Crystallography News

British Crystallographic Association

Issue No. 167 December 2023
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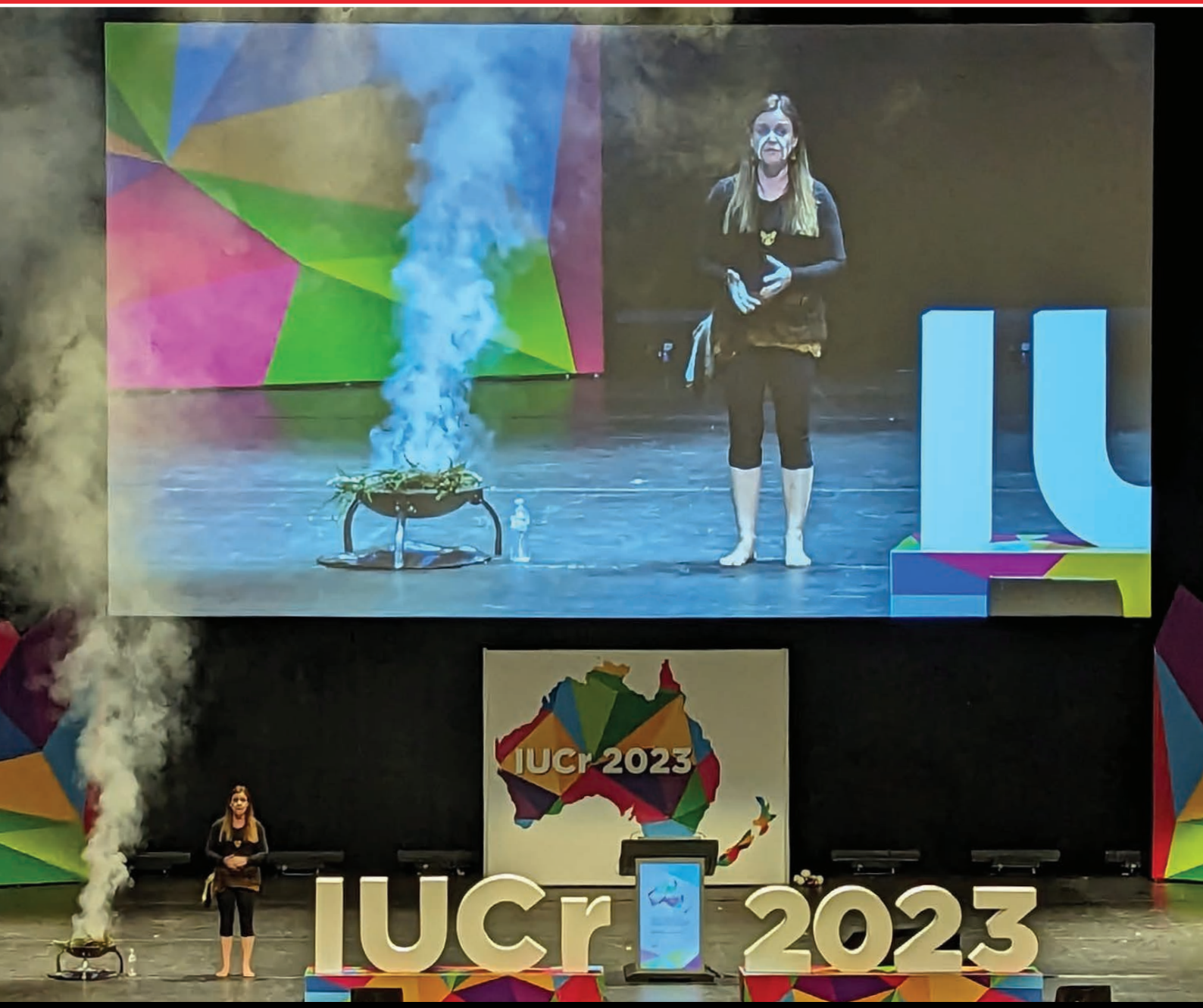

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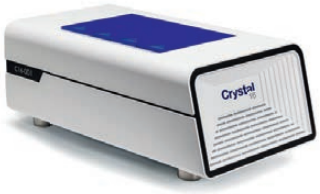

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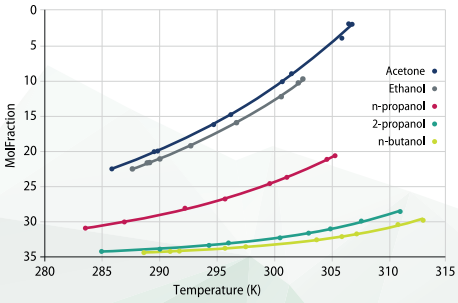

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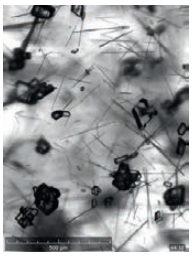
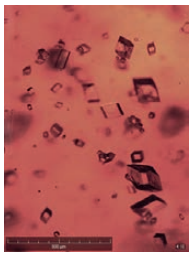


Polymorphic transformation



Coloured compounds

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British Crystallographic Association

Conference Bursaries 2024

Bursaries are available for BCA members to attend national and international crystallographic meetings, the eligibility criteria and application portal are available here:

https://crystallography.org.uk/prizes/bursaries

Bursary applications for the BCA Spring meeting should be made before the **31st January 2024**.

Successful recipients will be notified prior to the early bird deadlines.

*Later applications (after the early bird deadline) will only be considered at the discretion of the council.

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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 2024 issue are sent to the Editor to arrive before 25 January 2024.

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As required by the DATA PROTECTION ACT, the BCA is notifying members that we store your contact information on a computer database to simplify our administration.

These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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Contents

This month's cover:

Welcome to Country Ceremonial at the IUCr26 in Melbourne. Photograph by Glen Hebberd (Durham).

From the President

WELCOME to the December 2023 issue of *Crystallography News*. I think I can just about see a light at the end of the tunnel as I assemble this *penultimate* President's column; I hope that they have been more enjoyable to read than they are for me to put together!

This issue features some more reports from the BCA Spring Meeting in Sheffield earlier this year and from the recent SWSBC meeting. In addition, there is a round-up and highlights of the IUCr Congress and General Assembly in Melbourne, Australia, contributed by some of the BCA members who attended. I was personally disappointed that I was not able to make the trip to Melbourne, but I found that the write ups provide a useful impression of the scientific sessions and conveyed some of the excitement of being at such a large international meeting of crystallographers. The countdown to the next IUCr in Calgary, Canada has begun, and you can already sign-up for updates at the organisers' website (https://www.iucr2026.org/).

Thank you to the current BCA Nominating Committee for supporting the work of Council by finding candidates to serve in positions which are due to fall vacant. Although we haven't secured multiple nominations for posts this election cycle, this is not for lack of ongoing efforts to encourage BCA members to stand for election and the search process has identified some outstanding new Council members (see their statements later in this issue). For any members who would like to see more contested posts, please remember that you don't have to leave the hard work to the Nominating Committee: any two members can nominate someone for election to a post; all you need is their permission. I would like to welcome the new Council members from March 2024: President **Alex Gibbs**, Education and Outreach Coordinator **Ilaria Gimondi** and Council member **Jere Tidey**. In addition, thank you to **Lucy Saunders** for agreeing to take on the role of Bursary Coordinator from **Cheryl Doherty** who retires from Council next year. Notably, this is the first time that the BCA Council Officers and trustees (President, Vice-president, Secretary and Treasurer) will *all* be women since our foundation in 1982 – a statistically long overdue milestone; it will have been 28 years since the Council Officers were all men, if my quick check of historical *Crystallography News* issues hasn't missed any.

An outline of the programme of the 40th BCA Spring Meeting (Leeds, 25th - 28th March 2024) appears elsewhere in this issue – the only things missing are your contributed talks and posters. It is worth remembering that the abstract deadline will fall upon us before you have time to recover from the Christmas break – 9am on **Friday 19th January** for contributed talks (see https://hg3.co.uk/bca/). Registration is also now open – and please don't overlook the Early Stage Crystallographers Group satellite meeting on the first day: the speakers and poster presenters at these sessions are mainly students and other early stage researchers, but everyone is welcome to attend and support. The breadth and quality of science presented is always excellent. If you can cast your minds further ahead, planning for the 2025 Spring Meeting begins at the 2024 Spring Meeting – if you want to influence the meeting themes and sessions then start organising and lobbying your group representatives now.

The Early Stage Crystallographers Group (https://escg.crystallography.org.uk/) is the new name of the Young Crystallographers Group of the BCA. The change of name signals that the group welcomes researchers of any age who have recently begun to study or use crystallography. The name change has passed through the required approval of the YCG AGM (now ESCG) and requires some minor tweaks of the main BCA Statutes and Byelaws in order to make them consistent – this should happen at our AGM next year.

BCA Council has recently approved a BCA Events Code of Conduct which will apply to the 2024 Spring Meeting. The document sets out expected standards of conduct at BCA meetings and events: https://www.crystallography.org.uk/code-of-conduct. In an ideal world these standards of behaviour should be universal and would not need stating explicitly in a document, and of course I sincerely hope that situations do not arise which require them to be enforced in practice – however it is always better to set out clear expectations in advance. I would encourage everyone to be familiar with the code of conduct in order to support colleagues at meetings and being aware of where to report any occurrences of harassment that you may witness.

At the 2023 AGM we approved the creation of a new *Fellow* category of BCA membership and application for Fellow membership will be possible at renewal of membership for next year. The new membership category recognises those with an established career in crystallographic teaching or research and provides a way to support the organisation through the membership subscription. Qualifying members hold Fellow membership in addition to an existing class of membership. Fellows will normally have been members of the Association for at least five years, although the Officers can waive this requirement (for example for BCA members who have established a career outside the UK, or for members who have taken recent career breaks). Please be aware that if you currently pay by direct debit, you will have to fill in a form ahead of renewal in order to change your status. A reminder will be sent out with the annual renewal information.

Season's greetings and I look forward to seeing you at BCA 2024.

Richard Cooper
Oxford

BCA Council 2023

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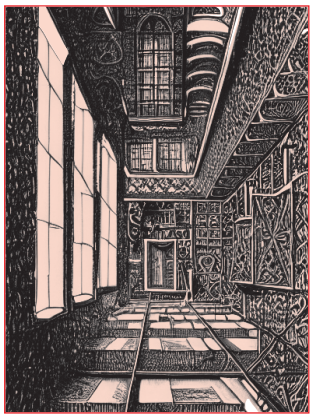
(The dates in parentheses indicate the end of the term of office).

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

From the Editor

IT is a great pleasure to report that this issue carries a detailed programme of the next BCA Spring Meeting in Leeds, 25 - 28 March 2024. We then have the three excellent candidate statements for elections to the BCA Council which are followed by a detailed report by John Helliwell (Manchester) on the truly outstanding IUCr26 Congress, held this year in Melbourne. This is followed by a report from John and Suzanna Ward (CCDC) on the IUCr General Assembly. We then have a series of excellent accounts by the Arnold Beevers Bursary winners of the Melbourne meeting. We continue reporting of the 2023 BCA Spring Meeting sessions and we have an account of the SWSBC meeting in July which was organised this year by Ivo Tews (Southampton) before taking another walk Down Memory Lane and looking at one or two crystallographers (sadly no longer with us) who changed field and we assess the impact this had on themselves and others!



As I had promised previously to institute a new column on ***Crystallographic Forteana*** and even generated some thematic artwork for the series in the last issue, with some trepidation, I think it is now time to bring these ideas to fruition. The word Fortean refers to anomalous phenomena and stems from the life and work of the American writer *Charles Hoy Fort* (1874 – 1932) who spent some years living in London to study at the British Museum. As mentioned previously, I am impressed that crystallographers have embraced anomalous phenomena for almost 100 years and indeed that *anomalous scattering* became one of the discipline's most powerful phasing tools, in the form of SAD and MAD. Fort's work is continued to this day, to some extent anyway, by the *Fortean Times* (FT), which members may have spotted in the larger reputable newsagents, usually at mainline railway stations. I have to admit that I struggle to read it from cover to cover because it can make you feel slightly queasy after a few pages and I am well aware that the anomalous phenomena reported in it may be slightly less reproducible than that which crystallographers are familiar with!

Purely as an example, the October 2023 FT issue has an interesting article[1] on the efforts by *Brother Jonathan* (a vintage phrase for our American cousins) to seek "transparency and accountability" through a Congressional hearing on "Unidentified Anomalous Phenomena" or UAP's for short – this is the new acronym for UFOs! The article alleges that whilst even NASA has a UAP Study Team (**https://science.nasa.gov/uap/**), sightings of UAP's are "grossly under-reported by pilots due to the stigma associated with the subject and the fear of professional repercussions." Crystallographers and future newsletter editors take note. Indeed, whilst the Pentagon has an All-domain Anomaly Resolution Office (**https://www.aaro.mil/**), the members of it are reported to have "not unreasonable anxieties about the career risks this would entail." So much for enlightenment, understanding and inclusivity in the modern scientific age! Anyway, even the FT reported "widespread disappointment at the lack of any new and convincing evidence" arising from the hearing. However it mentions the interesting idea of one former intelligence officer who claims that the "phenomenon itself is upset by the prospect of… disclosure." Ah, anomalous phenomena finally personified – they have life and are conscious! As strange as this concept may seem, I occasionally wondered if the complexity of the crystallographic phase problem was somehow due to the structure not wanting us to solve it!

Anyway, powerful as the phenomenon of anomalous scattering is, at least in macromolecular crystallography, we have to accept that time and tide wait for no one and, although SAD and to a lesser extent MAD are still popular, it is looking as though the wonderful developments in the AI field (another subject of great interest to the FT) will, sooner or later, supercede it as a phasing method[2].

Season's greetings from me too.

Jon Cooper
UCL

References:

1. Watson, N. (2023). UFOs over the Capitol. *Fortean Times* **436**, 28-31.
2. Terwilliger, T. C., Afonine, P. V., Liebschner, D., Croll, T. I., McCoy, A. J., Oeffner, R. D., Williams, C. J., Poon, B. K., Richardson, J. S., Read, R. J. & Adams, P. D. (2023). Accelerating crystal structure determination with iterative *AlphaFold* prediction. *Acta Crystallogr.* D **79**, 234-244.

Puzzle Corner

The challenge is to identify the plane group of each of the following wallpaper patterns which were photographed in a Venice hotel and very kindly sent to the editor by **John Lisgarten** (London).

(a)

(b)

BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
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- 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 **£850** for one year.

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The Cambridge Crystallographic Data Centre (CCDC): **https://www.ccdc.cam.ac.uk**

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- A copy of Crystallography News every quarter
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- 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 2024

Monday 25 March 2024

ESCG Early Career Satellite Meeting

Early Stage Crystallographers Group (ESCG)

13:00 – 21:00

The YCG satellite meeting is an opportunity for all early-stage crystallography researchers, 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

ESCG Opening Plenary:

Session Chair: **Rebecca Clulow** (Uppsala University)
Speaker: **Dr Lukáš Palatinus** (FZU – Institute of Physics of the Czech Academy of Sciences)

Small crystals, big results: the limits and prospects of electron crystallography

13:30 – 17:15

ESCG Research Sessions

Contributed talks from the ESCG community.

Session 1 Chair: **Joshua Morris** (Cardiff University)
Session 2 Chair: **Olivia Breen** (University College Dublin)
Session 3 Chair: **Sam Lewis** (Cardiff University)

17:15 – 17:45

ESCG Annual General Meeting

18:30 – 21:00

Flash Poster Presentations

Session Chairs: **Phillipa Partridge** (University of Edinburgh) and **Julia Gascol Cardona** (University of Strathclyde)

Researchers have an opportunity to present an overview of their poster in 30 seconds with one PowerPoint slide.

19:00

Poster Session with Dinner and Wine

21:00

Evening Concludes

Tuesday 26 March 2024

09:00 – 09:30

Parkin Lecture

Session Chair: **Thomas Hitchings** (University of Kent)
Speaker: ***TBC***

09:30 – 10:30

Session 4

Session Chair: **Anna Herlihy** (ISIS Neutron and Muon Source/Diamond Light Source)

10:30 – 11:00

Closing Plenary

Session Chair: **Jake Hill** (University of Bradford)
Speaker: **Dr Helen Ginn** (Hamburg Advanced Research Center for Bioorganic Chemistry)

Teasing out the secrets of subtle protein dynamics

Main Meeting

11:30 – 12:15

Lonsdale Lecture

Session Chair: **Dr Anthony Carter** (Pharmaron)
Speaker: **Dr Helena Shepherd** (University of Kent)

Thermally Responsive Molecules and Materials

13:00 – 13:45

CCG Plenary

Session Chair: **Mike Probert** (Newcastle University)
Speaker: **Aurora Cruz-Cabeza** (University of Durham)

If you can't beat the laws of thermodynamics, join them: Robust access routes to elusive polymorphs

14:00 – 15:30

Parallel Sessions

BSG: Getting the most from your protein crystals at the synchrotron
Session Chair: **Adam Crawshaw** (Diamond Light Source)
Keynote: TBC

Today automated data collection at the synchrotron has made collecting good quality data a trivial exercise, however, the development of unique instruments such as the long-wavelength beamline I23, in-situ diffraction beamline VMXi and the nanofocus beamline VMXm provide unique opportunities to collect data from the most challenging of samples. This session will introduce current data collection methodologies at the synchrotron and outline how to make the most of new, cutting-edge instrumentation that could unlock structures that were previously intractable.

CCG: Dynamics and Reactivity in Solids
Session Chair: **Erli Lu** (Newcastle University)
Keynote: TBC

By removing bulk solvents, the solid-state synthesis is a prime candidate for sustainable chemical synthesis technologies. But its potential is beyond merely being solvent-free: it could unlock otherwise impossible chemistry. To unleash the full potential of solid-state synthesis, it is crucial to understand the dynamics and reactivity in solids, which are incredibly challenging tasks. The aim of this session is to bring together a wide spectrum of cutting-edge advancements and global talents, from enabling in-situ monitoring methods to understand the dynamics, to ground-breaking reactivity which are inaccessible with the presence of solvents.

PCG/ESCG: Recent Developments in Software
Session Chair: **Dan Porter** (Diamond Light Source) and **Ben Tragheim** (University of Warwick)
Keynote: **Marcus Newton** (University of Southampton)

Advances in Processing and Analysis of Bragg Coherent Diffraction Imaging Data

Almost all forms of data processing, analysis and simulation require the use of some form of specialist scientific software. Developments of new functionalities in these software can provide faster and more accurate results, as well as providing new ways to interpret our data, driving scientific output and impact. Therefore, it is crucial that we continue to make advancements within this area of research. This session will highlight recent advances in software and ways in which we perform data analysis and processing, in all areas of crystallography and materials science. Abstracts are warmly welcomed from all members of the community, with early career researchers particularly encouraged to submit.

16:15 – 17:45

Parallel Sessions

BSG/ESCG Joint Session: Breaking the field boundary: careers between chemical and biological crystallography
Session Chair: **Jake Hill** (University of Bradford) & **Rachael Wilkinson** (University of Oxford)
Keynote: TBC

A career in crystallography can be varied and whilst chemical crystallography and biological crystallography can first appear very different, many skillsets of the chemical and biological crystallographer overlap. In this session the careers of those from both paths will be explored in addition to a discussion panel with emphasis on early stage crystallographers and how they can develop their careers in the field.

CCG: Mechanochemistry
Session Chair: **Guilio Lampronti** (University of Cambridge)
Keynote: TBC

Mechanochemistry is the field of physical and chemical transformations induced by mechanical force. It comprises a vast range of techniques, such as grinding, rolling, extrusion, mixing, cutting, the application of single pressure shocks or continuous pressure. Crystallographic investigations play an ever growing role in the study of the materials involved and the mechanisms of mechanochemical transformations. As mechanochemical methods produce virtually no waste and generally require less energy than thermal methods, they have been recognized as key for a sustainable future. They are used for the synthesis of new compounds and phases, as well as the control and optimization of known processes, with actual and potential chemical and pharmaceutical applications beyond the more traditional mechanical alloying and materials processing.

PCG: Phase Transitions
Session Chair: **Nilanthy Balakrishnan** (Keele University)
Keynote: **Claire Hobday** (University of Edinburgh)

Pressure Driven Phase Transitions: a Look to the Future of Refrigeration

Phase transitions are transitions between different physical states (phases) of the same substance. Sometimes the properties of a substance abruptly change, often in a dramatic way, by the changes in the specific volume and entropy. However, there are still many open questions across a host of scientific fields. This session aims to broadly cover phase transition phenomena in a diverse set of systems, including order/disorder, displacive transitions, and from crystals to amorphous. Talks from all areas of the scientific community are welcome.

18:00 – 18:45

BSG Plenary

Session Chair: **Rachael Wilkinson** (University of Oxford)
Speaker: **Prof. Syma Khalid** (University of Oxford)

When structural data gets messy: insights from molecular simulations

19:00 – 21:00

Poster Session with Dinner and Wine

Wednesday 27 March 2024

09:00 – 09:45

IG Plenary

Session Chair: **Tony Bell** (Sheffield Hallam University)
Keynote: **Simon Coles** (Southampton University)

A step change for single crystal structure determination: the new capabilities of electron crystallography

10:15 – 11:45

Parallel Sessions

CCG: Framework materials
Session Chair: **Georgia Orton** (University of Birmingham)
Keynote: TBC

Framework materials, such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs), have shown huge promise in a variety of applications. Developments in this rapidly moving field are typically underpinned by structural information provided by crystallographic techniques since the properties of frameworks are intrinsically related to their structures. Crystallography is a critical tool in areas including, but not limited to, elucidating the molecular-level structure of frameworks and encapsulated guests, understanding responses to external stimuli and reactivity within the framework and, in conjunction with complimentary techniques, exploring correlated disorder and glassy states.

IG/BSG: Exploring synergies at the small molecule-biomolecule boundary
Session Chair: **James Gordon** (Rigaku)
Keynote: **Duncan Johnstone** (GSK)

Title TBC

Small molecule and macromolecular crystallography have often involved differing methodologies and technique. Yet, techniques within macromolecular crystallography have recently shown promise for complex small molecules. This session explores the overlap between chemical and biological crystallography and how methods and understanding can be exchanged within these areas.

PCG: Electron Crystallography
Session Chair: **Matt Cliffe** (University of Nottingham)
Keynote: **Sean Collins** (University of Leeds)

Scanning Nanobeam Analysis of Defect Domains, Dislocations, and Disorder in Metal–Organic Frameworks and Molecular Crystals

Electron diffraction is one of the most rapidly developing areas of crystallography, due to the recent advances in instrumentation, software, and understanding. Electron crystallography, potentially enabling the measurement of single-crystal datasets from 'powder' samples, could be transformative and the nanoscale information available will shed light on the true heterogeneity of materials. This session will showcase the range of crystallography conducted using electron beams: from fundamentals of measurement and new modes of analysis through to its use to develop new understanding of materials' structure.

11:45 – 12:15

CCG Annual General Meeting
BSG Annual General Meeting
PCG Annual General Meeting

13:00 – 14:30

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.

Chemical Crystallography Group Prize for Younger Scientists

The CCG 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 Early Career Prize

The 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.

14:30 – 14:45

Exhibitor Forum

15:15 – 16:45

Parallel Sessions

BSG: Artificial intelligence in structural biology
Session Chair: **Georgina Menzies** (Cardiff University)
Keynote: TBC

Recent years have seen significant advances in the role of artificial intelligence within structural biology. This has included the improved prediction of protein structure by Alphafold 2/ESMfold as well as for molecular dynamic simulations. With AI an ever-increasing presence within the field this session explores how it is currently being used to best effect within the field.

IG/CCG: Crystallography and Systems under Mechanical Stress
Session Chairs: **Tony Bell** (Sheffield Hallam University) & **Adam Michalchuk** (University of Birmingham)
Keynote: TBC

Solid materials are exposed to a wide variety of mechanical stresses, whether they be engineering materials in a motor, pharmaceutical materials being ground or tableted, or even biological materials in the depths of the oceans. The explicit use of mechanical stress has also emerged as a tool to induce solvent-free chemical synthesis and to manipulate material functional properties like electronic conductivity, colour, and magnetism. This session will highlight exciting recent developments made to elucidate the effects of mechanical stress on material structure and function, demonstrating how structural insight into crystals and systems under mechanical stress forge breakthroughs across disciplinary boundaries.

PCG: Analysis of Local Structure
Session Chair: **Anna Herlihy** (STFC)
Keynote: **Phoebe Allan** (University of Birmingham)

Operando Studies of Local Structure in Battery Materials

There is an increasing awareness of the role that disorder plays in structure-property relationships of functional materials.

Disorder within crystal structures presents itself in a number of ways, with local structure probes such as total scattering, NMR, diffuse scattering, and EXAFS providing information on sometimes complex local behaviour which can be obfuscated by the relatively simple unit cell picture provided by average structure approaches. This session will explore the wide range of functional materials that benefit from local structure techniques and will highlight recent experimental developments including in operando and in situ methodologies.

17:15 – 18:00
Bragg Prize Lecture
Session Chair: **Professor Richard Cooper** (University of Oxford)
Speaker: **Professor Arwen Pearson** (University of Hamburg)

The future of macromolecular crystallography in the age of machine learning

Structure prediction tools have had a major impact on structural biology. What are the limits of these tools, and where are they creating new opportunities for the field?

18:00 – 19:00
BCA Annual General Meeting

19:30 – 01:00
Conference Dinner & Ceilidh

Thursday 28 March 2024

09:00 – 09:45
PCG Plenary
Session Chair: **Alex Gibbs** (University of St Andrews)
Speaker: **Dr Silvia Ramos** (University of Kent)

Structural Signatures of Metal-Insulator Transitions as seen by Polarisation Dependent X-ray Absorption Spectroscopy

10:15 – 11:45
Parallel Sessions

BSG: Breaking barriers with emerging technology in structural biology
Session Chair: **Hanna Kwon** (University of Leicester)
Keynote: TBC

Development of new technologies for the determination of protein structures in biology is moving at a rapid pace from instrumentation development in X-ray crystallography and cryoEM to the use of serial crystallography to improve mechanistic understanding of enzyme reactions. This session covers the current use of new and emerging technology within structural biology.

CCG: Molecular interactions and Supramolecular chemistry
Session Chair: **Krešo Bucar** (University College London)
Keynote: TBC

This session aims to provide a forum to both experimental and computational solid-state chemists to discuss the latest advances in understanding the nature of non-covalent interactions, molecular self-assembly and the engineering of materials with targeted properties. We particularly welcome contributions on the use of predictive models, computational methods, new or advanced techniques to characterise the solid state, and 'big data'.

PCG/IG: Energy & Sustainability
Session Chair: **Glen Hebberd** (Durham University)
Keynote: **Beth Johnston** (University of Sheffield)

Elucidation of the Structure and Local Diffusion Dynamics in Nickel Rich Layered Oxide Cathodes for Lithium-ion Batteries

The wide field of energy materials uses a variety of analytical techniques (crystallographic and non-crystallographic) to probe both the long-range order and the local structure to explore the composition, electronics, and dynamics of a material. This session will delve into all different forms of research that have links to sustainable goals such as the target for affordable and clean energy. This includes, but is not limited to, work on novel systems for energy capture, conversion, or storage; structure-property relationships; or any work undertaken using less energy-intensive synthesis methods than traditional routes. Abstracts from early-career researchers in this field are strongly encouraged.

12:15 – 13:45
Parallel Sessions

BSG: Open Session
Session Chair: **TJ Ragan** (University of Leicester)

This session will cover areas of structural biology within the breaking barriers theme.

CCG: Open Session
Session Chair: **Sam Chong** (University of Liverpool)

The Open Session for Chemical Crystallography invites research contributions that span the breadth of chemical crystallography. We welcome abstract submissions from researchers using experimental and computational approaches, diverse materials – including molecular and framework structures, organic and inorganic compounds – crystallographic phase transitions, crystal growth mechanisms, method development and more! Join us to share your innovative work and engage with the chemical crystallography community. Whether your research is fundamental or applied, this session provides a platform for showcasing diverse perspectives and methodologies.

PCG: Open Session
Session Chair: **Lewis Owen** (Sheffield)

This open session is a forum for research that falls outside of the targeted topics of other sessions. 'Physical' crystallography is interdisciplinary and intersects with many exciting fields. Whether your work is fundamental or applied, theoretical or experimental; whatever your material, whatever your technique, contributions from every corner of the physical crystallography community are welcome.

CLOSE OF CONFERENCE

BCA Council Elections 2024

Candidate statements

Nominations have been received for **President**, **Education Coordinator** and **Ordinary Member**.

Alex Gibbs (St Andrews)

President

Current Position
EPSRC Early Career Fellow, School of Chemistry, St Andrews.

Education and Career
MPhys, St Andrews, 2008.
PhD, St Andrews, 2013.
Postdoctoral researcher, Tokyo and Max Planck, 2012-2016.
Instrument scientist, ISIS, 2016-2020.
Currently PCG committee Chair 2020-2023.

Personal Statement
Alex completed her MPhys at the University of St Andrews in 2008 after originally starting out in chemistry. She stayed there for her interdisciplinary PhD with Prof. P. Lightfoot and Prof. A. P. Mackenzie on structure-property relationships and emergent states in transition metal oxides.

Following this, Alex took up opportunities to conduct research in Japan (at the University of Tokyo and RIKEN) and Germany (Max Planck Institute for Solid State Research in Stuttgart) focusing on the exploration of new quantum materials. With neutron scattering being a key experimental tool for her work, she then moved to a permanent position at the ISIS Neutron and Muon Source in Oxfordshire to follow her continued interest in high resolution neutron diffraction.

These research streams have now converged in her EPSRC Early Career Fellowship at the School of Chemistry at St Andrews in association with the Crystallography Group at ISIS. Her research is at the chemistry–physics boundary, studying structure–property relationships in quantum and functional materials.

She has been a member of the BCA since 2009 and the PCG committee since 2016, serving as Treasurer 2017-2020 and Chair 2020-2023.

Ilaria Gimondi (CCDC)

Education Coordinator

Current Position
Education and Outreach Officer at the Cambridge Crystallographic Data Centre (CCDC).

Education and Career
Bachelor and Master in Chemical Engineering, Politecnico di Milano, 2013 and 2015.
Ph.D. in Chemical Engineering, University College London, 2020.
Currently covering *ad interim* the Education and Outreach Coordinator position at the BCA.

Personal Statement
It is great to officially take on the Education and Outreach Coordinator position for the next term! As Education and Outreach Officer at the CCDC, I have had the pleasure to interact with the community over the last few years, both for training events and for outreach opportunities. In particular, I had the opportunity to collaborate with the BCA on the Elements in Crystal activities, the continuation of the International Year of the Periodic Table project. I have also worked together on the Crystal Battlecards, directly inspired by and showcasing the periodic table of elements and crystals created by our community (including some of you!), and a collection of short videos, curated by a PhD student from the University of Cambridge.

Recently I have been covering the *ad interim* Education and Outreach Coordinator role at the BCA. During this time, I have learnt how the council works (including having the honour to be part of the UK delegation at the IUCr conference!) and I have enjoyed discussing ideas and hearing from some of the members their views and plans for Education and Outreach at the BCA. Taking over the role for the next term, I wish to continue and expand these discussions and help delivering the BCA vision for education and outreach.

I believe it is important that education and outreach activities remain a focus for our community, and I am looking forward to working with you to support and inspire the current and next generation of crystallographers.

Jeremiah (Jere) Tidey (Warwick)

Ordinary member

Current Position
Research Technical Professional in electron diffraction (ED), University of Warwick.

Education and Career
MSci (Hons) Chemistry,University of Nottingham, 2008-2012.
PhD in Chemistry, University of Nottingham, 2012-2016.
Research Associate, University of Toledo, 2016-2019.
Research Fellow, University of Warwick, 2019-2021.
Research Fellow, University of Warwick, 2021-2023.

Personal Statement
Jere joins the BCA Council as Ordinary Member with an increasingly diverse background in diffraction. He completed his PhD in high-pressure crystallography of coordination complexes with Alexander (Sandy) Blake at the University of Nottingham, supplementing Sandy's training with the obligatory time-served at the BCA/CCG teaching school in single-crystal XRD. He promptly then moved to America in 2016 to join the Pinkerton group at the University of Toledo, Ohio. There, he spent three years performing variable-temperature charge-density studies on organic energetic materials. Upon returning, he joined the Senn group at the University of Warwick, traded the CCG for the PCG, and found himself powerless to resist the charms of high-resolution powder diffraction (albeit with a refreshing side-dish of HPXRD). In the wake of the COVID-19 pandemic, Jere returned to the BCA/CCG "Durham School", ascended to tutorship, where he hopes to remain engaged for some years to come. 2023 saw him finally lose touch with meaningful *R*-factors as he switched into a technical role at Warwick. He now serves as lead operator of the UK's first (just!) dedicated electron diffractometer, a Rigaku Synergy-ED, in partnership with the Simon Coles' team at the University of Southampton to form the UK's new National Electron Diffraction Service.

BCA Spring Meeting 2023, CCG Session Report

Databases and Associated Tools

TUESDAY afternoon of the Spring Meeting saw the CCG session on "Databases and Associated Tools", which covered a considerable breadth of chemical crystallography and showed how useful managing in-house data can be, alongside demonstrating the value of existing global repositories of crystal structures such as the Cambridge Structural Database (CSD).

The keynote presentation was given by **Matthew Kitching** (Durham) on "Identifying a hidden conglomerate chiral pool in the CSD." Matthew is a synthetic chemist with a particular interest in chirality, and he explained how conglomerate crystallisation leads to spontaneous chiral resolution during crystallisation. Such systems are, however, not commonly documented, and Matthew outlined previous and ongoing attempts to systematically search for chiral species in the CSD and understand the patterns and trends present in conglomerate crystals. He finished his presentation by posing a series of questions about the approach taken so far and the additional data that the community should provide to further increase the value of such datasets, which resulted in a lively discussion with the audience. This will certainly provide further interesting conversations in conferences to come.

The next talk was given **Tabbasum Naz** (Strathclyde) on "Digital transformation in pharmaceutical manufacturing" which described the outputs from the recent Digital Design Accelerator Platform (D-DAP) project. Tabbasum described the vastness and complexity of data sources that are crucial to pharmaceutical development and manufacturing, and how it is necessary to handle this data efficiently and consistently to enable the digitalisation of this key industry. She stressed the importance of making sure data is FAIR (Findable, Accessible, Interoperable, Reusable) so that information from a variety of instruments, techniques, and models can be efficiently combined and reused before describing how this approach can be expanded on for future projects much more easily if care is taken when starting out.

The third talk came from **James Osborn** (University of Liverpool) who described the development of a Python Machine Learning Toolkit for Powder Diffraction (PyMLPD) in a presentation on "Clustering of molecular organic crystals from powder X-ray diffraction data." The PyMLPD tool developed by James and colleagues uses a variety of machine learning techniques to automatically identify similarities and differences in powder diffraction patterns. James explained that this ultimately makes rapid identification of polymorphs a possibility, enabling screening of samples via PXRD without the need for inspection.

The final talk of the session was given by **Thomas Smith** (Newcastle) and was one of many across the meeting that described the outputs and challenges from the ENaCt (Encapsulated Nanodroplet Crystallisation) platform at Newcastle. In his presentation entitled "A highly integrated data management solution for parallel crystallisation experiments", Thomas described the vast quantities of data produced during parallel crystallisation experiments and demonstrated the impossibility of trying to manage all this information manually. Thomas outlined how a well-structured underlying data architecture, combined with user-sympathetic tools to store, manage and analyse this data, can provide a rich resource not just for the experimentalist at the time, but for future analysis for a variety of different purposes.

Andy Maloney
CCDC

IUCr 2023 Congress

THIS report complements the report on the IUCr 2023 General Assembly elsewhere in *Crystallography News* from Suzanna Ward (CCDC), Leader of the British Delegation. I was honoured to be a member of the Delegation.

At the Closing Ceremony we learnt from **Michael Parker** (Melbourne), the Chair of the Local Organising Committee, the statistics of the marvellous success of IUCr 2023. There were 1788 in person delegates and 82 virtual attendees, 34% female participation, then by country no surprise that Australia was top with 336 delegates, then Japan with 197, USA 173 and then UK with 158; overall there were 66 countries represented. There were 402 early career researchers and 16 attendees harnessed the childcare provision. By comparison, just to mention that I was at the 1987 Congress in Perth and from memory I think the total attendance there was 700 people. A big feature in the Melbourne Congress Centre Exhibition Hall was the presence of large-scale atomic and molecular models. The largest of all, assembled during the week by volunteers, was an atomic model of diamond. Michael again showed the impressive numbers that this diamond model comprised 59,956 atoms, 118,724 bonds, 24 layers, a bottom edge of 3.69 m, top edge 2.31 m and height 1.11m. It weighed 329 kg and of course took a week to build.

At one time I counted as many as 7 volunteers working on its construction. From the tweets by @SBattenResearch (Dr Stuart Batten based in Melbourne) Nature noticed the effort and the coordinator of the Guinness Book of World Records contacted IUCr2023 and is in the process of their certification checks. At talks by Australian presenters, as well as at the Opening Ceremony, respect was given to the indigenous peoples of Australia.

I arrived in time for me to present the opening lecture at the Workshop "A practical approach to synchrotron experiments" (https://iucr2023.org/workshops/). This finished with a lunch and panel discussion led by the organisers **Simon Grabowski** (Bern) and **Dubravka Sisak Jung** (Dectris) under the auspices of the Swiss Society of Crystallography. Then later in the afternoon I met the IUCr Executive Committee and answered questions on behalf of the IUCr Committee on Data, on the International Science Council's Committee on Data (CODATA) activities (https://www.iucr.org/iucr/ab.html/other-bodies/codata.html) and on our Book Series with Oxford University Press (https://www.iucr.org/publications/iucr-oup). On the next day the IUCr Committee on Data had organised a full day Workshop "Raw diffraction data reuse: the good, the bad and the challenging" (https://www.iucr.org/resources/data/commdat/melbourne-workshop).

Michael Parker (Chairman of the IUCr 2023 Local Organising Committee) opens IUCr 2023 with the "Acknowledgement of Country." With thanks to the IUCr 2023 Congress – photographed by SDP Media.

The opening ceremony was both spectacular and learned. First of all, we had the indigenous peoples of Australia smoke ceremony. The welcoming remarks portion then included an overview of all the sciences from the President of the International Science Council **Peter Gluckman** (Auckland). Then, the Ewald Prize lecture was presented by the awardee **Wayne Hendrickson** (Columbia). This was a tour de force of great depth within the theme of the crystallographic phase problem. We then proceeded to the welcome buffet, which for the first time included oysters, which was in the Exhibition Hall.

The Congress program was very busy with its parallel sessions but time keeping was a strict instruction to Chairs. I co-chaired two microsymposia, one on "Interoperability of Databases" and another on "Databases and data management." So, in one microsymposium that I attended, a time gap was adhered to due to a speaker's absence. This allowed relaxed chat amongst that session's audience which was rather pleasant actually. Of course, the overall purpose of the timekeeping was to make possible session-to-session hopping. The Congress Centre layout was straightforward as it was a simple walk between the rooms on the second floor.

The education session took building community trust as its theme. In this session, I presented a lecture on the role of the IUCr's crystallographic data science skills and the crystallographic information framework with an especial focus on training courses we had run in recent years; https://www.iucr.org/resources/data/commdat/vienna-workshop and https://www.iucr.org/resources/cif/comcifs/cifiesta-2019. Also, a recent education article I wrote with **Chiara Massera** (Parma) on trust published by the *Journal of Applied Crystallography*, handled by Editor **Louise Dawe** (Wilfrid Laurier), gave an important connected logic throughout my talk. See https://journals.iucr.org/j/issues/2022/05/00/dv5002/index.html.

I was involved with four different breakfast meetings, a type of timeslot that I started using in Montreal in 2014 simply because I found we could never find the best timeslot during the Congress day itself.

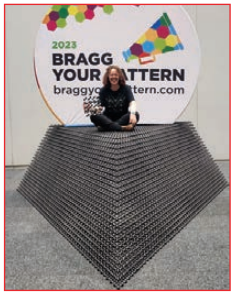
As well as the careful daily diary plan that I made for sessions that I must attend, there were unexpected delights. I found myself passing the NMR crystallography session and strayed in and stayed! Then at the Bragg Prize Symposium, awarded to **Arkadiy Simonov** (ETH Zurich) for his work on diffuse scattering, **Mike Glazer** (Oxford) in his introductory remarks as Chair showed a family movie clip of the Braggs, father and son, in the home garden chatting and smiling convivially with each other. This neatly refuting the notion that Lawrence Bragg was at loggerheads with his father, William Henry Bragg. Another unexpected delight was arriving at the poster of the Chair of the Prague Congress, **Radek Kužel** (Prague) which provided the details of the on-site and virtual participation at the 2021 Prague Congress which was hybrid. So, the poster showed statistics such as the ranking order by number of virtual sign-ins to lectures and to posters.

To sum up, I found this an excellent Congress. I tweeted my appreciation from @HelliwellJohn after the closing ceremony thanking the Congress organisers, the Exhibition Centre, Melbourne city and all of Australia. Like the Perth Congress in 1987 it is a privilege and pleasure to have taken part. The IUCr President **Hanna Dabkowska** (McMaster) formally closed the Congress in a heart-warming manner and emphasised that the Calgary Congress in 2026 awaits. This had been eloquently described by **Louise Dawe** (Wilfrid Laurier) a few minutes earlier on behalf of the Canadian National Committee for Crystallography, the American Crystallographic Association and the US National Committee for Crystallography.

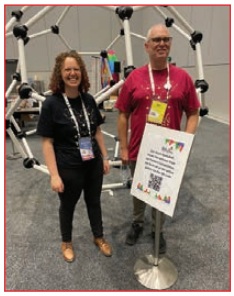
John R Helliwell
Manchester

*End of the session photograph for "Interoperability of Crystallographic Data and Databases" organised by **Ian Bruno** (CCDC) and **Alice Brink** (Free State, SA) neither of whom could attend the Congress. Left to right: **John Helliwell** (Session Chair and Chairman of IUCr Committee on Data), **Simon Coles** (incoming Chairman of IUCr Committee on Data), **Soorya Kabekkodu** (ICDD), **Suzanna Ward** (CCDC), **Toby Blundell** (Durham), **Thomas Smith** (Newcastle), **Brian McMahon** (IUCr), **Saulius Gražulis** (Vilnius and COD) and **Daumantas Matulis** (Vilnius). Photo taken on the camera of Saulius Gražulis reproduced under CC-BY.*

*Building the giant diamond model in the IUCr 2023 Exhibition Hall with **Sam Horrell** (DLS) kneeling atop the model.*



Rosemary Young (ANSTO) atop the completed giant diamond model. With thanks to the IUCr 2023 Congress – photographed by SDP Media.



*Rosemary Young (ANSTO) and **Alan Riboldi-Tunnicliffe** (ANSTO) next to their giant buckyball model in the IUCr 2023 Exhibition Hall. Photo taken by John Helliwell with their permission to reproduce here in Crystallography News. ANSTO is the Australian Nuclear Science and Technology Organisation.*

*The scene at the River Yarra in the morning; photo taken by **John Helliwell** (Manchester) walking en route to the Congress Centre which is nearby.*

Report on the IUCr 2023 General Assembly

Members attending: Ilaria Gimondi (CCDC), **Mike Glazer** (Oxford), **John Helliwell** (Manchester) and **Natalie Johnson** (CCDC) who on day 3 alternated with **Simon Coles** (Southampton). The UK has 5 votes allowing 5 members, one vote per member.

The 2023 IUCr General Assembly took place over three separate evenings in the Melbourne Exhibition and Congress Centre in August. The agenda is available here and included changes to memberships of the Union, financial reports, an update on prizes, publishing, outreach and education activities as well as commission and committee updates, elections and plans for future general assembly meetings. The formal minutes will be available in due course. The following items can be reported:

The African Crystallographic Association (AfCA) was officially voted in as a Regional Associate of the IUCr.

A proposal by the Polish Delegation, seconded by the French Delegation, to suspend Russia was not passed.

The Editor in Chief of IUCr Journals, **Andrew Allen** (NIST, USA) presented an overview of the journals and confirmed that to mark the 75th anniversary of the IUCr every presenter of an abstract, oral or poster, had been invited to submit an article to the appropriate IUCr journal. With revenues from the journals helping to support the activities of the IUCr all members were encouraged to consider submitting other articles to IUCr journals too.

The retirement of **John Helliwell** (Manchester) as Chairman of the Committee on Data, his role as IUCr Representative to CODATA and as Chairman of the IUCr OUP Book Series Committee was marked with applause by the Executive Committee and the Delegations. **Simon Coles** (Southampton) will be taking on the role of Chairman of the Committee on Data.

A presentation on the 2026 Congress and General Assembly in Calgary, Canada was given. It was confirmed that the 2029 Congress and General Assembly will be in Berlin, Germany.

Two preliminary presentations for the 2032 Congress and General Assembly bids were presented by China and by South Korea.

The elections to the IUCr Commissions were done individually, which also allowed for scrutiny of the gender balance of the new Commission membership; the percentages ranged from 14% to 44%.

The new President is **Santiago García Granda** (Oviedo, Spain), the new Vice President is **Graciela Delgado** (Los Andes, Venezuela) and the new General Secretary and Treasurer is **Trevor Forsyth** (ESS, Sweden). The new ordinary members of the Executive are **Susan Bourne** (Cape Town, SA), **Atsushi Nakagawa** (Osaka, Japan) and **Cristina Nonato** (São Paulo, Brazil). The current President **Hanna Dabkowska** (Hamilton, Canada) congratulated the new members and invited the old and new Executive Committees to meet together for a new smooth handover.

Suzanna Ward (CCDC, Leader of the UK Delegation) and **John Helliwell** (Manchester, Member)

Bursary winner reports on IUCr26, Melbourne 2023

Walking out into the fresh air of Melbourne Tullamarine Airport at 5 am was quite the treat after 27 hours of sitting in small airplane seats and aimlessly wandering around terminals in Dubai and Brunei. The long journey was more than worth it though as even before the conference had begun, we were enjoying the cultural highlights of the city: an AFL game at the MCG and a trip to the pub for the final of the Women's Football World Cup.

The busy arrival was followed by a couple of much quieter days to reset from the jetlag and prepare for the beginning of the main conference. Amazing performances from the First People of Australia and New Zealand set the scene before the Ewald Prize lecture by **Wayne Hendrickson** (Columbia). While most of this talk went way over my head, the story of his first conference which included his first ever flight on an airplane before meeting W. L. Bragg and Paul Ewald was quite enthralling. An incredible reminder of the connection to the original pioneers in our community, as well as the speed of development in technology and knowledge.

That evening, the social calendar launched with plenty of drinks in the conference centre, trays of oysters (not my favourite, would've been better off just taking a big gulp of sea water) and an exhibition of Australian animals such as Billy the koala.

The highlight of the first few days for me was the keynote lecture by **Graeme Day** (Southampton) on computational prediction applied to porous molecular materials. His talk focused on understanding why some higher energy porous forms can be isolated experimentally in some systems. The branched visualisations of structure-energy relationships helped to make the content instantly engaging and was thought provoking for considering the fluidity of organisation which can exist during crystallisation.

The Saturday afternoon session on "Nanocrystalline porous materials" had a variety of topics which all centred around electron diffraction. **Ken Inge** (Stockholm) showed the ability to alter synthesis workflows because they can be characterised from powder samples. **Sofiia Butonova** (Stockholm)

IUCr26 poster presenter ***Robert Carroll*** *(Southampton).*

discussed the development of new crystalline sponges for electron diffraction, demonstrating the combination of two exciting areas for crystallography research which may be explored further.

Amidst all the crystallographic content, some time was also dedicated to socialising/networking, and I am pleased to report Melbourne has a range of options to suit most crystallographers. This includes (but is not limited to): Kylie Minogue and Robbie Williams tribute acts which have multiple costume changes, student clubs which are inevitably accompanied by a few injuries/losses of personnel before entry, and karaoke bars which can house around 40 crystallographers per room (special thanks to Peter and Jürgen for being excellent duet partners). We were also fortunate enough to explore some more of rural Victoria, with the kangaroos and wallabies at Moonlit Sanctuary being definite highlights.

In the final two days of the conference I was able to present some of my recent work in the form of a poster. It was amazing to engage with researchers from the wider crystallographic community and discuss the difficulties we had encountered even when working in quite different topics. Many of the best insights I took away from the conference came from these conversations and they have left me excited for work I can become involved in after the final year of my PhD.

Robert Carroll
Southampton

As part of the IUCr's commission on structural chemistry, the second day of the IUCr's 26th congress featured a parallel session focussing on crystal growth and nucleation. Opening was **Alexandra Longcake** (Newcastle), giving an overview of the ENaCt process, and how it is offered as part of the suite of non-standard crystallisation/crystallography techniques offered through the UK's National Crystallography Service. She then went on to describe how the technique had been applied to a suite of 60 natural products with a 50% success rate, including the discovery of a new polymorph of Betulinan A!

Following was **Kasun Athukorala Arachchig** (Brisbane) who talked about how they had developed the ENaCt technique to grow crystals suitable for charge-density studies. They applied these developments to collect charge-density structures for Pt(acac)2 and some other organic ligands. He also touched on how they were aiming to apply the ENaCt technique to so-called "bendy" crystals, and integrating the technique into a micro ED workflow.

The first invited speaker was **Martin Adam** (Bruker), who was presenting their developments on chaperone-based crystallisation techniques. Their technique uses tetraadamantane (TAA) ethers to produce co-crystals of high enough quality to produce good structures on modern instruments. TAA chaperones produce an interesting alternative to classical crystallisation techniques for sample-constrained environments or "uncrystallisables", with the entire experiment possible to perform with no specialist equipment in one minute!

Next was an interesting talk from **Yui Wakasa** (Rikkyo), which involved crystal engineering techniques to grow crystals of highly-reactive germanium compounds. I found this talk super interesting because most crystallisation talks tend to focus on small organics/APIs/natural products etc, whereas Yui used her work on highly-reactive germylenes. She went on to discuss how her modified Trp* ligands were suitable for use in the synthesis of Ge-X (X=Chalcogen) containing compounds.

The final contributed talk was from **Jessica Metherall** (Newcastle), wherein she discussed applying the ENaCt technique to the formation of new pharmaceutically interesting co-crystals. She described the experimental methodology she created to leverage the high-throughput nature of the technique to screen large amounts of the co-crystal space using minimal amounts of compound, resulting in several previously unreported cocrystals.

Closing the session was **Helen Brand** (ANSTO), who walked us through a journey with the mineral Jarosite - an industrially relevant family of minerals. We learned how the Zn refining process requires its formation to remove Fe impurities, however, bioleaching operations need to suppress its formation in order to improve yield. These two competing needs both require an understanding into the crystallisation process of the mineral, and it was this process that Helen investigated using the SAXS technique at the Australian Synchrotron, ultimately finding that the mineral nucleates in a single-step process which is sensitive to pH and temperature. This was a very interesting session with a variety of crystallisation techniques, as well as a wide range of applications too. Crystal growth is one of the key challenges facing a lot of different industries and processes, and the work presented in the session proves that there are many talented and hard-working people on the case.

Tom Smith
Newcastle

After making the long journey to a rainy Melbourne, the conference kicked off with a fantastic opening reception. It was great to see so many crystallographers from around the world as well as lots of familiar faces from the UK. The Australian wildlife special guests were a particular highlight!

I began the first day of talks by attending the fascinating keynote from **Joanne Etheridge** (Monash) who gave a highly informative overview of using transmission electron microscopy to study functional materials. The rest of the day was spent hearing about diffuse scattering analysis in the afternoon microsymposium. Particular highlights were a talk from **Chloe Fuller** (Durham) on applying machine learning to separate diffuse components from scattering data and the talk by **Andrew Goodwin** (Oxford) on the aperiodic 'Truchet' tiling structure in TRUMOF-1.

On the second day I was particularly looking forwards to the microsymposium on phase transitions which included lots of talks on solid-state chemistry. This included a talk from **Emma McCabe** (Durham) on oxides and oxychalcogenides with layered structures and the complex structure-property relationships in these materials. **Chris Ridley** (ISIS) also discussed his work on Li_2CO_3, a significant industrial source of lithium, under pressure which he explored using neutron diffraction and density functional theory.

Another microsymposium I particularly enjoyed was on new software in powder diffraction. A wide range of new software and analysis techniques were introduced such as EasyDiffraction, a new analysis and modelling software currently being developed by **Andrew Sazonov** (ESS). **Matthew Rowles** (Curtin, Perth) also introduced pdCIFplotter for visualising diffraction data from pdCIF files. **Alan Coelho** (Brisbane) gave

a talk on new functionality in the TOPAS software which included highly informative background on least squares refinement.

Over the last half of the conference I attended a number of talks on solid-state functional materials including ionic conductors and ferroelectrics. The Inversion Symmetry Breaking microsymposium included talks from **Joachim Breternitz** (Berlin) and **Harry Lloyd** (Birmingham) on how perovskites with polar space groups can facilitate ferroelectricity. It was interesting to see how group theory could be applied to design new functional materials and several interesting discussions arose throughout the session. In the session on bond valence methods, there was a significant emphasis in the use of bond valence sum energy calculations to determine ionic diffusion pathways. The talk from **Sacha Fop** (Aberdeen) on a wide variety of proton conducting materials was a particular highlight and sparked lots of interest and discussion.

The final keynote I attended was given by **Ram Seshadri** (Santa Barbara) with the title 'How crystallography informs the design of functional materials.' He gave a fascinating overview of the broad range of functional materials including optical electronics, solid state white lighting and magnetocalorics. There was an overall emphasis on how structure can inform properties and materials design. I also appreciated his tribute to the pioneering work of Helen Megaw and Olga Kennard.

Overall, IUCr26 was a wonderful experience with some fantastic science and a successful emphasis on outreach and science communication through the 'Bragg your Pattern' project.

Ellie Dempsey
Edinburgh

I arrived in Melbourne, Australia about a week before the IUCr Congress started. It was great to have time to explore the local area and I particularly enjoyed travelling outside of the city centre to see some of the incredibly scenic beaches and meet some native wildlife, unique to Australia. I also loved the many markets around the city that showcased much of the local produce.

Before the congress officially kicked off, I attended some additional workshops which allowed me to gain hands-on experience with Bruker's new APEX5 software, while also giving me tips on how to recognise twinning or modulation from the frames of a diffraction pattern. These sessions also helped to demystify the different parameters that can be chosen during the data collection and processing stages of XRD analysis.

The opening ceremony of the congress was exceptional and demonstrated the importance of the spiritual connection that the Aboriginal peoples have with the land and water and how culturally significant this is to Australia. This welcome was directly followed by the Ewald Prize Lecture given by **Wayne Hendrickson** (Columbia) which summarised his fascinating work in developing the MAD and SAD structure solution techniques for macromolecules. In the evening the welcome reception was impressive, with a plentiful supply of food and drinks while zookeepers roamed the exhibition hall with koalas, joeys, and even a crocodile!

In the days following, the keynote talks were extraordinary. One particular highlight of mine was **Graeme Day** (Southampton), who delivered a nicely accessible talk that updated the community on his crystal structure prediction method and how this has been used as both a polymorph identification technique and a method to identify materials with promising electron transport properties.

The parallel sessions during the congress were so wide-ranging; it was incredible to find out how much work is being undertaken around the central pillar of crystallography. As someone who is keen on sustainability, I quite enjoyed the multiple talks involving lower-temperature intercalation reaction methods. In particular, the talk by **Yoshiyuki Inaguma** (Gakushuin), who explained how sealed-tube reactions can still be studied with *in-situ* XRD by using nickel, instead of quartz, ampoules due to their improved X-ray transparency.

Nearing the end of the conference, the W. H. and W. L. Bragg Prize was awarded to **Arkadiy Simonov** (ETH Zurich), who gave an incredible talk explaining 3D difference PDF maps and how these can be used to highlight some structural features that Bragg peaks alone cannot identify.

Presenting my poster during this congress gave me the opportunity to network with international colleagues and explain my field of research. This generated some useful discussions about alternative synthetic methods that may be worthwhile investigating and I received some great feedback which I can use for future events!

The congress was wrapped up with a "Night at the Museum" event which allowed everyone to relax and enjoy themselves, giving the opportunity to look around some of the exhibits, followed by live music and plenty of drinks to go around. Overall, this congress was a fantastic event, with such a great variety of work on display, and has allowed me to not only discover new options for my own research but also to explore some other exciting fields of crystallography, opening up new avenues for my future career.

Glen Hebberd
Durham

I had the delight of attending the 26th IUCr in Melbourne, Australia, this summer 2023. This prestigious conference kicked off with a terrific talk from the 13th Ewald Prize winner **Wayne Hendrickson** (Columbia) who developed the MAD/SAD methods for phasing. The conference therein covered a wide scope from AlphaFold, to a 173-protein cryoEM structure, to structure solution without phasing (!), a needle-in-the-haystack harvest-everything microED talk, XFEL and compact XFEL, 2-day membrane protein prep hacks with an anti-His antibody… this conference was fantastic!

In one crystallography talk, we were shown a glutamate-binding protein wherein the poly-glutamate tail extends out from the protein pore towards a positively charged patch that results in its cleavage – a neat mechanism! Another interesting talk was on *in vivo* crystallisation which surprisingly posed no problems for background noise and was a useful way to identify endogenous ligands. Interestingly, the intracellular compartment affected crystal size and shape. These crystals could be transferred to specialised chips and data collected in 12 minutes. When using an AlphaFold model for MR, one suggestion was to split the model into domains of high confidence and remove disordered regions then resolve from there with iterative refinement. Another discussion point was that AlphaFold models have low Ramachandran outliers which

A night at the museum of Melbourne.

is mostly great, but you should look at your plots graphically because big gaps in the secondary structure space/coordinates could indicate errors in modelling – a handy tip!

I came away from the conference feeling inspired and armed with some new ideas for my PhD project, including crystallisation techniques, SAXS, and fluorescence assay tips. The poster sessions were an excellent opportunity to engage with other PhD students at a similar stage in their career and to connect more generally. The food and drink provided throughout the conference was delicious – some of my favourites were the chocolate wall and the rendang curry. Coffee in Melbourne is also so good that Starbucks simply has not been able to take a hold there! We were all surprised to see a real live koala by the poster session. The local zoo visited the conference and we saw crocodiles, flying foxes, pygmy possums and snakes. The conference concluded with a 'Night at the Museum' party with an incredible live band performing dynamically on multiple stages, life-sized animal theatre, canopés and drinks – it was great fun!

Charlotte Manning
Reading

I arrived in Melbourne, Australia on the 20th August for the 26th IUCr congress after a flight of over 24 hours from Manchester. The IUCr is the largest worldwide gathering of crystallographers and it was my first time to attend such an international conference during my PhD. I had a fantastic experience, not only because of the thrilling presentations of the cutting-edge science and technology, but also the old and new friends that I met and made there.

Numerous pre-congress workshops were offered for attendance on the 21st and 22nd preceding the opening of conference. I attended "Olex2" and "Using the CSD to go from data to discoveries", learning how to use the software and picking up some useful tips through practical experience. The official opening started in the afternoon of the 22nd with the 13th Ewald Prize lecture given by **Wayne Hendrickson** (Columbia), followed by the amazing welcome dinner with the oyster buffet and other delicious Australian food. At the dinner, a Koala, baby kangaroo and other indigenous animals from the zoo were introduced, generating excitement from the attending researchers.

The meeting programme came after, spanning the next seven days, with multiple parallel sessions. I was inspired by several

*Bursary winner and IUCr26 presenter **Yichun Shen** (Manchester).*

plenary and keynote speakers. The talk impressed that me most was about exploring energy landscapes of crystals for functional materials and was given by **Graeme Day** (Southampton). The crystal prediction method would be important and valuable within my system. A particular highlight for me in the session presentation was by **Yi Zhou** (Shanghai) about confirming new MOF structures through low dose electron microscopy, which offered a clue regarding the structure characterisation of my single crystals. The coffee break and poster session were also good chances to communicate and make friends with the researchers in the same field all over the world.

I was very honoured to give an oral presentation on the third day of the conference to present my up-to-date work about the solution phase aggregation in a co-crystal system. I was also pleased to find that many international researchers expressed interest in my research, talking with me after the presentation and providing constructive feedback.

There was plenty of time for well-scheduled networking events such as the congress celebration party at the Melbourne Museum on the last evening of the conference, providing a large space and more relaxing atmosphere for social networking together with exploring the museum and dancing. Additionally, the sponsor exhibition and the sponsor lunch and dinner were good opportunities to know the latest technologies and equipment from the supporting companies.

The conference closed on the 29th August, and it was an irreplaceable opportunity for me to attend before I enter the writing-up phase of the PhD programme. After the PhD, I plan to do a post-doc. The conference brought great opportunities for me in terms of knowing more about the possibilities of career choices in the field, meeting potential supervisors, and gaining inspiration for my future career.

Yichun Shen
Manchester

*The photos were kindly provided by **Robert Carroll** (Southampton), **Glen Hebberd** (Durham) and **Yichun Shen** (Manchester).*

South West Structural Biology Consortium, Southampton 2023

THE 2023 SWSBC was held at the University of Southampton from 10th - 11th July 2023. This meeting is held each year and enables structural biologists at Exeter, Cardiff, Bath, Bristol, Reading, Portsmouth, Southampton, Sussex and UCL to meet and discuss research being performed in the region. The speakers are usually selected from early career stage researchers and the meeting involves a number of training workshops organised by CCP4 and CCP-EM. The meeting was generously sponsored by CCP4, ThermoFisher Scientific, Douglas Instruments, Constant Systems, Applied Photophysics, Molecular Dimensions, Starlab, Avantor, Dectris and Mitegen. Whilst Ivo Tews was in overall charge, the bulk of the organisation was done by others in the Southampton team, namely Abigail Sudol, Charlotte Cordery, Jack Stubbs, Martin Malý and Chris Holes.

The opening presentation was given by **Max Crispin** (Southampton) and was entitled "Antibody deactivation – therapeutic opportunities." The speaker described how antibody-coated red blood cells (RBCs) have a high clearance rate when injected into normal patients with low antibody levels. In contrast, cancer patients with high antibody levels, have a very low rate of clearance. As a possible route for cancer treatment using therapeutic antibodies the team are trying to eliminate the competing IgG and are using severe combined immunodeficient (SCID) mice for these studies. The project involves crystallographic studies of antibodies and several Fc structures have been determined. Attempts were made by mutagenesis to disrupt salt-bridges and thereby reduce the tendency of the Fc region to crystallise on its own. The bacterial glycosidase EndoS and protease IdeS are also being analysed by mutagenesis and structural studies in order to develop enzymes that could be used to degrade excess host IgG in the presence of a competing therapeutic antibody. The complexes of catalytically inactive mutants of both enzymes with engineered mutant IgG Fc have been determined. IdeS encases the antibody hinge region and EndoS makes extensive interactions via its carbohydrate binding modules (CBM's) with the Fc oligosaccharide in a 'flipped-out' conformation.

Max Crispin (Southampton) presenting the opening lecture at the 2023 SWSBC in Southampton.

The first session was chaired by **Martin Malý** (Southampton) and began with a lecture by **Aaron Wall** (Cardiff) who spoke on "Cross-recognition of bacterial and preproinsulin peptides by HLA-A*24:02-restricted T-cell receptors in type 1 diabetes." The speaker covered the T-cell mediated killing of β-cells of the pancreas in diabetes and how this might be an autoimmune response triggered by pathogens which happen to possess peptides similar to those of the host cells. The speaker described the use of *E. coli* to express the T-cell receptor 4C6 and HLA-A24 separately, both of which required refolding. Prior screening studies had identified a peptide with 5μM affinity for 4C6 and seeding allowed its co-crystallisation with 4C6 and A24. An Arg-Leu sequence within the peptide formed most of the contacts with a helix in the HLA molecule. Bioinformatics screening of bacterial genomes to identify those that might possess similar peptides is in progress. This talk was followed by a presentation entitled "Structural investigations into antibiotic hydrolysis by the KPC-2 β-lactamase" which was given by **Catherine Tooke** (Bristol). Catherine emphasised that antibiotic resistance is predicted to be a bigger cause of death than cancer by 2050 and went on to review the different classes of β-lactam. The use of inhibitors of β-lactam degrading enzymes (β-lactamases) is a verified means of overcoming antibiotic resistance. However, the enzyme mutates a lot, allowing pathogens to acquire resistance to a given antibiotic. The speaker described her work on the high resolution crystal structures of carbapenemase from *Klebsiella pneumoniae* with a range of β-lactamase inhibitors bound. This facilitated molecular dynamics studies as well as QM/MM simulation of the reaction mechanism, which involves the catalytic serine residue forming a stable acyl-enzyme intermediate. Her work shed light on the enzyme's relative efficiency in breaking down different possible tautomeric forms of the intermediate, thereby ruling out one possible reaction pathway. Modifying β-lactams to promote formation of the tautomer which cannot be hydrolysed may make them resistant to degradation by class A carbapenemases. Next up, **Dylan Ivory** (Exeter) gave a presentation entitled "Allosteric activation and inhibition of glycogen phosphorylase share common transient structural features." The speaker explained how glycogen phosphorylase, which catalyses the release of glucose from glycogen, is a good drug target for type II diabetes and potentially for metastatic cancer. Time-resolved experiments, using hydrogen/deuterium mass spectrometry, have precisely located dynamic structural changes in the enzyme during its regulation by both allosteric activators and inhibitors. H/D exchange of the enzyme's tower helices, which reside at the subunit interface, was found to increase in the presence of activators and inhibitors. Dylan explained how he plans to undertake molecular dynamics studies to investigate these effects further. Last but not least, the final speaker in this session, **Matilda Clark** (Portsmouth), gave a lecture on the interesting subject of "Biophysics to bioreactors: using small scale experiments to predict enzyme activity on a large scale." Matilda's lecture covered the chemical breakdown of polyester plastics and her work on expression and redesign of plastic-degrading enzymes with the aim of discovering enzymes that could be useful environmentally for recycling of plastic

The core of the SWSBC organising team in Southampton: ***Martin Malý, Charlotte Cordery, Abigail Sudol*** *and* ***Jack Stubbs****.*

The SWSBC local organising team: ***Daniel Burns, Hayden Fisher, Anjala Gammanpila, Isabel Elliott, Charlotte Cordery, Abigail Sudol, Jack Stubbs, Chris Holes*** *and* ***Martin Malý*** *(all Southampton).*

pollutants. Differential scanning and isothermal titration calorimetry (DSC and ITC) were used to determine the denaturation temperatures (T_m) of the expressed enzymes, which are typically in the 40 – 60 °C range. The effects of sequence and post-translational modifications on the stability are being analysed. The aim is to determine the optimal temperature for scaling the reaction conditions up for industrial bio-recycling.

After lunch and posters, the second session, which was chaired by **Abigail Sudol** (Southampton) began with a lecture by **Mathew McLaren** (Exeter) entitled "*In situ* structure of a dimeric hibernating ribosome from a eukaryotic intracellular pathogen." The speaker described cryoEM tomographic studies of the microsporidium *Spraguea lophii*. Microsporidia are parasites of all animals and generally have dimensions in the 1 – 4 µm range. They form single-cell spores which are stable for months on end and are spread by being ingested. The spores have an internal highly coiled 'polar' tube that is 150 nm thick and is injected into the host cell during an infection. The ribosomes on the inside of the polar tube followed by the rest of the spore's contents pass through the tube and into the host cell. A tomographic study of the polar tubes at 14 Å resolution showed that they are very rich in ribosome dimers (100 S) which are associated with the endoplasmic reticulum. It is suspected that this dimerisation is necessary to maintain the ribosomes in an inactive state while the spore is dormant. The speaker described spectacular EM studies of the monomeric ribosomes at 2.3 Å resolution and presented a model of the 100 S dimer which suggested that proteins eS12 and eS31 are involved in dimerisation. The speaker concluded by describing some focussed ion beam studies which suggested an eversion model for germination of the spore. The next lecture was given by **Mohinder Pal** (Sussex) whose title was "CryoEM structure of the R2TP chaperone and its role in macromolecular assembly." The speaker explained how R2TP forms a 500 kDa chaperone complex with HSP90, a heterohexameric AAA+ ATPase, which is required for the folding and stability of many other protein complexes and is essential for cell survival. R2TP requires additional protein co-factors in order to stabilise specific targets, e.g. TTT is required for it to act on mTOR kinase. Studies of the human and yeast chaperones have shown that in the 800 kDa complex of R2TP with TTT, it is the kinase domain of mTOR which is recruited by the TTT adaptor, although it retains kinase activity in the complex. Mohinder described many additional EM studies of the interactions with adaptors and the conformational changes during ATP hydrolysis. The next speaker, **Emma Buzzard** (Exeter) gave a prize-winning lecture on the subject of "CryoET for investigating the role of respiratory chain organisation in health and disease." The speaker described the electron transfer complexes of the inner mitochondrial membrane which assemble to form a higher order super-complex known as the respirasome. Ageing, cancer and degenerative diseases such as Parkinson's are associated with a decrease in stability of the respirasome. Emma described experiments using RNAi technology to artificially reduce respirasome stability in the worm *C. elegans* by knocking down an accessory subunit of complex I which normally allows it to interact with complex III. EM showed that the knockdown, which gives rise to impaired respiration, development and reproduction, was associated with aberrant cristae. More detailed studies of the ATP synthase by EM and fitting of an AlphaFold model of the structure suggested that the dimer angle is related the diameter of the crista. The following talk entitled "CryoEM structure and AlphaFold modelling of slipper limpet hemocyanin" was given by **Mark Young** (Cardiff). Like all arthropods and molluscs, the sequential hermaphrodite slipper limpet (*Crepidula fornicata*) relies on hemocyanin for transport of oxygen. The *C. fornicata* protein consists of decamers as well as di- and tri-decamers of a 350 kDa subunit. Each subunit consists of 8 functional units, each containing a copper centre for binding oxygen in which the O_2 molecule is held between two copper ions, each coordinated by 3 histidines. The EM structure of the protein has been solved at resolutions of 7 Å and 4.7 Å for the di- and tri-decameric forms, respectively, by fitting an AlphaFold model derived from transcriptome data for this organism. The decamers form partially capped cylinders which can form higher order assemblies and are heavily glycosylated. The next talk was by **Anil Jamithireddy** (Exeter) who spoke on "Exploring the catalytic core of yeast DNA-polymerase ε." The speaker explained how this enzyme has high replication fidelity and is the major polymerase in eukaryotes. Anil described the fingers, palm and thumb domain structure of the enzyme which has an iron-sulphur cluster involved in connecting the domains. The mutational removal of the 4Fe-4S cluster severely affects the polymerase activity but not the exonuclease activity. Anil's project is based on using thermofluor assays to determine the best metal ions to capture complexes with oligonucleotides. Last but not least in this session, **Hassan Akram-Sheikh** (Molecular Dimensions) gave a presentation entitled "New and exciting updates from Molecular Dimensions" describing items in their product range which assist with peptide and protein production, as well as the Shotgun crystallisation screen which is derived from conditions reported in the PDB, the Morpheus Fusion additive screen and the CSalt screen of 22 different salts.

After much-needed coffee, the final session of the day, chaired

by **Charlotte Cordery** (Southampton), began with a talk entitled "Time-resolved serial crystallography at I24" which was given by **Sam Horrell** (DLS). Sam explained how this beamline which is intended for microcrystals has two sets of focussing mirrors giving a 7 µm beam size with a flux of 10^{12} photons per second. The beamline has grid- and helical-scan capabilities and can do SAD and MAD, as well as uv/vis spectroscopy and serial crystallography. A slurry of 10^7 to 10^8 microcrystals per ml can be sealed between two Mylar films for serial work. Sam gave examples of 70 year old crystals of nudivirus being analysed by this method as well as time-resolved studies involving rapid mixing and light activation. The following speaker, **Christian Orr** (DLS) gave a presentation entitled "The Diamond standard: exploring unique beamline resources at DLS" in which he initially emphasised the long-wavelength capabilities of the *in vacuo* beamline I23. This can operate at wavelengths up to 2.9 Å and allow K-SAD phasing as well as work on S, Cl^- and Ca^{2+}. The speaker then introduced the VMXm micro and nano focus beamline which operates at 7 – 22 keV with a beam size of 0.4 – 10 µm. CryoEM grids are used to mount the samples. Christian concluded his lecture by outlining the VMXi crystallisation factory. The next lecture on "Sample delivery techniques to perform time-resolved serial crystallography at the XFEL Hub of DLS" was presented by **Anastasya Shilova** (DLS). Anastasya described the range of sample preparation techniques for XFEL studies including the use of chips which are filled with 4 µl of protein by a piezoelectric injector and the use of plastic tapes to introduce samples into the beam. The speaker described a time-resolved XFEL study of the binding of avibactam to β-lactamase which was shown to be complete within 2 ms. Next up, **Pedro Nunes** (DLS) presented on the subject of "The high-energy electron crystallography instrument: a tool for macromolecular structure determination" describing the HeX1 instrument which is under development at DLS. Pedro explained how electrons interact with matter more strongly than X-rays by a factor of 10^6 and are sensitive to the Coulomb potential rather than the electron density, as well as being good at locating hydrogen atoms which are elusive to X-rays. The instrument being commissioned is a 3 m long Cockcroft-Walton generator – a device which generates a high DC voltage from a low-voltage AC or pulsed DC input. The final talk of the day was given by **Ivo Tews** (Southampton) who pointed out that cryoEM is rapidly overtaking X-ray crystallography for determination of novel structures. Ivo also outlined some of the very interesting developments in the CCP4 software suite to do with generating restraints for ligands and carbohydrates as well as validation of structures. The newly-developed web-based version of Coot, known as Moorhen, was also described. This marked the end of the scientific programme for the first day and delegates then relocated to the Dancing Man Brewery in central Southampton for the excellent conference dinner. To the credit of the organisers, this involved a novel system for exchanging places that encouraged some very valuable cross-talk between members of the participating groups.

Bright and early the following morning, the first session was chaired by **Isabel Elliott** (Southampton) and began with a prize-winning lecture by **Rosie Mundy** (Cardiff) entitled "High resolution structure of HAdV-D10 determined by cryoEM." Rosie described how human adenoviruses cause a wide range of infections, are icosahedral and have a dsDNA genome. The D10 serotype causes mild ocular infections and has low seroprevalence suggesting that it may be useful in oncolytic virotherapy or vaccine development. The viral capsid consists of hexon assemblies with prominent, projecting fibre-knob structures at the penton vertices. A mutant form of the virus containing an A20 peptide from FMDV has been engineered by inserting the peptide into an exposed loop of the fibre-knob protein. The A20 peptide specifically binds the αvβ6 integrin which is expressed in epithelial cells and is a cancer-specific antigen. The 3.3 Å resolution structure of the engineered capsid has been determined by cryoEM along with a lower resolution structure of the fibre-knob. Currently transcriptomics experiments are underway to assess the safety of the virus for immunotherapy. Next up, **Becky Connors** (Exeter) spoke on how "CryoEM of the f1 filamentous phage reveals insights into viral infection and assembly." Becky described work on a shortened nanorod form of the M13 phage which is highly amenable to cryoEM. M13 itself is of interest in phage display screening and phage therapy of bacterial infections when antibiotics fail due to resistance. Use of the EBIC facility at DLS has yielded structures in the resolution range of 2.6 to 3.0 Å giving a complete model of the 80 nm nanorod, shedding much light on binding of the phage to the F-pilus during infection and packaging of the viral DNA during assembly of new phages. The next lecture on "Understanding the breakdown of enmetazobactam by the extended spectrum β-lactamase GES-1" was given by **Michael Beer** (Bristol). The structures of different forms of the β-lactamase inhibitors enmetazobactam and tazobactam bound to the GES-1 enzyme have been determined at high resolution by soaking crystals of the enzyme with each inhibitor for different times. Several breakdown products have been identified including the initial covalent intermediate and the occurrence of a lysinoalanine crosslink that can form with other β-lactamases has been ruled out. **Kyle Gregory** (Bath) then spoke on "Serendipity in crystallography" with respect to studies of two enzymes: botulinum neurotoxin (BoNT) and angiotensin converting enzyme (ACE), both of which adopted two crystal morphologies in the same growth conditions. BoNTs initially bind to polysialoganglioside at the nerve terminal where they are endocytosed and, being metalloproteases, they cleave SNARE proteins thus stopping neurotransmitter release and ultimately causing paralysis. The structure of a complex of BoNT with the receptor ganglioside has been determined revealing a Lys-Cys redox switch. The ACE enzyme consists of two metalloprotease domains with subtly different functions, the N-terminal domain being specific for bradykinin and the C-terminal domain for angiotensin II. The speaker described the structure of an ACE inhibitor complex which exhibits an open conformation due to movement of the lid domain. This session was followed by coffee and posters prior to the CCP4, CCP-EM and SAXS workshops which were run by **Martin Malý** (Southampton), **Tom Burnley** (STFC) and **Rob Rambo** (DLS).

Following lunch, **Jack Stubbs** (Southampton) chaired the first afternoon session which began with a presentation by **Patrick Shaw-Stewart** (Douglas Instruments) entitled "Sample preparation for routine and advanced structural biology, including serial data collection, microED and cryoEM." The speaker described the random microseed matrix screening method which can be carried out in microbatch and is easy to scale up. Patrick also described screening methods using dynamic light scattering to identify optimum conditions for cryoEM studies in which the protein should be monodisperse rather than aggregated. Following this talk, **Brooke Wain** (Portsmouth) gave a lecture entitled "Enzymatic degradation of crystalline polyethylene terephthalate (PET): discovery, engineering and structural characterization of novel plastic-degrading enzymes." The speaker emphasised the environmental problem of decades of accumulated plastic waste and the requirement for efficient bio-recycling strategies.

The intensely captivated SWSBC 2023 audience.

*Prize winners **Rosie Mundy** (Cardiff), **Emma Buzzard** (Exeter) and **Jack Stubbs** (Southampton).*

Enzymes which degrade PET, known as PETases, have great potential in dealing with this problem but are not able to act on crystalline PET which is generally more abundant than the amorphous form. Like all PETases, the enzyme studied, SfCut, is a cutinase consisting of a carbohydrate binding module and a catalytic serine esterase domain with a connecting linker region. The speaker described DNA screening and machine learning studies to identify the best enzyme for activity on crystalline PET as well as bioreactor work for scaling up to an industrial setting. **Bruce MacLachlan** (Cardiff) then gave a lecture entitled "Understanding the HLA class-II peptide presentation platform and its role in anti-SARS-CoV-2 T-cell memory." The speaker described structural studies of a class II HLA molecule with a variety of peptides derived from SARS-CoV-2 and demonstrated how the omicron variant evades recognition by the T-cell receptor due to mutations, one of which induces a frame shift in the binding groove of the receptor. This session concluded with a presentation by **Jemma Roberts** (Applied Photophysics) entitled "Orthogonal spectrometry – systems for analysis of protein stability and structural changes." Jemma's talk covered a range of techniques including CD and high throughput differential scanning fluorimetry (DSF) which can be used with small volumes to find optimum buffer conditions for protein stability or thermostable mutants using intrinsic protein fluorescence only.

The final session of the meeting, entitled "Electron diffraction" and chaired by **Ivo Tews** (Southampton), began with a presentation by **Simon Coles** (Southampton) on the subject of "Electron diffraction at the National Crystallography Centre." Simon began by describing some of the innovative techniques in use at the NCS and how the recent award of funding for a Rigaku electron diffractometer with a hybrid pixel detector will allow work on nanocrystals. ED data are collected by continuous rotation with this system, typically within 60 seconds. Although this is an exceptionally powerful technique, Simon emphasised that developments in the dynamical theory of ED will be required to achieve merging statistics that are comparable to those of X-ray studies. This is due to the fact that electrons interact so strongly with matter that multiple scattering becomes very significant. The next lecture was given by **Tarik Devron** (STFC) and was entitled "Software development for ED in macromolecular crystallography." The speaker emphasised that since the electron-atom interaction is a Coulombic one, current ED studies required adaptation of the X-ray form factors by the Mott-Bethe theory. Although this treatment allowed many structures to be determined by ED, further improvements stemming from the use of dynamical theory have allowed hydrogen atom positions to be determined experimentally. The speaker described the challenges of extending the theoretical work to macromolecular studies. The final speaker in this session, **Nick Harmer** (Exeter) gave a presentation entitled "Using microcrystals for structural biology: an unexpected journey." The speaker described the applications of microED and serial crystallography methods from an enzymologist's perspective, focussing on heptose isomerase from *B. pseudomallei*, which is a tetrameric enzyme that exhibits half-of-sites cooperativity. The speaker described efforts to obtain a microcrystalline sludge by a process of reverse crystal optimisation in order to pursue synchrotron serial crystallography studies at VMXm (DLS) and ID29 (ESRF). The best results were obtained by squeezing the microcrystalline sludge between layers of plastic film. This allowed the crystals to be soaked with substrate and the structures of the enzyme with substrate and product bound determined by varying the soak time.

The closing lecture of the symposium was given by **Phil Williamson** (Southampton) and was entitled "How does a neuro-inflammatory environment influence the onset and progression of neurodegenerative disease?" The speaker covered the deposition of Aβ fibres which occurs during calcium dyshomeostasis and went on to describe synchrotron CD and solid-state NMR studies of S100A9, a calcium-binding protein involved in inflammation and the immune response. S100A9 is amyloidogenic itself and promotes the formation of amyloid fibres in other proteins such as Aβ and α-synuclein. The use of insensitive nuclei enhanced polarisation transfer (INEPT) experiments to investigate mobile elements in fibrils was described along with studies of the influence of S100A9 on the polymorphism of α-synuclein by solid state NMR and EM. Phil gave an amusing ending to his lecture by briefly describing solid state NMR studies of fruit fly eyes expressing the amyloid protein tau. After questions, Phil masterfully brought the meeting to a close with the award of lecture prizes to **Emma Buzzard** (Exeter) and **Rosie Mundy** (Cardiff) along with poster prizes to **Adam Cutts** (Cardiff) and **Jack Stubbs** (Southampton). Special thanks were given to the local organiser **Ivo Tews** as well as to **Martin Malý** and **Chris Holes** for undertaking the bulk of the administration of the symposium.

Jon Cooper
UCL

I thank Martin Malý for the photographs.

Down Memory Lane

Staying on the crystallographic track with an answer to last issue's puzzle

IN the previous issue, I posed the question: "Which British scientist completed a PhD in what is now a rapidly advancing diffraction technique that was covered in the June issue, before going on to write a textbook on the subject and, in later life, becoming both the frontman and scapegoat for major infrastructure changes across the UK?"

The prize again goes to **Philip Bradfield** (Edinburgh) who replied 100% correctly within days saying: "The historical question has the answer: Richard Beeching who had been a proper scientist before leaving the tracks." Beeching's text book entitled "Electron Diffraction" was published in 1936 in the "Methuen's Monographs" series. Philip also mentions that "These little books are worth collecting, as also are those in the "Oliver and Boyd" mathematics series."

I realised that my quiz question was slightly disrespectful to someone who had both a brilliant scientific background and who went on to reach the lofty heights of corporate management, as well as gaining a life peerage. So let us try to redress this imbalance. Richard Beeching (1913 - 1985) obtained a first class degree in physics at Imperial College London where he then completed a PhD in 1936, having worked under the supervision of the Nobel laureate George Thomson whose own father, J. J. Thomson, another Nobel laureate, is credited with being the first to discover the electron. At this point I must accredit Wikipedia, with all of its wonderful clickable cross references, as my main source of information here. During the war, Beeching worked as a senior engineer in armaments and in 1948 he joined ICI, becoming Technical Director of the board in 1957. In 1961 he was given 5 years leave from ICI to become Director of the British Railways Board with the same salary that he had received from ICI – about 10 times the average UK house price at the time. His remit was to make the railways profitable at a time when their losses had trebled in the previous 3 years. In 1963 he published a report entitled "The Reshaping of British Railways" which proposed the closure of over 2000 stations and 5000 miles of track. In 1965, his next report proposed that less than half of the existing railway network should receive funding for further development. This subsequently proved to be a year of mixed blessings for him since on the one hand the new Labour government claimed in Parliament that he had been dismissed (something he denied) while on the other hand it gave him a life peerage and allowed him to return to the ICI board. He later pursued a succession of top-flight management roles in industrial, financial and legal circles.

Opinions amongst train buffs are highly polarised – while many say he ransacked the network, others say that he heroically saved the UK's rail system. The most succinct and balanced assessment of his work on the railways that I could find easily is given in an article[1] on the Network Rail website entitled "Dr Beeching's axe" and I have attempted a summary of this account. The key points are that whilst there was controversy on how Beeching's team collected data that would decide the fate of the railways, his report provided the first country-wide view of what was by then a nationalised industry. Following publication of the report, there was huge pressure for action and ultimately it was the successive governments of the 1960's and early 70's who decided which services were to be closed down. Many lines and stations targeted in Beeching's report were saved whilst others not shortlisted by him were nonetheless withdrawn. Some lines which had loss-making passenger services, remained open for freight, at least for some time. On the plus side, closure of less used local and rural branch lines removed bottlenecks and allowed growth of the popular inter-city services. Nevertheless, to the editor, closing stations in major towns with populations in excess of 50,000, such as Dudley, does seem a little extreme. As my final comment on the Beeching era, it is perhaps not surprising that, as an Imperial College man, he closed the direct line between Oxford and Cambridge.

Part of a cartoon by ***Michael Cummings*** *entitled "Talking of bottlenecks..." that was originally published in the Daily Express. It shows former electron diffractionist but, by then Director of the British Railways Board, Dr Richard Beeching. This image is in the Science Museum Group Collection (object number: 1980-7425) and is available under a Creative Commons BY-NC-SA 4.0 Licence.*

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Moving away from the railways, but still on a historical theme, one of my scientific heroes is the late A. D. Booth (1918-2009) who made absolutely pivotal developments in the subject of crystallographic refinement in the 1940's before changing track, although not quite as spectacularly as Beeching did, and moving into the computer science field. Booth was a brilliant mathematician who had completed a PhD with Gordon Cox (later Prof Sir FRS, with numerous military honours) in Birmingham on the refinement of crystal structures of explosives during the second world war. Booth's subsequent recruitment by J. D. Bernal to his laboratory at Birkbeck College in London is touched on by C. H. Carlisle in his unpublished memoirs: "Serving my Time in Crystallography at Birkbeck: some memories spanning 40 years, 1938 - 1978" (c/o Birkbeck College Library). The following is a very slightly shortened and reworded version of Carlisle's account. It is clear that whilst Carlisle had a huge respect for Booth's exceptional abilities, there are signs that questions over whose research projects, computing needs, sand castles, etc, were most important, might have slightly strained their relationship!

"I would like to say a few words about Andrew Donald Booth and his contribution – or as it turned out, his lack of it – to our need for computers in our crystal structure determination work, particularly on viruses and proteins. Booth was undoubtedly an enthusiastic and affable character, very energetic and hard-working and, in some respects, ahead of his time in

some of his ideas. The results of his efforts and foresight in developing his own section, without doubt led the College to start a Department of Computer Science, so successfully run by its first Professor, one of Donald's former students, Peter King, and I regard this as a tribute to Donald. In my remarks about him, I confine myself to the relevance of his researches to the crystallographic side of the Research Laboratory in Torrington Square. For instance, I would mention his acquisition of a computer from International Computers and Tabulators (ICT, later ICL) for his own research which was never used by him, the attempt we made to use it after he left us, and as a result of all this, the realisation by the College, after all, that it might be to its advantage to have its own computer, but which, alas, never materialised. However, there is a little story that I would to relate."

"It was either in the Autumn of 1944 or the Spring of 1945 that Donald, a very young PhD, from Birmingham, gave a paper on refinement procedures in crystal structure analysis, at a crystallography meeting in Oxford. He talked with great authority on the subject, for such procedures were new to us and even to the old-stagers like Lawrence Bragg and Bernal, who were sitting next to each other at that meeting. In his talk, Donald went on to mention the use of computers which such refinement procedures required, which must have impressed quite a few at the meeting. It so happened that I was sitting behind Bragg and Bernal while Donald was giving his talk, and after it, with a somewhat stunned look, Bragg turned to Bernal and I heard him ask, "Who is this chap Booth?" Bernal was non-committal, for I'm not sure whether he had set eyes on Booth before either. Later, I was not surprised to find that Donald was one of the group who were invited to join Bernal's research team in August 1945."

"Donald's job, as I have said, apart from delving into the theoretical aspects of X-ray diffraction, was also to design and construct an electronic computer for crystallographic computations and for use by those more directly involved in physics research. I would repeat that it is true we never had a computer or anything remotely resembling a computer from Donald which would have been of use to us for our crystallographic calculations, but I would hasten to add that Donald was, I believe, ahead of his time in designing computers. He is supposed to have built four small valve-operated ones, very small by our requirements today; one went to Imperial College, another to British Rayon Research Limited, the third to Norway and the fourth to Physics at UCL."

"From personal recollections, Donald was fast getting out of touch with the rapid advances that were being made, by the mid-fifties, in crystallographic techniques. But he was at the same time moving fast up the ladder; one has only to go through the College Reports to see this. In 1954 he was made Reader in Computational Methods, by conferment of title. In 1958, the Computer Laboratory, as Donald's section was named, was made into the Department of Numerical Automation. (Note that the parent body, the Crystallographic Research Laboratory, which was now a part of the Physics Department, had to wait a further six years before it was given due recognition as a Department in its own right.) In another College Report (1958/59), reference is made to the testing of a program for French-English translation on the University "Mercury" computer, but it turns out that: "the machine is unsuitable for any operations other than trivial ones involved in arithmetical calculations." So Donald had moved into a new field, that of language translation by computers."

"In 1960/61, ICT made available to Donald a type 1400 computer reputed to be twice as fast as "Mercury", in recognition of "his pioneering efforts in the Computer Field, and especially for his work in mechanical translation and in promoting the study of the analysis of language." The cost of housing and commissioning this new giant in the School of Hygiene and Tropical Medicine, for there was not space for it in the College, was made possible by a grant of £10,000 from the Nuffield Foundation. In 1962, however, Donald was appointed Professor and Head of Department of Electrical Engineering at the University of Saskatchewan. The College was certainly sorry to lose him, but was left with a very large computer on its hands."

"My reason for leading up to this point was that even before I knew anything about the ICT 1400, as I have said before, I had always felt that it might be to the Crystallography Laboratory's and/or the College's advantage if we had our own computer. This feeling was strengthened all the more' when on learning about Donald's acquisition I asked him if we in Crystallography might use it. "Not on your life, Harry", said he."

After Birkbeck, Booth went on to an illustrious academic career in Canada, becoming the President of Lakehead University, Ontario until his retirement in 1978. Sadly, the model of mainframe computer that he left behind in London came nowhere near to being a commercial success for ICT, probably due to it being the last of their valve-based machines before the product line was fully transistorised. In fact, according to Roger Johnson's online article entitled "The School of Computer Science and Information Systems: A Short History" (Birkbeck, 2008), the machine given to Booth was the only one of that series ever made[2].

So given that we have looked at two diffractionists who were led away from their discipline, one by the lure of executive management and the other by the pursuit of more fundamental computer science questions, what do members advise for trying to stay on the crystallographic track?

References:

1. https://www.networkrail.co.uk/who-we-are/our-history/making-the-connection/dr-beechings-axe/
2. https://www.dcs.bbk.ac.uk/site/assets/files/1029/50yearsofcomputing.pdf

Andrew Donald Booth was Reader in Computational Methods at Birkbeck College London before moving to the University of Saskatchewan in 1962 where he became Dean of the College of Engineering. This photograph is copyright of the University of Saskatchewan (University Archives and Special Collections, A-3328) and is reproduced with permission.

Meetings of interest

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

BSG Winter Meeting 2023

Date and time: Monday 11th December 2023, 10.00 am – 5.30 pm.
Venue: The Dorothy Crowfoot Hodgkin Building, University of Oxford, Oxford, OX1 3QU.

Speakers include:
Jo Parker (Oxford) – *Drug recognition and transport via solute carriers*
Xiaodong Zhang (Imperial) – *title tba*
Andrew Carter (MRC LMB) – *Cargo transport by dynein/dynactin*
Giulia Zanetti (UCL Birkbeck) – *Membrane trafficking mechanisms in the early secretory pathway*
Elton Zeqiraj (Leeds) – *Discovery of molecular glues that regulate activity and conformation of dynamic protein complexes*

For more information and registration, please visit: **https://registrations.hg3conferences.co.uk/hg3/frontend/reg/thome.csp?pageID=107555&eventID=275**.

BCA Spring Meeting 2024

Date and time: Monday 25th - Thursday 28th March 2024.
Venue: University of Leeds.

The annual Spring Meeting of the BCA brings together all four subject groups and the Early Career Stage Crystallographers group for a three-day conference in the UK.

For more information and registration, please visit: **https://registrations.hg3conferences.co.uk/hg3/frontend/reg/thome.csp?pageID=103723&eventID=267**.

Hot Topics in Contemporary Crystallography 6 – Advanced Macromolecular Crystallography Workshop

Dates: 7th - 12th Apr 2024.
Venue: Dubrovnik, Croatia.

The workshop is organised by the Croatian Association of Crystallographers (CAC).

For more information and registration, please visit: **https://htcc6.org/**.

The Zürich School of Crystallography – Bring Your Own Crystals

Dates: 17th - 29th June 2024.
Venue: University of Zurich, Switzerland.

The Zurich School of Crystallography teaches small-molecule single-crystal X-ray structure determination and consists of lectures, computer exercises and practical work.

For more information and registration, please visit: **https://www.chem.uzh.ch/linden/zsc/**.

ECM34

The European Crystallographic Association (ECA) and the Italian Association of Crystallography (AIC) are hosting the 34th European Crystallographic Meeting in Padova (Italy) 26 - 31 August 2024.

The organisers of this event are **Gilberto Artioli** (Chair), **Giuseppe Zanotti** (Co-chair) and further details can be found here: **https://www.ecm34.org**.

News from the CCDC

Data Release (September 2023) To 1.25M and Beyond

The September update of the Cambridge Structural Database (CSD) added 13,367 new experimentally determined structures, resulting in 14,166 new entries. The CSD now contains over 1.25 million structures, a significant number of these coming from BCA members. One more major data release is planned before the end of the year, it will include new entries and improvements and edits to existing entries. Find out more about our releases and if the final update is now available **here**. These newly added structures offer invaluable insights and discoveries that will contribute to advancing research in various fields.

If you are one of our thousands of contributors to the CSD don't forget to check out our social media channels in December to participate in **#CSDWrapped!**

Recent Blogs

Catalyst Ligand Design using CSD-CrossMiner

Researchers from the University of Leeds and the CCDC have developed a computational workflow for ligand discovery in catalysis with the **Cambridge Structural Database (CSD)**, as reported in ***Catalysis Science & Technology***. In this work, **CSD-CrossMiner** is used for catalyst design and development, highlighting the power and versatility of the tool that is usually used to identify lead compounds in pharmaceutical development. **Read more**.

Co-crystallization: a Tool to Tune the Pharmacokinetic Profile of Drugs

New blog based on the article "Celecoxib-tramadol co-crystal: a randomized 4-way crossover comparative bioavailability study" that investigates the pharmacokinetic profile of a co-crystal drug and compares it to its single components. **Read more**.

Upcoming Events

Visit our events page at **https://www.ccdc.cam.ac.uk/community/events/** for more details on dates and topics.

Webinar: How Rapid Assessment of Molecular Geometries Can Help the Structure-Based Drug Designer

It is well recognized that the pre-organization of a ligand into a low-strain binding conformation is a valuable objective in drug design. Mogul software from CCDC enables a rapid assessment of the geometry of a 3D model. During this webinar, John Liebeschuetz, Computational Chemist at Astex Pharmaceuticals, will demonstrate recent work using Mogul, which validates the proposition that strained or unusual molecular geometries are seldom encountered in optimized drug molecules. When they do appear, they are often indicative of a crystallographic artifact. **Register here**.

If you would like to suggest topics for our workshops, webinars, and CSDU online training modules in 2024, please email us at **hello@ccdc.cam.ac.uk**.

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Ana Machado
CCDC

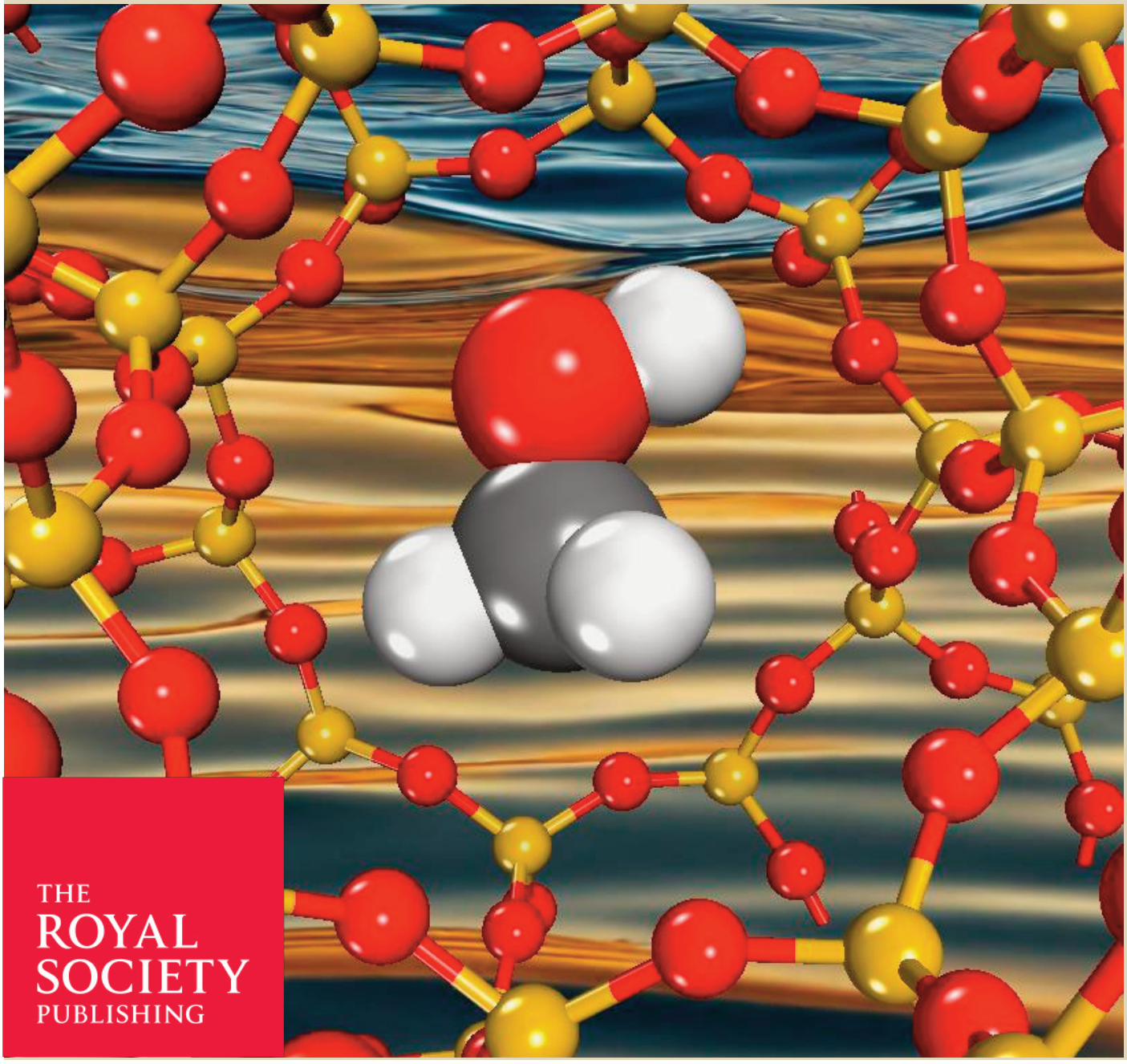
PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A

MATHEMATICAL, PHYSICAL AND ENGINEERING SCIENCES

Exploring the length scales, timescales, and chemistry of challenging materials

Theme issue compiled and edited by C. Richard A. Catlow, Chris Howard, Andrea Sella, Ana Jorge Sobrido and Martin Wilding

Part 1: published 28 August 2023
Part 2: published 11 September 2023



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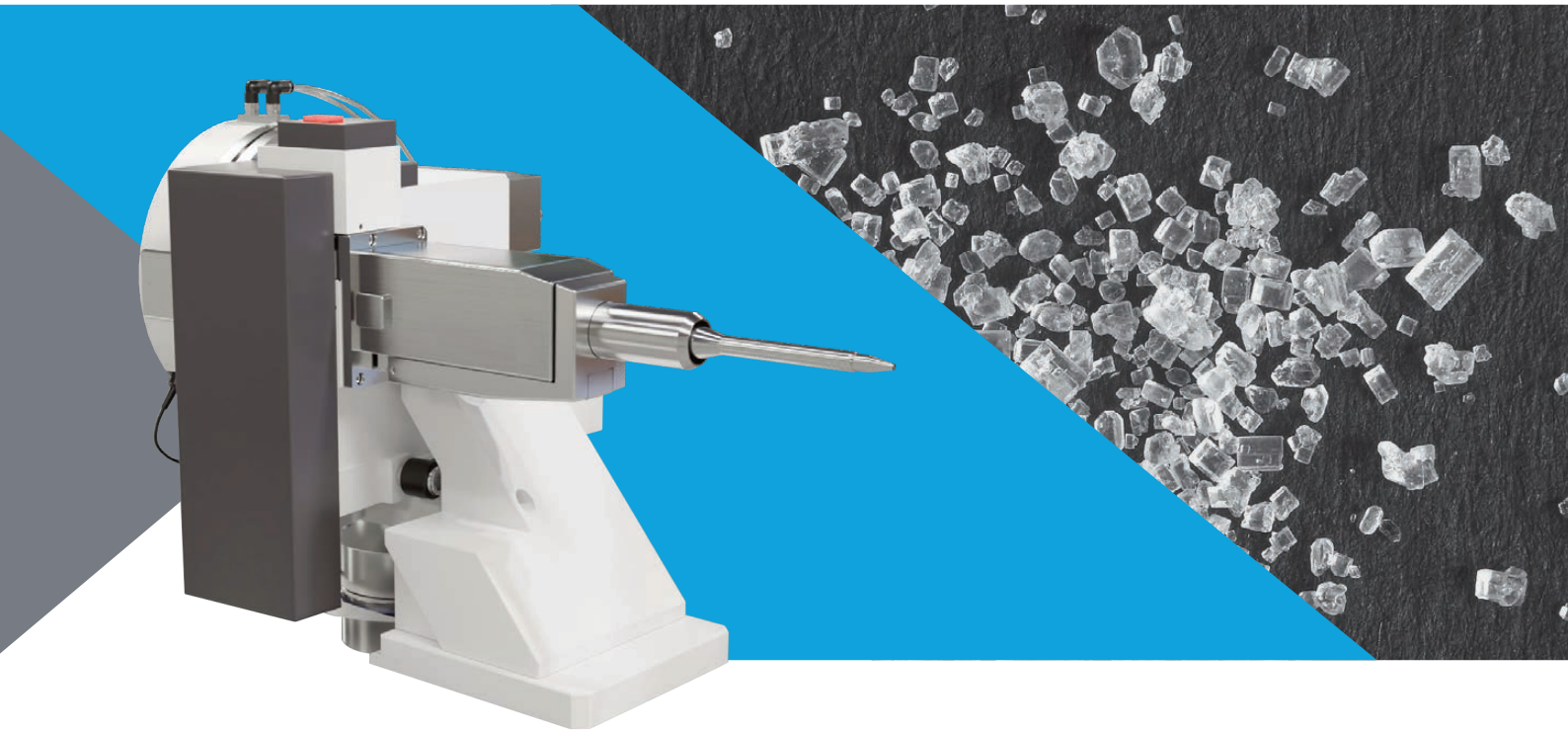

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