to approve the bid or not was to be held in GA3 (see below). There was also a 'planting a flag' bid from the German Crystallographic Association (GDK) to host IUCr28 in 2029 in Berlin, led by **Manfred Weiss** with **Udo Heinemann** and **Christian Lehman**. There was also a bid from the Chinese National Committee of Crystallography led by **H. Liu** for IUCr29 in 2032 in Xian, the ancient capital of China. The IUCr President remarked that these indications of interest to host the future IUCr Congresses from adhering countries through to 2032 were most welcome as they gave chance for stable planning for those years.



*A scene from the third General Assembly session, chaired by IUCr President **Sven Lidin** (right), immediately following the announcement of **Hanna Dabkowska** as his successor as President. Also in the image are **Luc van Meervelt**, outgoing IUCr General Secretary and Treasurer, and **Alex Ashcroft**, IUCr Executive Secretary. (Image: IUCr.)*

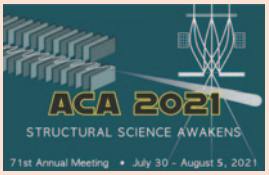
At GA3, we voted to approve the Calgary bid to host IUCr27 in 2026. We also received a planning update report from the IUCr26 hosts in Melbourne, Australia which was warmly received. We learnt that the Womens' World Cup Soccer tournament would be in Australia, culminating in the final in Sydney a few days before the IUCr26 Congress. GA3 also involved voting on candidates for the IUCr Executive Committee. The new President was approved by acclamation: **Dr Hannah Dabkowska** from Canada. Likewise, the candidate for Treasurer **Bo Brummerstedt Iversen** from Denmark was elected by acclamation. There were two candidates for IUCr Vice President: **Santiago Garcia Granda** from Spain and **Radek Kuzel** from the Czech Republic. **Santiago Garcia Granda** was elected. There were then ten candidates for three vacancies as Ordinary Members of the Executive Committee. After multiple rounds of voting, after the Congress had concluded, the three members elected were **Angela Altomare** (Italy), **Thomas Proffen** (USA) and **Manfred Weiss** (Germany). The IUCr President had already noted within the General Assembly that the IUCr appreciated very much, and thanked the Delegations in presenting such a fruitful number of very worthy candidates for consideration in the election.

John R Helliwell
University of Manchester
Chair of the UK Delegation

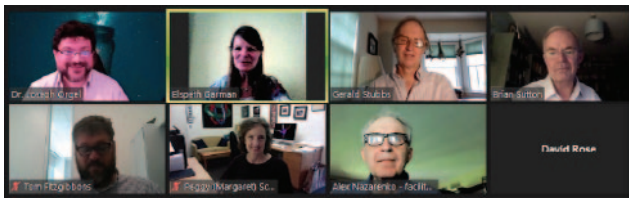
Structural Science Awakens: 71st Annual Meeting of the American Crystallographic Association – July 30th – August 5th Virtual

WHILE an in-person meeting was not possible this year, several BCA members took part in this year's ACA Annual Meeting. The following two sessions may be of particular interest to BCA members.

You may also be interested to know that the abstracts for the 2021 ACA meeting are available at https://journals.iucr.org/a/issues/2021/a1/00/.



'Rosalind Franklin: 101st Anniversary' session



Speakers at the Rosalind Franklin session.

It is 101 years since the birth of Rosalind Franklin, famous for her part in the unravelling of the structure of DNA. However, this great achievement constituted only a small part of her scientific output in a career which was sadly cut short due to her untimely death at the age of 37.

In the ACA session entitled 'Rosalind Franklin: 101st Anniversary', chaired by **Joseph Orgel** (Illinois Institute of Technology) and myself, her enormous contributions to our understanding of the chemistry of coal, of the structure of DNA and of the three-dimensional arrangements of viruses were explored in depth, with talks on all three aspects of her work. To introduce her, I gave a general biographical overview of her family and career, tracing her life from her birth in London in July 1920 as the second in a family of 5 children, through her education at a boarding school in Bexhill-on-Sea from ages 9 to 11, and as a daygirl to St Paul's Girls' School in London. On leaving school, she went to Paris, beginning her lifelong love of France and all things French. She perfected her spoken French and developed a passion for hiking and mountains. She then studied Natural Sciences with a focus on

Chemistry from 1938-41 at Newnham College, Cambridge. Her final year research project went well and was supervised by Fred Dainton, a photo- and polymer chemist. However, she did not actually 'graduate' until 1948 since degrees were not awarded to women by Cambridge until 1947, whereas in Oxford they did so from 1921 onwards. There followed a 4th year research scholarship from Newnham from 1941-42 which she did not enjoy, and then a move to the British Coal Utilisation Research Association (BCURA) in Kingston where she carried out research for a Cambridge Ph.D. For her first postdoctoral position she happily returned to her beloved France and worked from 1947-51 in Paris, studying the crystallography of coal and graphite under Jacques Mering at the Laboratoire Central des Services Chimiques de l'Etat (a Government Lab). At the beginning of 1951 she moved back to England, taking up a 3-year Turner and Newall Fellowship at King's College, London to work under John Randall, and carried out her famous experiments on DNA fibres. She stayed for only three years before moving to Birkbeck College where she carried out ground-breaking work on the structure of viruses (see below). A fuller account can be found in[1] and the further reading referenced therein.

The second talk in the session was a detailed description by **Alexander Nazarenko** (SUNY Buffalo State College) of (arguably) the first observation of covalent aromatic bond electron density which was made by Rosalind. She published her results in Nature in 1950[2] and showed that it is necessary to consider electrons as being located between two carbon atoms, missing in the then-popular independent atom model. Much later, more accurate experiments[3] confirmed her results, and her methods are particularly successful in describing aromatic organic molecules, which exhibit similarity to graphite bonding. The speaker pointed out that there are no references to paper [2] in any of the work on multipole models or, more recently, quantum chemistry enhanced crystallography (and *vice versa*), and that appropriate recognition of Franklin's impact on charge density research is long overdue.

The next speaker, **Margaret Schott** (Northwestern University) explained Franklin's significant, fundamental and long-lasting contributions to our understanding of the molecular structure of sp2-based graphitic carbon materials, studies which continued until her death. In particular, she investigated the process of graphitization using X-ray diffraction techniques and developed a structural model illustrating the potential of crystallites to fuse into well-ordered graphite, as well as its vulnerability to changes during oxidation[4]. Interestingly, the speaker had tracked down the talks on coal given by Franklin around Europe in 1953 when she was already at King's, and which included visits to Yugoslavia, Germany and France.

As highlighted by the following contributor, **Thomas Fitzgibbons** (DOW Chemical Company), Franklin's very careful measurements of the density of different coals in a range of solvents allowed her to formulate a quantitative model of the graphitic grain growth during carbonization of graphitizing and non-graphitizing carbons as a function of temperature which is still of great relevance, guiding research and development of new carbon materials today. Her model, since modified by other researchers, is still being used to design molecular sieves using the carbonaceous gas separation membranes formed from the carbonization of polymeric precursors[5].

Rosalind Franklin is best known for her work on DNA (1951-53), and in particular, for the famous 'Photograph 51' of B form (92% humidity) DNA, seen without her knowledge by James Watson in early 1953. **Brian Sutton** (King's College, London) addressed the fascinating question of how near Franklin herself was to uncovering the structure of DNA, coming to the conclusion that she was in fact tantalisingly close to an accurate description. Tragically, she died never knowing that her data had played such a key role in establishing DNA's structure, but today her contribution is fully appreciated and she rightly receives the recognition due to such an extraordinarily gifted scientist.

The final talk in the session was given by **Gerald Stubbs** (Vanderbilt University) with backup from **Joseph Orgel** (Illinois Institute of Technology), and described Franklin's tobacco mosaic virus (TMV) work, carried out with Aaron Klug, Kenneth Holmes, and John Finch at Birkbeck College. The speaker had worked as a postdoctoral researcher with Ken Holmes, and then continued to investigate TMV in his own lab. He described how the detailed structure published in 1989, 31 years after Rosalind Franklin's death, confirmed numerous results from her work, and that this remarkable achievement reminds us of both her genius and in particular of her vision.

The session was attended by over 85 people, several of whom contacted the organisers afterwards to say how much they had enjoyed learning more about Rosalind Franklin's work.

Elspeth F Garman
Oxford University

References:

[1] Rosalind Franklin 1920–1958. E.F. Garman, *Acta Cryst.* **D76**, 698 (2020).
[2] Influence of the Bonding Electrons on the Scattering of X-Rays by Carbon. R.E. Franklin, *Nature* **165**, 71 (1950).
[3] Bonding effects in graphite. G. Moss, *Acta Cryst.* **A34**, 91 (1978).
[4] Changes in the Structure of Carbon during Oxidation. R.D. Watt & R.E. Franklin, *Nature* **180**, 1190 (1957).
[5] Hyperaging Tuning of a Carbon Molecular-Sieve Hollow Fiber Membrane with Extraordinary Gas-Separation Performance and Stability. W. Qiu *et al*, *Angew. Chem. Int. Ed.* **58**, 1170 (2019).

Warren Award to Professor Jacqueline Cole

The ACA Warren Award was established in 1970 by students and friends of Professor B. E. Warren on the occasion of his retirement from the Massachusetts Institute of Technology. The award recognizes an important recent contribution to the physics of solids or liquids using X-ray, neutron, or electron diffraction techniques. Previous Warren Awardees from the UK include Michael Hart (1970, with Ulrich Bonse) and Ian Robinson (2000). It is awarded once every three years.

This year, the Award was made to Professor **Jacqueline Cole**, who holds the Royal Academy of Engineering Research Professorship in Materials Physics at the University of Cambridge, where she is Head of Molecular Engineering (**https://www.phy.cam.ac.uk/directory/colej**). Jacqui's acceptance talk entitled 'Molecular Engineering of Single-crystal Optical Actuators' was begun with her mentioning that the research she was describing was mainly done at Argonne National Laboratory. In addition to Cambridge, her affiliations included ISIS and Argonne – amongst others *(see Figure 1 below)*.

There is a wide range of materials that can form switches at the nano scale of relevance to envisaging light driven molecular rotors, optical data storage and through to quantum computing. An example of one of the few compounds of generic formula that shows photo-isomerization is $[Ru(SO_2)(NH_3)_4X]Y$ *(see Figure 2)*, where the SO_2 group manifests solid-state linkage photo-isomerization, X is the trans-ligand to SO_2 and Y is a counterion. Spanning a large range of literature from the last decade, including much of her own, Jacqui presented the development of this family of materials towards their applications. Her studies included a range of advanced *in situ* light-induced X-ray diffraction (well known to crystallographers as photo-crystallography) and *in situ* light-induced single-crystal optical absorption spectroscopy microscopy experiments. Together these captured the phenomenon in its light-induced states. Her results are contributing to a knowledge base of structure-to-function relationships within the overall goal of being able to engineer these materials at the molecular scale for a given device application.

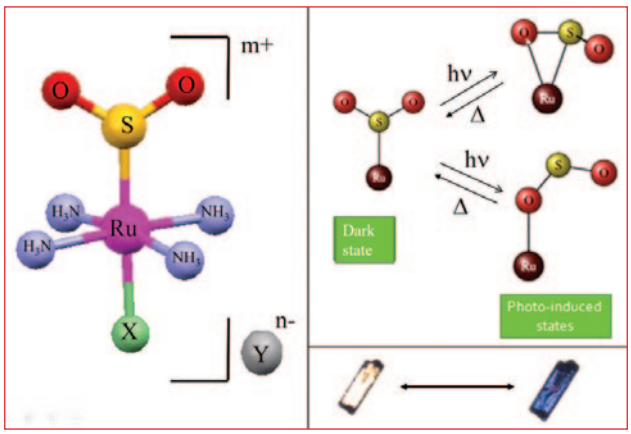


Figure 2: Photo-induced SO_2 linkage isomerism.

More details of Jacqui's science can be found in the references she cited in her Warren Award abstract: https://ww2.aievolution.com/acas/index.cfm?do=ev.viewEv&ev=1420

Highlights from the Proceedings of the 2021 ECA Council Meeting

THIS year's meeting of the Council of the European Crystallographic Association (ECA) took place over two lunchtimes on the 16th and 18th of August this year. This meeting, attended by the ECA Executive Committee, the ECA national member representatives, and a number of invited attendees, is an opportunity to discuss business pertinent to crystallography throughout the ECA region, which currently covers Europe, the Middle East, and Africa. ECA Council meetings take place annually, normally during a European Crystallographic Meeting (ECM) or an IUCr Congress. This year's Council meeting was a hybrid meeting, much like the IUCr Congress itself, with remote attendees dialling in to a Zoom meeting hosted by the Executive Committee in Prague.

2021 saw the completion of several ECA Executive Committee members' three-year terms in office, and consequently ballots were held to elect candidates to a number of official positions. **Marijana Đaković** (University of Zagreb, Croatia) was elected President, succeeding **Udo Heinemann** (Freie Universität Berlin, Germany) who takes up the position of Past President. **Arie van der Lee** (Université de Montpellier, France) was elected Vice-President, while **Andy Maloney** (Cambridge Crystallographic Data Centre, UK) was elected Secretary. This year saw **Alessia Bacchi** (Università di Parma, Italy) and **Carl Henrik Gørbitz** (University of Oslo, Norway) complete their respective terms as Past President and Officer for Grants. **Klaudia Hradil** (TU Wien, Austria) was elected to the latter position. The remaining members of the Executive Committee remain in their previous offices: **Jacob Overgaard** (Aarhus University, Denmark), Treasurer; **Jan Dohnálek** (BIOCEV, Czech Republic), Officer for Interest Groups; **Delia Haynes** (University of Stellenbosch, South Africa), Officer for National Members; **Consiglia Tedesco** (Università di Salerno, Italy), Officer for Education.

ECA Council Meetings are also an opportunity to hear about the progress towards the planning of future ECMs and to receive and vote for bids for prospective meetings. The 33rd European Crystallographic Meeting, ECM33, will take place in Versailles, France, from 23rd – 27th August 2022. Planning is well underway for this meeting set to take place in a magnificent venue, and the organisers are optimistic that a full programme can be delivered in person. Further information can be found on the conference website: https://www.ecm33.fr/. ECM34 is scheduled to take place in Padova, Italy, from the 20th – 24th August 2024, and a successful bid from Lviv will take ECM35 to Ukraine in 2025.

Of particular interest to younger members of the crystallographic community, the ECA Council heard a report on the 6th European Crystallographic School (ECS6), which took place virtually in Budapest, Hungary, in July this year. European Crystallographic Schools combine lectures and hands-on tutorials to provide attendees a fundamental understanding of the principles underpinning crystallography. Each school is unique, however, and offers a variety of topics to cater to a broad range of interests. ECS7 will take place during 2022 in Lisbon, Portugal, and a successful bid to host ECS8 in Berlin, Germany, in 2023 was received. For further information on the ECS, please visit https://ecanews.org/european-crystallography-school/.

Andy Maloney
Cambridge Crystallographic Data Centre

South West Structural Biology Consortium Meeting 2021 – 14-15 July 2021 – Virtual

Report on the software talks

A Guide to the Offline Graphical Interfaces of CCP4

After the Wednesday morning break, **Kyle Stevenson** (STFC) gave a presentation on the CCP4i2 GUI, a modern interface to CCP4 which gives users access to advanced pipelines which cover all aspects of structure solution, from data integration to deposition. Kyle guided us through the installation and use of CCP4i2, introducing us to the integrated web browser and project viewer, and the new documentation. Projects may be started from the browser or from an existing project panel, and can be transferred between different machines using the intrinsic import/export functionality. The task menu in the project viewer lists all the pipelines that can be run from the GUI and also shows the data available (stored in your home directory in CCP4I2_PROJECTS). The full suite of programs for X-ray structure determination covers:

- *Data integration* – DIALS, MOSFLM & XDS (separate download).
- *Data reduction* – AIMLESS free-R set & Matthews coefficient widget.
- *Experimental Phasing* – Phaser, SHELX & CRANK2.
- *Molecular Replacement* – Phaser, Molrep and automated MR with SIMBAD, AMPLE, MORDA and MrBUMP. Some of these pipelines (*ab initio* ARCIMBALDO & AMPLE) can be very CPU intensive and are best run on the server.
- *Model building* – Coot, BUCCANEAR (auto), PARROT (density modification), SHELX, ARP/wARP and CCP4MG.
- *Refinement* – REFMAC5 & LORESTR (low resolution pipeline).
- *Full Ligand support* – Automated solution of isomorphous ligand complexes and ACEDRG (a stereo-chemical description generator).

Structure solution can often be straightforward with high resolution data and Kyle demonstrated two phasing examples, using gamma adaptin (SAD using CRANK2) and beta lactamase with inhibitor (MR using Phaser). Figures of merit appear in the results tab and generally the default settings phase the data well – a quick REFMAC5 run and then visualisation in Coot show that the structure is pretty much solved with the default program settings. Documentation has recently been overhauled, and now covers tutorials and road show material, which gives users multiple examples to look over, and up-to-date information is also available online. CCP4i2 is currently being expanded and refined with the addition of MolProbity for validation, a new shift-field refinement program, support for further phasing and refinement tools, and a new automated model builder which is in development by York University. IRIS is also being introduced for graphical per-residue validation and an improved PDB deposition task is in development.

Solving Structures Online with CCP4 Cloud

After lunch, **Eugene Krissinel** (STFC) gave an interesting presentation entitled *'Solving Structures Online with CCP4 Cloud'*. CCP4 Cloud acts as a client for running processes both locally and on CCP4's clusters, in a manner similar to CCP4i2 but with representation of structure solution projects in the form of branching processes, created either by the researcher or with automatic workflows. Eugene took us through registration and then demonstrated the three CCP4 Cloud modes:

1. *Web-only* – for running all tasks on the Web. This mode is suitable for all platforms that can run ordinary web browsers, including tablets and smartphones. However, a few tasks, including Coot, are not supported in this mode. Structures and electron density can be can be visualised in the embedded UglyMol viewer, which mimics Coot, but does not allow modification.
2. *Remote* – for running mostly on the Web (certain graphical applications like Coot which are run locally on the user's computer are seamlessly integrated with the project and data in the Cloud). Local CCP4 setup is still required in this mode; however, it benefits from Cloud's computing power, centrally maintained software and databases, online projects that can be shared between team members and data backup.
3. *Desktop* – for running CCP4 Cloud completely locally, making it a mere alternative to CCP4i2.

CCP4 Cloud is configured with a special *config* utility, which allows choice of browser and also monitors regularly for CCP4 updates. Note that remote and desktop clouds do not automatically talk to each other; however they can export/import projects.

After importing the reflection dataset (hkl) and the protein sequence, the AU contents and space group are determined and a simple auto MR should give a decent structure solution. As a structure solution project usually involves repeats of certain actions and branching, a project in CCP4 Cloud has a tree-like structure. The particular state of a structure solution may be viewed as a conceptual box (structure revision) containing various data items (e.g. the reflection dataset, composition of the AU, phases, coordinate model, ligands, heavy atom substructure and others). As the project develops, structure revisions are passed from one task to another, getting updated with new or improved data (such as atomic coordinates, phases, ligands), until the structure is considered solved. For

guidance, the CCP4 Cloud Roadmap suggests groups of tasks appropriate to each stage of structure solution, with accompanying detailed commentary and movies.

Eugene then demonstrated the automated structure solution of gamma protein, importing the reflection and sequence data from CCP4 Cloud examples. Ligands are not present in this case, but if they were, the corresponding CIF file with crystallographic restraints could have been imported as well, or such restraints could be generated in-project with the Make Ligand task (using a SMILES string or the standard 3-letter code), or alternatively in Coot. In the Autostart mode of CCP4 Cloud, the structure solution workflow develops automatically (around the use of the MrBUMP pipeline in the example given), with one job appearing after another (every job in CCP4 Cloud corresponds to a particular task such as data reduction, search model preparation, phasing and so on). Failed jobs can simply be cloned and rerun with altered parameters. Projects can be annotated and repetitive jobs archived to keep project representation concise. Special care should be exercised when working with Coot – before exiting, always make sure to 'save coordinates' without changing the filename and job directory offered by default. Structure quality may be assessed through the analysis provided in the Refmac task, which also includes MolProbity reports. When the structure is complete, it should be prepared for deposition with the dedicated Deposition task. This task will also acquire the wwPDB validation report on the achieved structure quality and completeness level. The report's checklist must be checked before structure deposition.

Apart from the demonstrated *automatic* mode there are also *standard* (full list of tasks for manual operation) and *hop-on* (for continuing projects started elsewhere e.g. CCP4i1) modes. There is an initial disk space limit of 10GB per user and a CPU limit of 24hrs daily/240 hours monthly. If these quotas are exhausted, an increase can be requested from the CCP4 Cloud maintainers, or alternatively, completed projects may be exported to a local computer for personal archiving.

The CCP-EM software suite for cryo-EM

The Wednesday afternoon scientific session continued with a talk in which **Colin Palmer** (STFC) introduced CCP-EM which supports users and software developers in computational aspects of EM. The CCP-EM software suite is a range of utilities, all behind a common Python framework, covering:

- *Cryo-EM data processing (single particle reconstruction)* – RELION 3.1.
- *Map optimisation (sharpening/blurring/denoising)* – MRC to MTZ, LAFTER, LocScale and Confidence Maps.
- *Docking/model building* – MOLREP, BUCCANEER and DockEM.
- *Automated refinement* – REFMAC5 and Flex-EM.
- *Interactive refinement* – CCP-EM Coot & Chimera.

Validation for cryo-EM is a developing subject and cryo-EM structures are not always up to the standards of crystal structures. *Half-map Validation* is built into the Refmac refinement pipeline - it refines the model against one half-map and checks it against the other half-map for over-fitting. More recently CCP-EM have developed a *Model Validation tool* which will run multiple validation metrics for various aspects of model geometry and fixed density, giving an overview table of local & global statistics and a to do list of residues to check in Coot, grouping the problems into clusters.

Colin stressed the importance of depositing your cryo-EM structures in the EMDB & PDB and your raw data in EMPIAR, as this helps with method development. The talk ended by discussing the following recent developments:

- CryoEF (analysis of the angular distribution in cryo-EM reconstructions).
- SIDESPLITTER (extension of LAFTER for half-map comparison-based denoising).
- Difference Maps (highlighting the presence or absence of a ligand).
- HARUSPEX (AI based colouring of secondary structures in maps).
- CoVal – A server that extends the model validation tool to structures from SARS-CoV-2 and maps mutations identified from public genome databases.

Forthcoming Developments will include the *Servalcat* Python refinement pipeline as the primary way of running REFMAC5, and integration of RELION more closely into CCP-EM (both will be brought together in an integrated pipeline in Python3 which will take care of job control, scheduling and metadata extraction). In the long run there will be a new user friendly GUI with full scripting capability for developers and the ability to add third party plugins.

CCPNmr Analysis Version-3: modern software for integrated NMR analysis

On Thursday morning, **Vicky Higman** (Leicester) from the CCP for biomolecular NMR (CCPN) development team presented on CCPNmr Analysis Version-3. Written in Python 3, Version 3 is more user-friendly than Version 2 and also a lot more flexible, with the facility to write macros to adapt the program to your own needs. The new NMR Exchange Format (NEF) now enables seamless integration with other programs, enabling more accurate and wide-ranging exchange of data than was possible with the Format Converter in Version 2.

Vicky took us through the different stages of an NMR project to show how V3 can help: CCPNmr Analysis enables interactive phasing (including selecting traces in different planes) to obtain the parameters needed for processing with nmrPipe. To visualise processed data the spectrum can be dragged and dropped together with the FASTA file and the sequence is automatically appended (much easier than V2). Backbone assignment has also been made more user friendly in V3 through drag and drop of matched C^{α}s and C^{β}s to connect residues. The sequence appears at the foot of the window and possible matches to the sequence based on typical chemical shifts are indicated, giving sequence-specific assignment options. Structure calculation involves exporting the processed data to NEF and reading this file into X-PLOR (works well), CYANA or ARIA (final bugs still being ironed out). The CCPnmr software has improved violation analysis tools (previously a problem in V2 because of incorrect import of stereospecific assignments). Finally, structure deposition is easy, as both the PDB and BMRB now accept NEF files.

For binding studies and titrations the Chemical Shift Perturbation Analysis module displays binding curves and shift differences

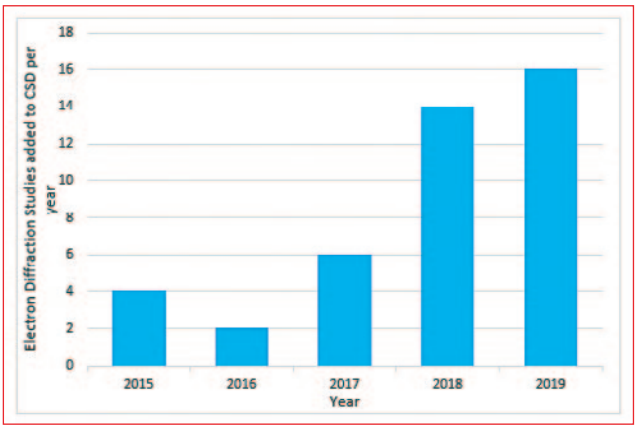
as an interactive histogram. Results can also be viewed directly on a structure in PYMOL. An additional Dynamics module (coming soon) will fit each residue and produce similar graphs with export to RELAX allowing more specialist fitting. Any features not yet implemented in CCPNmr can be created using a macro on the Python console (many Python libraries are already included). Each user will have to decide when they are ready to move to from V2 to V3!

The SWSBC 2021 conference organisers would like to thank the CCP speakers for such excellent and informative reports.

Raj Gill
University of Portsmouth

News from the Cambridge Crystallographic Data Centre (CCDC)

TO date, solving structures of potential therapeutics using X-ray diffraction (XRD) has been an assumed, pivotal step in the drug development process. However, a recent paper[i] shows how microcrystal electron diffraction (MicroED) is growing to obtain the structures of potential pharmaceuticals. As MicroED can work with crystals of almost any size, it can get over the problem of having to grow large crystals, which can be a serious bottleneck.



As evidenced in the figure, developments in automated data collection and data processing have led to increased interest in electron diffraction as an XRD alternative. Currently, there are over 100 unique datasets determined using electron diffraction in the Cambridge Structural Database's (CSD's) June 2021 web and desktop offerings.

Information on accessing and depositing electron diffraction structures in the CSD can be found on the CCDC website at https://www.ccdc.cam.ac.uk/Community/blog/2020-05-04-electron-diffraction-data-in-the-csd/.

Reference:
i J.F. Bruhn *et al.* https://www.frontiersin.org/articles/10.3389/fmolb.2021.648603/full.

PCG Intensive School in Physical Crystallography

THE next PCG Intensive School in Physical Crystallography will be held in the summer of 2022 – dates tbc.

This school is aimed at anyone who is interested in learning about advanced topics in physical crystallography from experts in the field. Information about the previous school, held in 2018, can be found here: https://pcgschool2018.wordpress.com/ and the 2022 school is likely to follow a similar format.

Further information will be circulated in due course. In the meantime, please contact **Alex Gibbs** (a.gibbs@st-andrews.ac.uk) with any questions, comments or suggestions.

ISIS Endeavour Project

Endeavour – addressing real-world challenges, for the next decade and beyond, through state of the art instrumentation at the ISIS Neutron and Muon Source.

THE ISIS Neutron and Muon Source[i] is a major centre for research in the physical and life sciences. Primarily funded by the U.K. Government, the facility is operated by the Science and Technology Facilities Council at the Rutherford Appleton Laboratory in Oxfordshire. Since starting operations in 1984, ISIS has continually worked to innovate and develop its instrumentation suite, so as to maintain its ability to contribute to societally-relevant, high impact research. The next stage of this development is the Endeavour[ii] programme. Endeavour builds on the strong foundation of the 29 neutron and 5 muon instruments that ISIS currently operates, and that support the research activities of close to 1,700 scientists each year. Endeavour will provide ground-breaking scientific capabilities and research capacity in priority thematic areas such as Clean Growth, Advanced Manufacturing, and Biosciences and Healthcare.

Within the Endeavour programme a broad range of projects is currently being developed, with the aim of delivering a balanced portfolio of instruments that will greatly enhance the facility's capability to address the ever more challenging questions around the structural and dynamical properties of matter in the physical and life sciences. Endeavour will take full advantage of developments in areas such as sample environment, multi-modal measurements and machine learning. Instrumentation for next generation crystallography is undeniably going to play a major role in this research agenda. Currently within Endeavour there is a range of projects linked to structural characterisation: the next-generation high-resolution power diffractometer (HRPD-X); the construction of a new single crystal and thin film cold neutron diffractometer (WISH-II), complemented by a polarised neutron capability on the existing WISH instrument; the provision of a new engineering instrument optimised for characterising real-world industrial components (e-MAP); a new large-molecule diffractometer for single crystal studies of biomolecules and functional materials (LMX); and an upgrade to the liquid and amorphous materials diffractometer to enhance its suitability for enhanced parametric and isotopic data collection paradigms that are required to address modern chemical-, materials- and life-science challenges (SANDALS-II).

At the present time, the programme and instrument project details are being refined and the business case for Endeavour is being developed. Subject to a positive, timely funding decision, the materials structure-related projects that could be delivered over the next 5-10 year timescale are summarised below.

HRPD-X

The current High Resolution Powder Diffraction (HRPD) instrument is a flagship for both the ISIS Facility and the U.K. powder diffraction community, whilst also setting a benchmark for high-resolution facilities elsewhere in the world. The HRPD-X[iii] project is a major upgrade to the current HRPD instrument, which will expand its user base into many new research areas. It is essentially a complete rebuild of the instrument beyond the end of the neutron guide, with the major advance in performance provided by a significant increase in the solid angle of detector coverage (by a factor of four overall and with a 90-fold increase at $2\theta < 80°$), whilst maintaining the high $\Delta d/d$ re solution currently offered. To accommodate the upgraded instrument and improve the working environment, it will be necessary to completely rebuild the current building, and a detailed layout has been developed in collaboration with a team of external architects.

In terms of scientific applications, the powder diffraction community is amongst the largest and most productive at ISIS, being drawn from diverse fields covering chemistry, physics, materials, earth and planetary sciences, engineering and cultural heritage research. The HRPD-X upgrade will expand the current instrument's scientific domain in many areas, including high resolution studies of complex organics and inorganics; catalytic and energy-related materials; organic-inorganic composites; samples under hydrostatic and uniaxial pressures; materials with incommensurate nuclear and magnetic structures and/or large unit cells; measurements using applied fields in complex sample environment; novel *in situ* studies; rapid parametric studies at high resolution and studies of small samples. In summary, the HRPD-X upgrade will maintain HRPD's place at the forefront of the world-wide diffraction community.

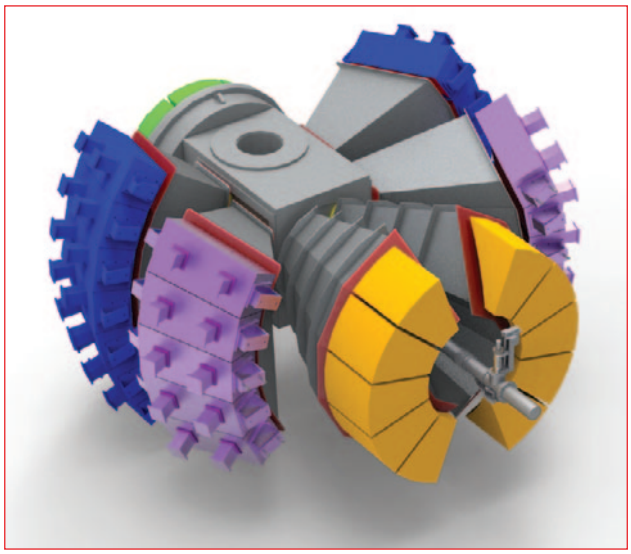


Figure 1: *Engineering model of the enhanced detector coverage planned for HRPD-X.*

WISH-II and polarization option on WISH

This project is twofold: building a new single crystal and thin film cold neutron diffractometer WISH-II[iv] with a large continuous detector coverage (approx. 2.4π) and an upgrade to the existing WISH beamline to implement polarized neutron measurement capability.

Primarily designed as a magnetic powder diffractometer, the excellent characteristics and flexibility of WISH have seen its scientific programme extend into new areas such as magnetic thin films and energy materials, establishing an unrivalled reputation within the international user community. The consistently high demand for beamtime and impressive scientific output of WISH naturally provide a strong basis for a further development towards another cold neutron diffraction instrument on the second target station. The WISH-II project will deliver a new cold neutron diffractometer optimized for the study of small single crystals and thin films, whilst also allowing powder experiments. Its large detector coverage will be a great advantage for thin film experiments, since several symmetry-equivalent directions will be measured at the same time, whilst structural studies of many large unit cell materials, such as metal organic frameworks, zeolites and complex magnetic systems, will become tractable.

A complementary proposal for the installation of a polarizer and an analyser on the current WISH instrument is also being developed, which will enable new types of experiments with drastically reduced incoherent scattering from hydrogen and precise reconstruction of spin-density maps. Moreover, diffraction data collected using polarised neutrons are sometimes the only way to establish a unique description of the magnetic structure. Taken together, the two projects promise transformative breakthroughs in important research areas, including advanced manufacturing and the development of new materials for clean growth.

e-MAP

e-MAP[v] is a new diffractometer for the application of neutron diffraction techniques in areas such as 3D residual stress mapping of large and complex-shaped components with high spatial resolution. The specification for the new e-MAP instrument has been chosen to lie between that of the existing ENGIN-X and IMAT instruments at ISIS, with increased flux compared to ENGIN-X and better $\Delta d/d$ resolution than IMAT. As a consequence, the flux and resolution characteristics will allow: 3D residual stress mapping; high spatial resolution; large, thick, heavy and complex-shaped components;

What have neutrons ever done for us?

The June 2020 issue of *'Elements'* magazine (elementsmagazine.org) focussed on the use of neutrons in mineralogy, geochemistry and petrology. The Editorial in that issue is reproduced below by permission of the Mineralogical Society of America and the author. Some among us may have some idea of who the names might (playfully) refer to…

Rich: Alright everyone, settle down. I hereby call this extraordinary meeting of the Society for the Protection of Analytical Methods [SPAM] to order. Brothers and sisters, we face a grave threat. For decades we've provided X-rays and electrons to study the structure and properties of natural materials – everything a mineralogist could ever dream of. But now this!

[Frantically waves the "Exploring Earth and Planetary Materials with Neutrons" issue of Elements.]

They are threatening to take it all way from us! They've bled us dry! They've taken everything we had, and not just from us, but from our fathers, and from our fathers' fathers.

Nancy: And from our fathers' fathers' fathers.

Rich: Yeah.

Nancy: And from our fathers' fathers' fathers' fathers.

Rich: Yeah, all right Nancy. Don't labour the point. But what have neutrons ever done for us?

David: Hydrogen?

Rich: What?

David: Well, they do scatter pretty well off the lighter elements.

Rich: Oh. Yeah, yeah. They do do that I suppose, yeah.

Jodi: And magnetism.

Nancy: Oh yeah, the magnetism Rich! Remember what it used to be like trying to determine magnetic structures?

Rich: Yeah. All right. I'll grant you hydrogen and magnetism are two things that neutrons can do pretty well.

Jodi: And the vibrational spectroscopy.

Rich: Well, yeah, obviously the vibrational spectroscopy. I mean, that goes without saying, doesn't it? But apart from the hydrogen, the magnetism, and vibrational spectro...

David: Isotopic substitution!

Nancy: Neutron activation analysis!

Jodi: Total scattering!

Rich: Yeah, yeah. All right. Fair enough.

David: All those disordered structures…

Nancy and Jodi: Oh, yes!

David: Yeah. Yeah, that's something we'd really struggle with without neutrons.

Nancy: Small angle scattering, tomography of nanoporous structures!

Jodi: And we can make complex sample environments, Rich.

David: Yeah, given how weakly neutrons interact with matter, let's face it, they're the only ones who could get through some of the high pressure rigs we have in a place like this.

All: Heh heh heh.

Rich: All right, all right. But apart from hydrogen, magnetism, lattice dynamics, isotopic substitution, chemical imaging, disordered structures, 3-D imaging, and the ability to build complex sample environments, I ask you: what have neutrons ever done for us?

Nancy and David: Well, I guess we'd better read the issue and find out **http://elementsmagazine.org/past-issues/exploring-with-neutrons/** …

Richard Harrison, Principal Editor Elements
University of Cambridge

near-to-surface measurements; process measurement (e.g. *in situ* welding); *in situ* loading and special environments; long-term tests (e.g. creep). The high neutron flux will allow *in situ* and *in operando* experiments at realistic (i.e. industrially-relevant) time scales and under complex stress conditions. The instrument will also have a large laboratory space to store special sample environments and carry out offline long-term tests, e.g. creep experiments, where intermittent measurements are required.

Together with the facilities offered on ENGIN-X and IMAT, e-MAP will form a suite of world-leading instrumentation. It represents a step change in the ability to study real-world engineering components at ISIS, exploiting advanced neutron characterisation techniques to address a diverse range of technologically-relevant problems.

LMX

LMX[vi] is a new single crystal diffractometer to be located on the second target station at ISIS, optimised for studies of large molecule systems and with applications across a range of research areas in the fields of structural biology, macromolecular chemistry and functional materials.

The vast majority of structural studies of large molecule systems are performed using X-rays at synchrotron sources. Despite being considered a more 'niche' technique, its neutron counterpart has proved to be highly successful for many decades, originally at reactor-based (monochromatic) facilities and then at spallation (pulsed) sources. A major focus has been on providing complementary information to X-rays, especially on the location of light atoms in the presence of heavy ones and, in particular, the hydrogens which are often the key to understanding interactions in biological processes and drug binding sites. As the only dedicated single crystal diffractometer at ISIS, SXD has made significant contributions in the area of 'small molecule' chemical crystallography (with unit cell volumes typically up to around 10,000Å^3). However, the past 20 years or so have seen increased demand for the study of larger molecular systems. LMX will be designed to accommodate unit cell volumes up to ~2,000,000 Å^3, a 200-fold increase on SXD. As such, it will meet the needs of new research groups whose requirements cannot currently be met at the facility, across topical areas such as supramolecular chemistry, hybrid organic-inorganic complexes that exhibit mixed properties, molecular magnets, framework materials, organometallic chemistry, catalysis and biomolecular science.

SANDALS-II

Since entering operation 32 years ago, the existing SANDALS instrument has helped catalyse a strong national and international research programme in light-element-bearing disordered materials science, and has delivered major impact in many research fields and industries where molecular liquids and glasses play key roles. The SANDALS-II[vii] project now aims to build on this strong foundation to deliver a significantly upgraded facility with a factor 5 improvement in overall performance. This step-change in capability is needed to allow the facility to better meet the increasingly complex research requirements that are required for making significant advances in our structural understanding of fields such as amorphous pharmaceuticals, catalysis, energy materials and green chemistry.

The proposed upgrade of the existing instrument has four key components that will enhance its count rate, stability, reciprocal space resolution, kinetic capabilities and reduce its background. These project components are **i.** a complete modernisation of the performance-critical forward-scattering detector banks, doubling solid angle coverage in the 3° to 40° scattering angle range with detector modules offering enhanced efficiency; **ii.** the replacement of the existing small sample enclosure with a much larger vacuum tank to minimise background contributions to the scattering patterns; **iii.** the installation of a new 90° detector bank to provide enhanced reciprocal-space resolution capabilities that are required for better understanding of crystalline and partially crystalline samples; and **iv.** a general upgrade of the detector block house temperature and humidity controls, to enhance the overall stability of the instrument. Collectively these upgrades will make SANDALS-II the ISIS instrument of choice for time-resolved, parametric, and large sample-set, disordered and complex materials studies on length scales up to 5nm.

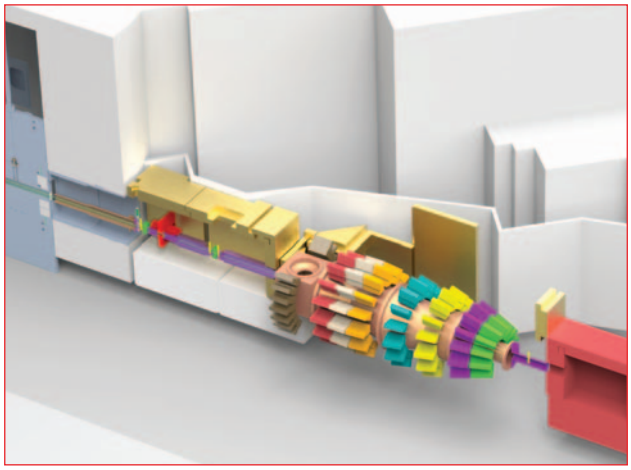


Figure 2: Outline design of the proposed SANDALS-II diffractometer, showing the enhanced forward-angle detector coverage, large sample and detector vacuum tank, and proposed high-resolution 90° detector bank.

In this short update, we have focussed on the projects of direct relevance to chemical and magnetic structure characterisation. The broader programme encompasses the unique properties of neutrons and muons to not only access structure but also kinetics and dynamics. New and transformative capabilities are proposed for spectroscopic measurements applied to a broad range of systems from biology through to quantum matter. The Tosca+ and Osiris+ spectrometers will receive significant flux increases through guide and secondary spectrometer developments. The gains will be widely applicable in catalysis and energy materials. Mushroom is a new concept in inelastic indirect geometry spectrometers which will open up this powerful technique to new materials and systems, particularly those which are only available in small sample volumes. SuperMuSR is an upgrade to the existing MuSR muon instrument and will deliver an order of magnitude increase in count rate and time resolution allowing the instrument to push into new domains of magnetism and superconductivity research. Increasingly, research questions will require a detailed knowledge of both the structure and dynamics of complex materials hence the balance of the Endeavour programme.

The new capabilities of Endeavour will broaden the applicability of neutron and muon techniques to ever more realistic and complex systems and thereby enable the community of users to deliver significant impact on real-world challenges. For further information please visit the Endeavour webpages[ii].

Acknowledgements

The authors wish to acknowledge fully the broad range of contributors to Endeavour. The Endeavour programme is only possible with the combined effort and support of the ISIS user community, the facility's scientific, engineering and technical teams, the facility's advisory boards, and the many business development support teams across UK Research and Innovation. We are particularly grateful to the academic and industrial communities who have shaped the scientific case for Endeavour and who are fully engaged in its development through activities such as our user meetings and the Endeavour Programme user meetings[viii].

Daniel Bowron, Sara Fletcher, Stephen Hull, Phillip King, Sean Langridge
ISIS Neutron and Muon Source, Rutherford Appleton Laboratory

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vi https://www.isis.stfc.ac.uk/Pages/LMX.pdf
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The Rosalind Franklin Institute Opens

THE Rosalind Franklin Institute, based at the Harwell Science and Innovation Campus, was opened on 29 September by **Prof. Lynn Gladden**, EPSRC Executive Chair. The Institute is developing cutting-edge biological imaging technologies to help address major health research challenges. Technologies developed to date include world-first time-resolved electron microscopes, technology for imaging cells in 3D at atomic resolution, chemical tools for protein modification and labelling and mass spectrometry equipment with high fidelity sensitivity for tissue imaging. At the opening, the Institute Director (and renowned crystallographer) **Prof. James Naismith** said: ***"The work we do here will provide major factor-of-ten leaps in our ability to see and understand life"***.

L to R: ***Dr Vivienne Cox****, Franklin Chair;* ***Dr Noor Shaker****, Founder of Glamorous AI;* ***Prof. James Naismith****, Institute Director;* ***Prof. Dame Lynn Gladden****, Executive Chair, EPSRC;* ***Dr Richard Henderson****, MRC-LMB. (Image: Rosalind Franklin Institute).*

Conferences celebrating PDB50

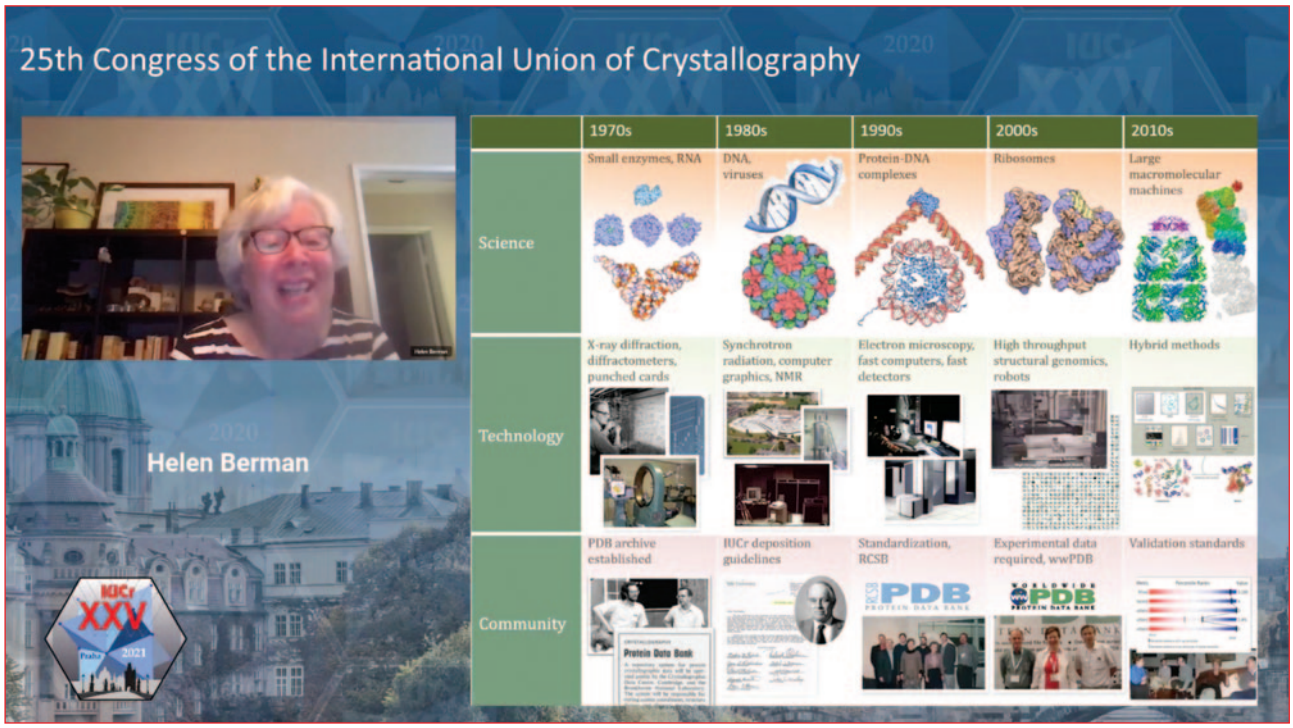
THERE are several conferences celebrating the 50th anniversary of the Protein Data Bank (PDB). Some have already happened, and more are planned for later this year. These have featured, or will feature, a wide range of contributors describing the historical development of the PDB, as well as a diverse range of themes of biological structures and methods for their determination, principally involving X-ray crystallography.

The wwPDB Foundation started the PDB50 celebrations in May as a virtual event of the American Society of Biochemistry and Molecular Biology[i]. Then the ACA 2021 Transactions Symposium, over two full sessions, was devoted to joining the celebrations on the 50th anniversary of the founding of the Protein Data Bank ('PDB50')[ii]. The IUCr25 Congress[iii] had major contributions to mark the PDB50th. The American Chemical Society[iv] (this latter jointly with the CCDC), the European Molecular Biology Organisation[v] and the Biophysical Society of Japan[vi] continue these.

At the IUCr25, one of the three Plenary Lectures was on the PDB and was delivered by **Helen Berman**, who was there at the PDB's inception in 1971 at the Cold Spring Harbour Quantitative Biology Symposium on the 'Structure and Function of Proteins at the Three-Dimensional Level', which she described, and onwards to the present day (see figure). Helen was Director of the Nucleic Acid Database and a Director of the RCSB Protein Data Bank. Other Directors of the PDB at different stages, and PDB-related people in turn, chaired the several sessions at the American Society of Biochemistry and Molecular Biology event: **Tom Koetzle**, **Joel Sussman**, **Shoshana Wodak** and **Janet Thornton**. In 2003, the Worldwide Protein Data Bank (wwPDB) was formed to maintain a single PDB archive of macromolecular structural data that is freely and publicly available to the global community. It consists of organizations that act as deposition, data processing and distribution centres for PDB data.

At the ACA2021 one of the founder depositors in 1971, **Wayne Hendrickson**, described the evolution of the PDB in the context of diffraction, as well as molecular biological, methods and their radical developments over the last five decades. The current landscape of all the structural databases to which crystallography is the dominant depositor as a method was captured in the IUCr25 session entitled *Exemplary practice in chemical, biological and materials database archiving* chaired by **Suzanna Ward** of the CSD and **Genji Kirusu** of PDBj. This included talks on the CSD by **Ian Bruno**, the RCSB PDB by **Stephen Burley**, the ICSD by **Annett Steudel**, the ICDD by **Stacy Gates-Rector** and PDBj by **Genji Kurisu**. The origins of the PDB were also mentioned in the IUCr Ewald Prize Lecture presented by **Suzanna Ward** on behalf of **Olga Kennard**.

The PDB was jointly launched in 1971 by the Brookhaven National Laboratory on Long Island USA, led by **Walter Hamilton**, and the CCDC in Cambridge UK led by **Olga Kennard**. Looking to the future, the IUCr25 had a session entitled *Integrative structural biology: The next 50 years of the Protein Data Bank* chaired by **Stephen Burley** and **Dina Schneidman**. This reflected the variety of experimental



Helen Berman presenting her plenary lecture on the PDB at IUCr25. (Image: IUCr.)

methods used in structural biology and their integration via bioinformatic and modelling tools. This was envisaged to reach cell biology by **Andrej Sali** of the University of California San Francisco. As Chair of **Helen Berman**'s Plenary Lecture at IUCr25 I concluded the session by offering a vote of thanks on behalf of all depositors and users of the PDB to Helen and all involved in making the PDB what it is today, a fantastic resource.

To return to the inaugural event celebrating the PDB50th at the ASBMB in May, the U.K. was represented in the speakers by **Tom Blundell** who presented a personal history of five decades of structural biology and the PDB, from early work with insulin through HIV-1 protease inhibitor development to recent work on the characterization of large complexes using 3DEM. Also, he recounted his co-founding of Astex Therapeutics to do fragment-based drug design. The current Director of the RCSB PDB **Stephen Burley** discussed the influence of the PDB on the process of drug discovery and the massive impact the modern PDB has had on new FDA drug approvals. Between 2010 and approximately 2018, nearly 200 new molecular entities approved by the FDA as drugs and over 70 new cancer drugs have had a basis in thousands of three-dimensional macromolecular structures archived by the PDB representing approximately 100 billion dollars in NIH funding.

To conclude this report I recall the very memorable description by **Jenny Martin** of the University of Wollongong, Australia in her talk at the ASBMB event entitled *Science, crystallography, reflections: A journey with the PDB over 35 years*. Jenny summarised the 'Top 5 Reasons to Love the Protein Data Bank' as:-

> *"(1) open access data with myriad uses conforming to FAIR principles, (2) a collaborative community with research integrity, (3) the availability (early in the life of the archive) of personalized PDB codes, (4) expert curation, visualization, and analysis of structural data, and (5) the protein structure diversity available in the PDB and the 'wonder and awe of Nature' that it engenders."*

Jenny's abstract and those of the other speakers at the ASBMB event have been highlighted subsequently at the RCSB PDB website[vii].

John R. Helliwell
University of Manchester

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Obituary

Jack Dunitz:
9th March 1923 - 12th September 2021.

It was with deep sadness and a huge feeling of loss that we learned of the passing of Jack Dunitz at the age of 98. Jack was Emeritus Professor at ETH, Zürich, where he worked from 1957 until he retired formally in 1990, although for years he continued to travel, give talks and to meet fellow scientists.

Jack was always an inspiration to many of us reading this newsletter today, and we grew up with his papers and incredible insight into our subject and the clarity of his talks, where we were lucky enough to have enjoyed those wonderful times. I can recommend a very recent interview with Jack and the ACS Editor in Chief, Erik Carreira which is in the link below. Despite his age, Jack demonstrates so well his sense of humour and intellect, which shine through in this interview.
https://bit.ly/jack-dunitz

I met Jack first in Oxford in Dorothy Hodgkin's lab in the mid/late 1960s and it was wonderful as a young D.Phil. student to have had that opportunity, as Jack was already such a well-known name in our field. Subsequently I got to know Jack well and we met at many conferences, at the Erice Crystallography Schools, the regular CCDC student days and a memorable visit to my lab. in Durham. It was always a bonus to sit and listen to him talking, explaining things to the students, asking just the right questions and always enjoying the interaction with other chemists and crystallographers. Jack was without doubt wonderfully inspiring and such a human and knowledgeable face of crystallography.

(Image: Judith Howard)

His legacy to us all is enormous and Jack will be remembered for the way he taught and inspired others, in particular the young, the kindness he showed to nervous students and the patience he demonstrated to new comers to our field who were keen to learn the basics and more, from Jack himself.

Jack was born in Glasgow, went through school there and entered Glasgow University in 1940 to read chemistry, encouraged by his school chemistry teacher who had 'made the subject interesting'. For his graduate studies, Jack was assigned to the lab. of J. Monteath Robinson, who had demonstrated the power of isomorphous replacement, but Jack did not use that in his doctoral studies, nor the 'heavy atom' methods, but they had explored the 'new' Patterson function. After his Ph.D. he travelled south to Oxford to join Dorothy Hodgkin's lab., to learn about structure solution from 3 dimensional diffraction data and here he spent two years [1946-48] before taking up a postdoc in Caltech with Linus Pauling [1948-1951]. There followed another period at Oxford [1951-1953] and a further 2 years at Caltech and NIH [1954-1955] where he worked with the biophysicist Alex Rich to establish a lab. of structural research at Bethesda. Jack was recruited in 1956 by Sir Lawrence Bragg to join him at the Royal Institution, London and it was from there that he was appointed to the position at ETH, Zürich as Professor of Organic Chemistry (1957), where he established X-ray crystallography as the essential tool for chemical structure analysis.

Jack received many honours and awards in his life, including a number of Honorary degrees, the Paracelus Prize 1986 (Swiss Chemical Society), the Aminoff Prize 1990 (the Royal Swedish Academy of Sciences), the membership of several National Academies and he was elected FRS in 1974.

Jack's research took him into many 'new' areas and upon each he made a significant impact, changing the way we see and understand chemistry today. He studied the structure and reactivity of medium ring compounds, ion specificity of biologically important ionophores and demonstrated the importance of structure-energy relationships. He derived the Bürgi-Dunitz Angle with his colleague Hans-Beat Bürgi, which changed our understanding of chiral reactions and helped direct syntheses of enantiomerically pure compounds. He pioneered use of the very early Cambridge database (CSD) to gain new insights into families of structural data and showed how to use these results in a predictive manner. He became involved with the CCDC as a Governor and Trustee of the Board and continued to attend their student days into his 90s. The students loved to see him and, nervously, try to answer Jack's penetrating questions. Jack was deeply interested in the expanding and now commercially important study of polymorphs; in experimental charge density; all forms of hydrogen bonding – which had started in his doctoral thesis; phase transformations in the solid state and crystal structure prediction.

In the late 1940s he had worked with Verner Schomaker at Caltech to determine the structure of cyclobutene by gas-phase electron diffraction, another pioneering breakthrough. His work in Oxford, with Leslie Orgel, in determining the structure of ferrocene was a true landmark in organometallic chemistry (1953) and in that famous year, together with Dorothy Hodgkin on a visit to Cambridge, they witnessed the exciting new structure of DNA built by Watson and Crick. It was also the year he married Barbara Steuer, with whom he had recently celebrated their 68th wedding anniversary.

Jack was a deeply committed scientist and chemist, someone who loved his research work and his teaching and this he never stopped doing. His love of chemistry and science was paramount, but his interest in the arts and in music was also for him a very positive part of his life. Jack and his wife Barbara had been keen hikers into the local mountains of Switzerland and he was known to be doing serious exercise and swimming into very recent old age. I met Jack twice when he was over 90, once in Paris for the International Year of Crystallography (2014) and again in Cambridge to celebrate, with Olga Kennard, 50 years of the CSD (2015). It was great to see that he hadn't lost his love of science and sharp, enquiring mind at all.

We shall miss Jack's regular presence at so many of our crystallography meetings, but we can enjoy his legacy and whatever each of us recall about meeting him and sharing his time to discuss our subject, to which he was so passionately and so deeply connected for his entire lifetime.

In his autobiography [La Primavera] Jack wrote *'If I had another life, I would be happy to live it along much the same lines as I have lived this one'.* How wonderful an epitaph?

We think now of Barbara, their children (2), grandchildren (6) and great grandchildren (8) and extended our sincere sympathy to them all from the BCA.

Judith A. K. Howard
Durham University

Further reading: La Primavera. An Autobiographical Essay. *Helvetica Chimica Acta* **96**, 545 (2013).

The Royal Society's Biographical Memoir of Michael Woolfson has now been published. It is available to be read freely online at **https://royalsocietypublishing.org/doi/10.1098/rsbm.2021.0018.**

Jack Dunitz chatting to Andrei Batsanov. (Image: Judith Howard)

Meetings of interest

IN the continuing pandemic situation, many meetings are being cancelled or postponed. At the time of writing, all the meetings listed here were scheduled to go ahead either in-person or online, but there are likely to have been further changes since going to press. Further information may be obtained from the websites given. Assistance from the IUCr website is gratefully acknowledged.

Note that many online meetings charge little or no registration, so if there's a topic that's of particular interest but you'd rather not travel, you might check it out. Also, some meetings listed with a location may be running a mixed in-person/online format.

If you have news of any meetings to add to future lists, please send them to the Editor, **john.finney@ucl.ac.uk** .

6th Dec 2021 - 8th Dec 2021
Asia-Pacific Cryo-EM Symposium
Online.
https://www.apac-cryoem.org/

6th Dec 2021 - 17th Dec 2021
ICTP School on Synchrotron Light Sources and their Applications
Online.
http://indico.ictp.it/event/9645/

16th Dec 2021 - 17th Dec 2021
Italian Crystal Growth 2021 – Crystal Growth: from Theory to Application
Torino, Italy.
https://www.icg2020.net/

5th Jan 2022 - 7th Jan 2022
CCP4 Study Weekend: Current Trends in Macromolecular Model Refinement and Validation
Nottingham, U.K. and online.
https://cvent.me/YPqVd0

10th Jan 2022 - 14th Jan 2022
17th Jan 2022 - 21st Jan 2022
Rigaku School for Practical Crystallography
Online.
https://rigaku.zoom.us/webinar/register/8616327516193/WN_ApzzrLF5QC6aAd_CVPbevg

11th Jan 2022 - 14th Jan 2022
16th International Conference on Surface X-ray and Neutron Scattering (SXNS16)
Lund, Sweden.
https://www.sxns16.org

17th Jan 2022 - 22nd Jan 2022
Third Pan African Conference on Crystallography
Nairobi, Kenya.
https://pccr3africa.org/

24th Jan 2022 - 28th Jan 2022
Cryo-electron Tomography/MRC Training
Online.
https://astbury.leeds.ac.uk/facilities/wellcome-mrc-training-in-cryoem/

31st Jan 2022 – 3rd Feb 2022
Natural and Artificial Metalloenzymes: Faraday Discussion
Online.
https://rsc.li/metalloenzymes-fd2022

9th Mar 2022 - 12th Mar 2022
4th International Conference on 3D Cryo-EM Image Analysis
Lake Tahoe, U.S.A.
https://cryoem.bcm.edu/events/view_workshop/15

28th Mar 2022 - 30th Mar 2022
Understanding Crystallisation: Faraday Discussion
York, U.K.
https://www.rsc.org/events/detail/41849/understanding-crystallisation-faraday-discussion

6th April - 8th April 2022
Advances in Protein Folding, Evolution and Design
Bayreuth, Germany and online.
https://apfed22.uni-bayreuth.de/

24th April - 26th April 2022
Neutron & Muon Science User Meeting
Warwick Conference Centre.
https://www.isis.stfc.ac.uk

31st May 2022 - 3rd Jun 2022
17th European Powder Diffraction Conference – EPDIC17
Šibenik, Croatia.
https://www.epdic17.org/

3rd Jun 2022 - 11th June 2022
Erice School: Crystallography under Extreme Conditions
Erice, Italy.
https://crystalerice.org/2022/

3rd Jun 2022 - 11th June 2022
Erice School: Diffuse Scattering
Erice, Italy.
https://crystalerice.org/2022/

5th Jun 2022 - 10th June 2022
28th EUCHEM Conference on Molten Salts and Ionic Liquids
Patras, Greece.
https://euchemsil2022.org/

9th Jun 2022 - 10th June 2022
Assembling Matter at all Scales
Dresden, Germany.
https://www.max-bergmann-symposium-2022.de/

19th Jun 2022 - 30th June 2022
Zürich School of Crystallography 2022: Bring Your Own Crystals
Zürich, Switzerland.
https://www.chem.uzh.ch/linden/zsc/index.html

4th Jul 2022 - 6th Jul 2022
Emerging Inorganic Materials in Thin-film Photovoltaics: Faraday Discussion
Bath, U.K.
https://rsc.li/photovoltaics-fd2022

10th Jul 2022 - 16th Jul 2022
16th International Conference on the Physics of Non-Crystalline Solids
Canterbury, U.K.
https://sgt.org/mpage/PNCS16

13th Jul 2022 - 15th Jul 2022
Challenges in Biological Cryo-electron Microscopy: Faraday Discussion
Sheffield, U.K. and online.
https://rsc.li/bio-cryo-electro-fd2022

29th Jul 2022 - 3rd Aug 2022
72nd ACA Annual Meeting
Portland, OR, U.S.A.
https://www.amercrystalassn.org/future-meetings

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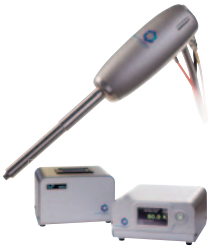
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