Crystallography News

British Crystallographic Association

Issue No. 163 December 2022
ISSI 1467-2790

Meeting reports: ECM, ACA … and isotopes!

Take the guesswork out of crystallization studies and see the results for yourself

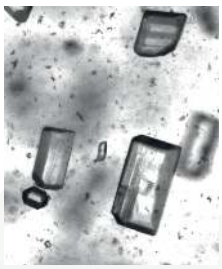
EVERY PICTURE TELLS YOUR STORY

Access crystallization and formulation information at mL scale with the Crystalline PV/RR

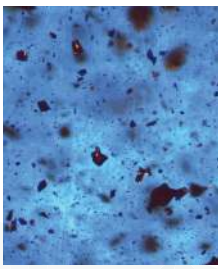
- AI-based image analysis
- Improved optics with resolution of 0.63 microns per pixel
- Advanced analytical features
- Ready for robotic integration

Crystal LINE

Visualise particles clearly with the improved front light and color camera options

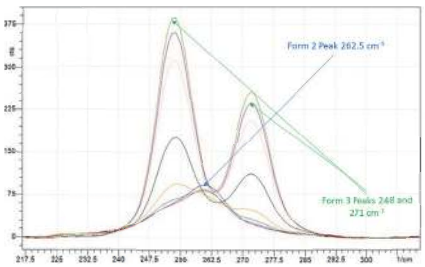


Nucleation within droplet

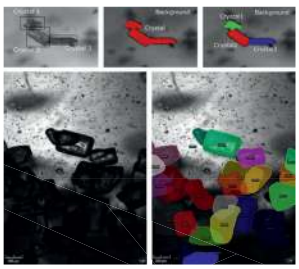


Colored particle view imaging

Use advanced analytical features such as Real time Raman



Control processes better with AI-based software analysis



Please contact us for more information
info@crystallizationsystems.com
crystallizationsystems.com
Tel: +31 72 30 200 40

Pyrietstraat 2
1812 SC Alkmaar, The Netherlands

Follow us on

Technobis
CRYSTALLIZATION SYSTEMS

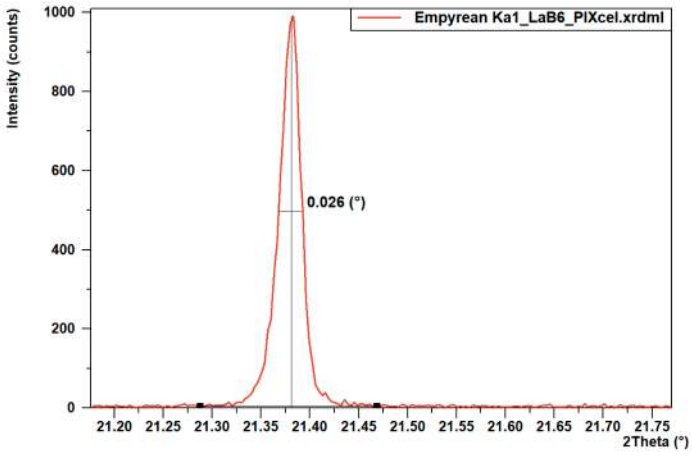
HIGH-RESOLUTION CRYSTALLOGRAPHY

scan me

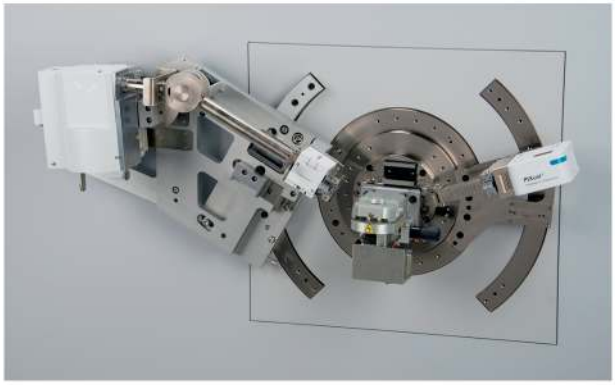
Learn More

Crystallographic analysis requires the highest quality diffraction data for accurate determination of atom positions and lattice dimensions, including:

- High resolution, expressed by the FWHM.
- Symmetrical peak shapes.
- High peak-to-background ratio.
  - Excluding scatters not related to the sample.
  - Excluding sample fluorescence by 1Der the high energy resolution detector.
- Excellent linearity of data across the 2-theta range.



The Empyrean Alpha-1 provides the highest quality diffraction data, second only to the best synchrotron beam line diffractometers.



1Der detector

www.malvernpanalytical.com/empyrean

Malvern Panalytical
a spectris company

British Crystallographic Association

Conference Bursaries 2022 and 2023

Bursaries are available for BCA members to attend national/ international crystallographic meetings in 2022 and 2023.

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

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

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

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

BCAIG

Contents

BCA Administrative Office,
4 Dragon Road
Harrogate HG1 5DF
Tel: +44 (0)1423 529 333
e-mail: bca@hg3.co.uk

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 2023 issue are sent to the Editor to arrive before 25 January 2023.

Editor: John Finney
Department of Physics and Astronomy and London Centre for Nanotechnology, University College London, Gower Street, London WC1E 6BT
e-mail: john.finney@ucl.ac.uk

Deputy Editor, Dave Allan
e-mail: dave.allan@diamond.ac.uk

The British Crystallographic Association is a Registered Charity (#284718)

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.

Printed by North Wolds Printers
83 Halifax Way, Pocklington Industrial Estate, Pocklington, York, YO42 1NR
Tel: 01759 303944
Web: www.northwolds.co.uk

This month's cover:

Images from ECM33. Credits: Léa Barbazanges (background); John Helliwell, Laura Martin, Andrea Sharpe

From the President

WELCOME to the December *Crystallography News!*

Over the summer, research integrity has been under the spotlight following the publication of a preprint 'Better Living through Coordination Chemistry: A descriptive study of a prolific papermill that combines crystallography and medicine' by David Bimler, which flagged a hoard of recent publications with potentially fabricated results, including crystallographic structures[1].

The publications in question are linked to 'papermills', which produce ghost-written papers for the benefit of a customer. The mills also organize citation pools to boost references to other publications in the pool. The papers highlighted by Bimler contain spurious citations which are unrelated to the content of the paper, and they all targeted therapeutic applications of framework materials.

It is easy to imagine that such arrangements could lack scientific rigour, and there is an implication that the crystal structures themselves are suspect. Bimler refers to "Imaginary Metal-Organic Frameworks and their wholly invented therapeutic applications" and published commentaries on the preprint have also assumed this is the case. Unfortunately, a quick analysis of one of the identified publications is consistent with this assumption: it is trivial to find a published crystal structure with identical parameters, but a carbon swapped for nitrogen in the framework linker – a highly unlikely coincidence.

Historically this type of problem is not limited to atomic resolution crystal structures: fraud has been uncovered in macromolecular structural databases. Nor is it exclusive to crystallography – examples include manipulation of IR spectra and Western blot electrophoresis images to fit the conclusions of the paper.

Gaming of the publication metrics erodes trust in both people and metrics. This may be an inevitable human response to the 'metrification' of success, and it renders metrics useless – a 2021 study found that the rank correlation coefficient of author h-index in physics with scientific awards fell from 0.34 in 2010 to 0.00 in 2019, demonstrating that surrogate targets of success cease to be useful once deployed in the real world[2].

As a consequence, the literature becomes polluted with made-up experiments, manipulated results, and conclusions. This could send entire research areas (e.g. catalysis, energy storage, gas storage, crystal structure prediction and design, etc.) off track for many years, pursuing unreproducible results or failing to explore avenues that have apparently already been exhausted.

There is cause for hope – it appears likely that at least some of the identified structures would not have made it into the crystallographic journals (IUCr) without raising some alerts due to their similarities to existing crystal structures. As a community of reviewers, editors and data users, we can be more likely to spot problems if we have some awareness of the patterns of fraud being perpetrated (see the preprint[1] and references therein). Remember that the goal of the fraud is not to deceive the world about some new material, but a much more mundane gaming of a publication metric, and it seems that is where the patterns will be found to detect these problems.

Thanks to the current BCA Nomination Committee, chaired by Claire Wilson, for supporting the work of Council by identifying and nominating candidates to serve in positions which are due to fall vacant. One candidate for an Ordinary Member of Council was nominated, and we look forward to welcoming Briony Yorke when she joins following the 2023 AGM. In addition, I am extremely grateful to Claire Naylor for agreeing to return as BCA Treasurer for another three-year term. The treasurer role is one of the most important in the Association, as they assist with the finance planning events and ensure we meet our legal and ethical obligations to continue operating as a charity.

I am also delighted to announce that the 2023 BCA Prize Lecture will be given by Professor Aurora Cruz-Cabeza from Durham University. Aurora's research focuses on developing understanding and control of the solid-state forms and properties of molecular materials, addressing phenomena such as polymorphism, solvation and desolvation, through combinations of experimental and computational studies. In addition to her frequent and enlightening scientific contributions to crystallographic meetings, she has also supported BCA events by getting involved in the organization and chairing of meetings. I very much look forward to seeing her BCA Prize Lecture presentation 'Beyond the bulk: when shall we care about surfaces in molecular crystals?' at the 2023 Spring Meeting.'

Many details of the programme of the 39th BCA Spring Meeting (Sheffield, 3rd-7th April 2023) appear elsewhere in this issue, but there's no harm in duplicating the reminder that the abstract deadline for contributed talks is 9 a.m. on Friday 20th January (see **https://hg3.co.uk/bca/**). When registering I urge you not to overlook the Young Crystallographers Group satellite meeting on the first day: the speakers and poster presenters at these sessions are mainly students and early stage researchers, but everyone is welcome to attend and support, and the depth and breadth of science presented is always excellent.

Looking ahead, Peter Moody and Hanna Kwon (University of Leicester) have generously agreed to jointly chair the Scientific Programme Committee for the 2024 Spring Meeting – planning details for that meeting will follow in future issues and the first steps to form the committee will take place at the 2023 Spring Meeting.

In our September Council meeting we decided to make an administrative change to tackle a growing problem of out-of-date contact details for our Honorary members. All benefits of Honorary membership will remain, but contact details will be confirmed each year in order to continue to receive postal copies of Crystallography News. If you believe you should receive a quarterly copy of CN but don't (how are you reading this?) please drop an email to our membership services **bca@hg3.co.uk**.

As mentioned briefly in the last issue, work is commencing to produce a short history of the BCA comprising historical articles, photographs and some new perspectives on the Association. If you would like to be involved in contributing, please get in touch (don't wait for an invitation).

Richard Cooper

[1] **https://www.researchsquare.com/article/rs-1537438/v1**

[2] V. Koltun and D. Hafner. PLOS ONE 16(6), e0253397 (2021). **https://doi.org/10.1371/journal.pone.0253397**

BCA Council 2022

COUNCIL OFFICERS

President (2024)
Prof Richard Cooper
Chemistry Research Laboratory, Mansfield Road, Oxford, OX1 3TA
president@crystallography.org.uk

Vice President (2025)
Suzanna Ward
The CCDC,
12 Union Road,
Cambridge, CB2 1EZ
ward@ccdc.cam.ac.uk

Secretary (2025)
Dr Lauren Hatcher
School of Chemistry,
Cardiff University Main Building, Park Place,
Cardiff, CF10 3AT
secretary@crystallography.org.uk

Treasurer (2023)
Dr Claire Naylor
SPT Labtech Ltd
treasurer@crystallography.org.uk

ORDINARY MEMBERS

Dr Lucy Saunders (2025)
Diamond Light Source,
Harwell Science and Innovation Campus,
Didcot,
Oxford, OX11 0DE
lucy.saunders@diamond.ac.uk

Dr Cheryl Doherty (2024)
Bursary Officer (2019-present)
GSK
Stevenage
Herts, SG1 2NY
cheryl.x.doherty@gsk.com

Dr Hazel Sparkes (2023)
Department of Chemistry,
University of Bristol,
Cantock's Close,
Bristol, BS8 1TS
Tel: 0117 331 8298
hazel.sparkes@bristol.ac.uk

GROUP REPRESENTATIVES

Biological Structures
Dr Mark Roe
School of Life Sciences,
University of Sussex,
Falmer,
East Sussex, BN1 9RQ
Tel. 01273 678863 (Office)
Tel. 01273 872896 (X-Ray Lab)
M.Roe@sussex.ac.uk

Chemical Crystallography
Dr Gary Nichol
University of Edinburgh,
Joseph Black Building,
Edinburgh, EH9 3FJ
Tel: 0131 650 4806
g.s.nichol@ed.ac.uk

Industrial
Dr Helen Blade
AstraZeneca,
Macclesfield Campus,
Macclesfield,
Cheshire, SK10 2NA
Helen.Blade@astrazeneca.com

Physical Crystallography
Dr Helen Playford
Building R3, Room 1.22
STFC ISIS Facility,
Rutherford Appleton Laboratory,
Didcot, OX11 0QX
Tel: 01235 446890
helen.playford@stfc.ac.uk

Young Crystallographers
Dr Anthony Carter
Pharmaron Hoddesdon,
West Hill Innovation Park,
Hertford Road,
Hoddesdon, EN11 9FH
Anthony.Carter
@pharmaron-uk.com

CO-OPTED MEMBERS

Programme Chair (2023)
Dr Helen Playford
Building R3, Room 1.22
STFC ISIS Facility,
Rutherford Appleton Laboratory,
Didcot, OX11 0QX
Tel: 01235 446890
helen.playford@stfc.ac.uk

EDUCATION & OUTREACH

Dr Christine Beavers
Rigaku
Christine.beavers@rigaku.com

GROUP CHAIRS

Biological Structures
Dr Katherine Brown
Cavendish Laboratory,
Department of Physics,
University of Cambridge,
J J Thomson Avenue,
Cambridge, CB3 0HE
kb518@cam.ac.uk

Chemical Crystallography
Dr Michael Probert
School of Natural and Environmental Sciences,
Newcastle University,
Bedson Building, Newcastle upon Tyne, NE1 7RU
Tel: 0191 208 6641
Michael.Probert@newcastle.ac.uk

Industrial
Dr Helen Blade
AstraZeneca,
Macclesfield Campus,
Macclesfield,
Cheshire, SK10 2NA
Helen.Blade@astrazeneca.com

Physical Crystallography
Dr Alexandra Gibbs
School of Chemistry,
University of St Andrews,
North Haugh, St Andrews,
Fife, KY16 9ST
Tel: 01334 464212
a.gibbs@st-andrews.ac.uk

Young Crystallographers
Dr Anthony Carter
Pharmaron Hoddesdon,
West Hill Innovation Park,
Hertford Road,
Hoddesdon, EN11 9FH
Anthony.Carter
@pharmaron-uk.com

EX-OFFICIO MEMBERS

Past President
Prof Simon E V Phillips
Department of Biochemistry,
University of Oxford,
South Parks Road,
Oxford OX1 3QU
Simon.Phillips@rc-harwell.ac.uk

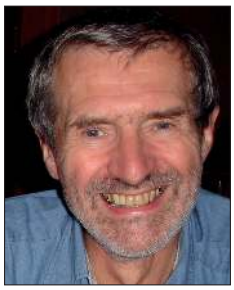
Webmaster
Dr Claire Hobday
University of Edinburgh,
Joseph Black Building,
David Brewster Road,
Edinburgh, EH9 3FJ
Claire.Hobday@ed.ac.uk

Editor "Crystallography News" Prof John Finney
Department of Physics and Astronomy and London Centre for Nanotechnology,
University College London,
Gower Street, London,
WC1E 6BT
john.finney@ucl.ac.uk

(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



THE contents of this bumper issue is good evidence that the crystallographic conference situation is – after two Covid-affected years – returning to normal. Not only does the (temporal) density of meetings of interest seem to be increasing (see the list towards the end of this issue), but in the meeting reports that make up the bulk of this issue we have pictures of real people in real places back on the crystallographic conference circuit. No more screenshots of arrays of disembodied heads staring into their computer screens!

As the summer past saw the 33rd European Crystallographic Meeting (ECM) in Versailles, you'll find several reports from colleagues who participated in the meeting. Reading them certainly made me wish I'd been there, so I hope you pick up from them something of the science – as well as getting positive vibes about the good person-to-person interactions that have been thin on the ground in the last two years. I'm also pleased we have three reports from Bursary holders (two from the ECM, one from the 72nd Annual Meeting of the American Crystallographic Association) – these underline the value of our bursary schemes to our up-and-coming young colleagues, and consequently to the health of our science.

In addition to the ECM and ACA reports, I've been (yet again?) a little self-indulgent in reporting on three meetings of particular interest to me which focussed largely on the use of isotopes in structural science. All were in-person ones, and the only thing I got infected with was good science and good fellowship! With continuing developments at central facility neutron sources, the power of isotope substitution is opening the door even wider to understanding structure and function in increasingly complex – and frequently 'disordered' – biological, chemical, and physical systems. What struck me forcibly was that this increased capability is enabling us to do serious work on complex systems of applied interest and importance that have until now seemed intractable.

This mention of central facilities and 'applied' science reminded me of a recent review, commissioned by the Institute of Physics, on the value of major UK National Science and Technology Facilities, which include the Diamond Light Source and the ISIS Neutron and Muon Source that are of particular interest to us. This independent review's conclusions are very positive. To quote from the report[1]:

> 'The findings of the review show that the UK's major national science and technology facilities provide world-leading capabilities for scientific research and technology development, and that the benefit and value of these facilities goes far beyond infrastructure, providing a hub to grow expertise and support industry. These centres of excellence, located throughout the UK, are being used by academia and industry to tackle some of the world's biggest challenges such as generating low-carbon energy, fighting climate change, improving quality of life, developing advanced manufacturing techniques, and supporting the national space strategy.'

Things have clearly moved on a very long way from the early days of the Daresbury synchrotron and the beginnings of ISIS, when us oldies cut their central facilities teeth. And remembering the two attempts to close down ISIS that we fought off when I was at ISIS some 30 years ago, this ringing endorsement was music to my ears!

There was also good news recently for AlphaFold, on which David Jones and Janet Thornton updated us in the September *Crystallography News*. One of this year's Breakthrough prizes[2] ($3 million to the winners!) has been awarded to the researchers behind this system, with Demis Hassabis and John Jumper of DeepMind being recognised for creating this artificial intelligence protein structure prediction tool.

In following up this award, I noticed that the Breakthrough Prize for Fundamental Physics has been awarded to four founders of the field of quantum information. This may not be of major interest to most crystallographers[3], but it was to me as I had worked (but – I hasten to add – not on quantum information) with one of them, Charles H. Bennett of the IBM Thomas J. Watson Research Center.

Following my first IUCr Congress (Stony Brook 1969), on the basis of a talk I gave there on random packings, I was invited to Harvard to discuss the relevance of my work to amorphous metals with David Turnbull's group. One of his team was Charles, but his schedule meant we couldn't get together before the time I was due to leave on the last train to Kingston, Rhode Island, where I was staying with a crystallographic friend and his family. So Charles insisted on joining me on the train to discuss things – despite the fact that he wouldn't be able to get back to Boston until horrendously late. The on-train discussion that followed turned out to be very useful to me, not only with respect to the average coordination number in a random close packing (not as abstruse a topic as you might think!), but it also established a relationship that led to further discussions on computer simulations of aqueous systems, and later joint publication on other work. Strange meetings can have good consequences...

One further point that came to mind in remembering Charles Bennett was that this was in the very early days of computing – you fed in a punched paper tape (or cards if it was a 'posh' IBM machine) and got out a printout of the results of the computation to ponder over. No typing on a VDU, or visualisation of structures on a screen (we were all physical model builders then!). But Charles wanted to visualise sphere packings on a screen, so wrote some code to display our models of simple liquids and amorphous metals. And in writing that, he said the most difficult thing was to program hidden line removal! How far we have come since then – think computer gaming as well as macromolecular display!

Enough of oldie ramblings. Now read on about what's been happening today in structural science!

John Finney

Footnotes:

[1] The report is at **https://www.iop.org/strategy/productivity-programme/major-national-science-technology-facilities**. And if you look carefully at the image at the top of that page, you'll perhaps recognise our Council Member Lucy Saunders at work on the Diamond diffraction beamline I11!

[2] **https://breakthroughprize.org/Laureates/2**.

[3] At least not yet. But perhaps in the future – their work may have laid the groundwork for the development of the quantum computers that might one day be of interest to crystallographers.

Puzzle Corner

Our intrepid puzzle setter thought it was about time to try a letter substitution code.

This is a short encouraging quote from Kathleen Lonsdale, originally from a talk to sixth formers:

> **"Szxsbeskos ofk jbekq f yekg wi owkteovewk vafv el mklafysfjrs. Vas loeskvelv ykwhl vafv as cfu afts vw bsvbfos lwcs wi ael lvsxl, vafv as vfysl hbwkq vmbkekql; jmv as afl kw gwmjv vafv as el cwtekq ek vas beqav gebsovewk, vafv ael mkgsblvfkgekq el qbwhekq, stsk vawmqa ev el recevsg ju ael vwwrl fkg ael whk ekvsrreqskos."**

Can you decode the letter to letter correspondence?

Solution to September's puzzle:

[The geometric mean of two positive numbers $\sqrt{(ab)}$ is always less than the arithmetic mean $[0.5(a+b)]$. Can you prove this?]

If $\sqrt{(ab)}$ is less than $(a+b)/2$,
– then $ab < (a^2 + 2ab + b^2)/4$.
Therefore $4ab < a^2 + 2ab + b^2$.
So $0 < a^2 - 2ab + b^2$
Therefore $0 < (a - b)^2$ which is clearly true for any two different* positive numbers.

QED.

*One member has pointed out that the above doesn't hold for two positive numbers *that are the same*. While apologising for not being more precise, our puzzle setter has suggested that two positive numbers implies two *different* ones – and has commented that the concepts of arithmetic and geometric means of a number with itself might be a little bizarre!

BCA Spring Meeting 2023

PLANNING is well advanced for the 2023 BCA Spring Meeting to be held at the University of Sheffield, so put the dates in your diaries! Details and titles for sessions are given below to inspire you to start thinking about contributing oral or poster abstracts.

Abstracts can be submitted at https://hg3.co.uk/bca/. The submission deadline is 9 a.m. on Friday 20th January 2023.

YCG Early Career Satellite Meeting

Monday 3 April 2023

Young Crystallographers Group (YCG)

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. It is run by fellow early career scientists.

13:00 – 13:30

YCG Opening Plenary

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

Speaker: **Mark Senn** (University of Warwick)

Symmetry assisted insights into ferric material

13:30 – 17:15

YCG Research Sessions

Contributed talks from the YCG community

Session 1 Chair: **Rebecca Clulow** (Uppsala University)

Session 2 Chair: **Josh Morris** (Cardiff University)

Session 3 Chair: **Alex Campbell** (University of Edinburgh)

17:15 – 17:45

YCG Annual General Meeting

18:30 – 21:00

Flash Poster Presentations

Session Chairs: **Phillippa Partridge** (University of Edinburgh) & **Julia Gasol 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

BCA 2023 Main Meeting Programme

Tuesday 4 April 2023

09:00 – 09:30

Parkin Lecture

Session Chair: **Aly Abdeldaim** (ISIS Neutron and Muon Source/University of Birmingham)

09:30 – 10:30

YCG Research Sessions (continued)

Session 4

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

10:30 – 11:00

Closing Plenary

Session Chair: **Lee Birchall** (University of Kent)

Speaker: **Lauren Hatcher** (Cardiff University)

Dynamic X-ray diffraction in photoswitchable materials design

MAIN MEETING

11:30 – 12:15
Lonsdale Lecture

Session Chair: **Anthony Blue Carter** (Pharmaron)

Speaker: **Kate Brown** (University of Cambridge/ University of Texas at Austin)

13:00 – 13:45
PCG Plenary

Session Chair: **Lewis Owen** (University of Sheffield)

Speaker: **Bo Brummerstedt Iversen** (Aarhus University)

XFEL Crystallography in Materials Science

14:00 – 15:30 Parallel Sessions
CCG/YCG: Crystal Growth

Session Chair: **Jonathan Foster** (University of Sheffield)

Keynote: **Katharina Edkins** (University of Manchester)

Making (the right) crystal grow

PCG/CCG: Software for Data Processing & Analysis

Session Chair: **Dean Keeble** (Diamond Light Source)

Keynote: **Jeremy Frey** (University of Southampton)

Regardless of whether you collect data on a laboratory diffractometer or at a central facility, there's a good chance an experiment performed today will take less time than the same experiment performed a few years ago. This means we're collecting more samples, more complex data, and more data points. Our ability as crystallographers to keep up with these experiments is now entirely dependent on the software tools we use to analyse our data, in many cases without supervision. This session will explore recent developments in processing and analysis software and will consider what we will need to do in the years to come to continue to exploit the ever-accelerating data collections.

BSG: Complementary Methods for Structural Biology

Session Chair: **Andrew Burnett** (University of Leeds)

Keynote: **Henrike Mueller-Werkmeister** (University of Potsdam)

The structural information and functional insight obtained from X-ray crystallography can be enhanced using complementary methods, such as optical and X-ray spectroscopies. These provide insight into a wide range of physical properties otherwise not accessible by crystallography. This session highlights the use of complementary methods in structural biology.

16:15 – 17:45 Parallel Sessions
CCG: Databases and associated tools

Session Chair: **Andy Maloney** (CCDC)

Keynote: **Matthew O. Kitching** (Durham University)

Using Crystallography and Crystallographic Databases for Selective Organic Synthesis

Crystallographic studies have provided the community with a vast number of high-quality crystallographic data, collated by organizations such as the CCDC, ICDD, and PDB. In addition to the collation and curation of these data, these organizations, alongside other individuals and groups, have provided us with a vast range of digital tools that allow us to readily analyse and extract the data we require from them. This session will highlight some high impact uses of crystal structure databases and associated software/digital tools that have provided us with a great insight into the solid state and structural chemistry.

PCG: Phase Transitions

Session Chair: **Arianna Minelli** (University of Oxford)

Keynote: **Siân Dutton** (University of Cambridge)

'Phase transitions' are in many ways an old topic that could be considered only part of textbooks. However, a lot of aspects are particularly challenging and there are still many open questions across a host of scientific fields. The aim of this session is to broadly cover these phenomena in a diverse set of systems, from chemistry to biology and from crystals to amorphous. Abstracts are invited from all areas of the community.

BSG: Dynamic Structures

Session Chair: **Stephen Muench** (University of Leeds)

Keynote: **Doryen Bubeck** (Imperial College London)

Despite the great steps we have made in solving the structures of proteins and protein complexes, we often look at proteins in a 'static' context. This session is about understanding the dynamics of proteins, from different conformational states, how protein complexes are formed and the role of dynamics in function.

18:00 – 18:45
CCG Plenary

Session Chair: **TBC**

Speaker: **Kim Jelfs** (Imperial College London)

Exploring Supramolecular Materials with Computation

19:00 – 21:00
Poster Session with Dinner and Wine

PCG Winter Meeting

The 2022 Winter Crystallography Meeting will be held on 6th February 2023 at the Rutherford Appleton Laboratory (RAL).

Registration will be free of charge and will include lunch and refreshments. Unfortunately we will not be able to offer reimbursement of travel costs. However there will be a remote attendance option for those who are unable to travel to RAL.

While it will be a slightly smaller scale meeting than previous years we are putting together a packed programme that we hope the community will enjoy!

More details will be available soon at **http://www.pcg-scmp.org/**

Wednesday 5 April 2023

09:00 – 09:45

IG Plenary

Session Chair: **Helen Blade** (AstraZeneca)

10:15 – 11:45 Parallel Sessions

CCG/PCG: Teaching Crystallography

Session Chair: **Emma McCabe** (Durham University)

Keynote: **A. M. Glazer** (University of Oxford)

Experience in teaching aspects of crystallography to undergraduates

With the significant advances in instrumentation and software, the practical aspect of using crystallography in research is far more accessible to students and researchers. The talks in this session highlight the ways in which crystallography is taught to students have evolved, as well as the aspects that haven't changed. The session gives an opportunity to present and discuss different approaches to crystallography teaching, and to reflect on strategies that will equip and inspire the next generation of crystallographers.

IG: Industrial Crystallography for Pharmaceuticals

Session Chair: **Helen Blade** (AstraZeneca)

Keynote: **Andy Maloney** (CCDC)

The use of crystallography within the pharmaceutical industry is applied in a variety of application. This session will cover practical and computational methods using crystallography to aid in drug development, developing control strategies and predictive approaches. Talks from the perspectives of crystallisation, solid form and particles will be welcome.

BSG: Science for Better Research

Session Chair: **Sam Horrell** (Diamond Light Source)

Keynote: **TBC**

New experimental methods are driving advances in structural biology, and take as much time and development as the biological questions they help to answer. This session focuses on new experimental methods and techniques that make it easier to answer important biological questions.

11:45 – 12:15

CCG Annual General Meeting

PCG Annual General Meeting

BSG Annual General Meeting

12:45 – 14:00

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.

14:00 – 15:15

Exhibitor Forum

Session Chair: **Tony Bell** (Sheffield Hallam University)

15:15 – 16:45 Parallel Sessions

YCG/PCG/CCG: Central Facilities Panel Discussion

Session Chairs: **Ben Tragheim** (University of Warwick) & **Natalie Pridmore** (University of Bristol)

A panel session where panellists will each have 10 minutes to present on opportunities and new developments at national facilities. There will be a particular focus on the instrumentation and types of experiments that are possible, and examples of exciting research being carried out because of it. Presentations will be followed by a full panel Q&A session.

IG: Industrial XRF

Session Chair: **Tony Bell** (Sheffield Hallam University)

Keynote: **Paul Bingham** (Sheffield Hallam University)

XRF analysis of feldspars and silicate glass: effects of melting time on fused bead consistency and volatilization

X-ray Fluorescence (XRF) spectroscopy is a complementary technique to X-ray diffraction (XRD) which is extremely useful in analysis of industrial materials. This session will cover the use of XRF for analysis of industrially relevant materials. Talks will be welcomed on all aspects of XRF work, done with or without the complementary use of XRD.

BSG: Science for Better Health and Wellbeing

Session Chair: **Paula Salgrado** (Newcastle University)

Keynote: **TBC**

Structural biology plays a key role in addressing the mechanisms leading to disease, and the design of new therapeutics and diagnostics. This session will focus on new advances in structural biology that lead to better health.

17:15 – 18:00

BCA Prize Lecture

Session Chair: **Richard Cooper** (University of Oxford)

Speaker: **Aurora Cruz Cabeza** (Durham University)

18:00 – 19:00

BCA Annual General Meeting

19:30 – 01:00

Conference Dinner

Thursday 6 April 2023

09:00 – 09:45

BSG Plenary

Session Chair: **TBC**

Speaker: **Simon Newstead** (University of Oxford)

Decoding the role of solute carrier membrane proteins in health and disease

10:15 – 11:45 Parallel Sessions

CCG: Powder Diffraction for Chemical Crystallography

Session Chair: **Iain Oswald** (University of Strathclyde)

Keynote: **Kenneth Harris** (Cardiff University)

Enhancing structure determination from powder diffraction through multi-technique synergy

This session will focus on the use of powder diffraction for chemical crystallography, particularly where single crystal investigations may falter, for example, *via* reconstructive phase transformations or *in situ* investigations *etc*. We welcome contributions that use multiple techniques in conjunction with Powder XRD to elucidate the structure and enhance our understanding of the solid state.

PCG: Sustainability

Session Chair: **Gabriel Perez Garcia** (ISIS Neutron and Muon Source/Faraday Institution)

Keynote: **Xiao Hua** (University of Lancaster)

The design, development and understanding of materials for improved sustainability requires the use of a variety of techniques and methods across a broad range of length scales. This session will explore sustainability in materials from different approaches, including, but not limited to, structure-property relations, methods for analysis, and novel systems. Abstracts related to the development of new data analysis and processing methodologies to investigate specific phenomena, or the investigation of local structure and its impact on sustainability, are particularly welcomed.

BSG: Computational Crystallography

Session Chair: **Keitaro Yamashita** (LMB MRC Cambridge)

Keynote: **Elspeth Garman** (University of Oxford)

Developments in computational methods and software programs underpin structural biology as a field. Further developments help us make full use of experimental data. Computational methods also streamline the pipeline of structure solution (from data collection to refinement and validation). This session will highlight developments in computational approaches to biological structural studies.

12:15 – 13:45 Parallel Sessions

CCG: Crystal Structure Prediction

Session Chair: **Louise Price** (UCL)

Keynote: **Lily Hunnisett** (CCDC)

The CCDC Blind Tests: Showcasing the triumphs, challenges, and evolution of Crystal Structure Prediction

Crystal structure prediction (CSP) is a rapidly advancing field and is one that shows great promise for thorough assessment of the solid form landscape of a molecule of interest. This session aims to highlight the use of CSP in the community, recent advances in the area as well as the current challenges encountered in the field.

PCG: Open Session

Session Chair: **Alex Browne** (University of St Andrews)

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.

BSG: 'Difficult Density' Workshop

Session Chair: **TBC**

CLOSE OF CONFERENCE

ISIS Neutron Training Course

28th February - 9th March 2023

The ISIS Practical Neutron Training Course is a hands-on course aimed at Ph.D. and post-doctoral researchers who have little or no experience of neutron scattering, but whose future research programme aims to make use of neutron scattering techniques at ISIS.

The course is free to participating students, and includes free accommodation at Cosener's House in Abingdon, and travel expenses within the UK.

The closing date for applications is imminent – 9am (UK time) on 5th December. More details are available at **https://www.isis.stfc.ac.uk/Pages/ISIS-Neutron-Training-Course.aspx**

BCA Council Elections 2022

Candidate statements

NOMINATIONS for Treasurer and Ordinary Member of Council have been received. The short CVs and statements produced by the candidates are given below.

Treasurer Candidate:

Claire Naylor

Current position:

Product Marketing Manager, Quantifoil Micro Tools GmbH, June 2020-present.

Education and Career:

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

BCA and other roles:

Industrial representative ECA Council, 2018-2021; Biological Structures Group Committee Member 2018-present; Biological Structures Group C-Chair 2019 BCA Spring Meeting.

Statement:

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

The move to industry, first to Molecular Dimensions and more recently to Quantifoil, may at first sight appear to be a step away from research. However, Quantifoil has always prided itself on working closely with academics, facilitating their research by offering the ability to customise products to researchers' requirements as well as commercialising new technologies developed in universities. In addition, I have driven Quantifoil's engagement with the community in a wider sense: participating in conferences and other events. It has been my pleasure to serve as BCA Treasurer for the last few years, and having gained experience and knowledge of the role I am keen to use that in another term. The nomination for Treasurer of the BCA Council is an honour, and I would be delighted to continue to serve the community in this position.

• • •

Ordinary Member Candidate:

Briony Yorke

Current Position:

Assistant Professor in Structural Biology, University of Bradford (2020 – present).

Education and Career:

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

BCA Related Activities:

2023 – Programme Organiser BSG at the BCA Spring Meeting, Sheffield.

2022 – Organiser CCP4 Northern Protein Structure Workshop, York.

2022 – Judging Panel 'Judith Flippen-Anderson Structural Dynamics Poster Prize at BCA'.

2021 – Present member of CCP4 Working Group 2.

2020 – Diamond I24 KMX upgrade working group member.

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

Research Interests:

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

Statement:

I am very excited to have been nominated for the position of Ordinary Member on the BCA Council. Ever since my first BCA Spring Meeting in 2010 I have felt proud to be a member of the crystallographic community. I have been inspired by my crystallographer mentors and peers to overcome adversity and be ambitious in my career. Mentorship from senior crystallographers has been transformative to my approach to not only science but to life and I am grateful for the opportunities that have been provided to me through the BCA community. In 2017 I was awarded the Parkin Lecture Prize by the YCG and in 2020 I was awarded the BSG early career prize. I am currently organising the BSG stream for the 2023 Spring Meeting and have also taken a leading role reviving the CCP4 Northern Protein Structure workshop aimed at providing post-graduate researchers with a friendly environment in which they can present their work and network with their peers. I believe that it is my duty to give back to the community that has given me so much. I will use this opportunity to provide opportunities to the next generation of crystallographers focusing on developments in time-resolved crystallography.

Biological Structures Group Winter Meeting 2022

Dynamic Structural Biology · The Crick Institute · London
Monday 12th December

Our Winter meeting is based around current research in Dynamical Structural Biology.

Protein structures are inherently flexible, and this flexibility is vital for the biological functions they perform. Researchers are now utilising cryo-EM and serial diffraction amongst other methods to understand the relationship between protein motion and activity. The meeting will provide a review of current progress in this interesting area – see **https://bsg.crystallography.org.uk/** for the full programme.

Please note that we have tried to keep registration costs low (£50 for BCA members, £80 to include BCA membership; £40 and £20 for students; £20 virtual attendance). However, if you are a student and/or young researcher and are in need to support to attend this meeting then please contact our secretary Dr Mark Roe (m.roe@sussex.ac.uk) to discuss your circumstances.

REGISTER NOW

https://www.eventsforce.net/hg3/245/register

In addition to organising meetings, a key role of the BCA Biological Structures Group is to promote the development of structural biology, particularly through supporting workshops, training and other events aimed at students and early career researchers. We receive many requests for support and profits from this meeting will be used to support as many of those events as we are able.

Many thanks to our exhibitors:
Rigaku Europe SE, Douglas Instruments, Dectris, Molecular Dimensions and SPTLabtech

Meeting Reports
33rd European Crystallographic Meeting

POSTPONED from 2021 by the Covid pandemic, the 33rd European Crystallographic Meeting (ECM) finally took place in Versailles from 23 to 27 August 2022. Several BCA members attended and participated in the meeting, and I'm grateful to the authors of the following reports for making me wish I had been there! I hope you also enjoy reading these reports, which include two from BCA Bursary holders, and a summary of the ECA Council Meeting.

Bursary Report

The journey to the ECM began with a (very) early departure from Newcastle train station, before catching the Eurostar to Paris. Transfer to Versailles involved experiencing the pre-warned stress of the Paris metro system and we arrived a few hours before the conference commenced. This was my first time in Versailles, and I could not have asked for a nicer location to have my first ever European crystallography meeting.

The conference started with the opening ceremony, including an interesting talk on the symmetry of the palace gardens. The session was then followed by the Max Perutz Prize, awarded to our very own Bill Clegg for his meritorious achievements in crystallography. The evening ended with opening drinks and the first pizza trip (of many!) to the local Italian restaurant.

The main meeting followed over the next few days and involved three parallel sessions. For me, the highlights were the sessions discussing crystal engineering with respect to co-crystallisations. During these days I also got to present a poster on the work I have been undertaking. These poster sessions not only allowed me to share my research, but also gave me a great opportunity to find out about the inspirational work going on internationally within other groups.

There was plenty of time for networking with well-scheduled events including coffee breaks after each session. The conference meal which involved a cruise along the Seine was a huge highlight of the trip and the view of the Eiffel Tower sparkling as we were getting off the boat will be unforgettable. I also really enjoyed the sponsor exhibitions, allowing me to talk to the companies about their new technologies and equipment, along with collecting my annual stash of pens.

The conference came to a close on the evening of the August 27th with poster prizes and awards, before saying goodbye to our new friends over our 3rd pizza at the local Italian restaurant. I greatly anticipate the next ECM event and I cannot wait to see everyone again soon.

Jessica Metherall
Newcastle University

• • •

Being at ECM33 Versailles

Introductory remarks

Nearly 900 participants converged on Versailles for ECM33. The Congress Centre was adjacent to the Versailles Palace, a place I had visited in 1968 on a school trip aged 15. Of course, the Palace dominated the scene as it did then. The magnificent gardens lay behind the view from the Congress Centre, but we had chance on the evening after the closing ceremony to join in viewing the fireworks event whilst listening to music and strolling in the gardens with friends and colleagues. The weather was fine and warm throughout. Within the sessions, those being careful about Covid-19 and wearing masks, included myself and to my impression most of the Italian crystallographers, at least the ones that I knew. One of my Australian friends was carrying a CO_2 monitor, where high levels were a sign of poor ventilation and thereby indicating a higher risk of SARS-CoV-2 levels. Our registrations and other detailed arrangements, hotels and so on, were efficiently managed by Hopscotch Congress Organisers. There were 27 commercial exhibitors and 6 representing the L' Association Française de Cristallographie (AFC), ECM34 Padova, ECM35 Lviv, ECA, IUCr and IUCr2023 Melbourne. At the Exhibition was a beautiful artwork entitled MICAPENROSE (figure 1).

Figure 1 At the ECM33 Exhibition: MICAPENROSE Léa Barbazanges (Avec la collaboration de S. Ravy). Credit: Léa Barbazanges. See also the short movie clip viewing this display from different angles https://www.youtube.com/watch?v=GZYfaOi1Lcw.

There were Plenary lectures: 'Fighting the enemy: understanding SARS-CoV-2 and its disease-causing mechanisms' by **Joakim Esbjörnsson** from Lund, and 'Code crack of colour diversity of inorganic pigments' by **Maguy Jaber** from Paris. There were public lectures by **Delphine Cabaret** from Paris on 'René-Just Haüy and the birth of modern crystallography' and by **Philippe Dillmann** from Gif-sur-Yvette on 'A scientific yard next to the restoration yard of Notre-Dame de Paris'. The Prize lectures were: the Perutz Prize Lecture by **Bill Clegg** (Newcastle) entitled 'Communicating crystallography', the Alajos Kalman Prize Lecture by **Eric Collet** (Rennes) on 'The key role of crystallography in the understanding of magnetic molecular materials' and the Bertaut Prize Lecture by **Lukáš Gajdos** (Grenoble) on 'Neutron protein crystallography for deciphering lectin glycan interactions involved in bacterial infection'. There were Keynotes from the U.K.: 'Diversity in crystallography: fact or fiction' presented by **Elspeth Garman** (Oxford) and 'Structural chemistry of layered hybrid perovskites' presented by **Philip Lightfoot** (St Andrews).

CCDC Workshop on Day zero.

I arrived a day early to learn about how to get the most out of chemical, materials and biological structures using the latest developments being made by the Cambridge Crystallographic Data Centre (CCDC) at their day-long workshop. This was in the University of Versailles approximately a half hour walk from the centre of Versailles. To my knowledge this was the first time that the CCDC had brought in biological structures as a topic into their learning workshops. This involved learning about the biomolecular graphics program Hermes to accompany their chemical crystal structures program of long standing, Mercury. A new product suite within Mercury called CSD-Particle was also demonstrated that enabled the rapid analysis of the mechanical and chemical properties of crystalline particles.

Microsymposium on Reproducibility in Crystallography

Chiara Massera, from Parma, and myself were independently asked to chair a microsymposium entitled 'Reliability in Crystallography'. I suggested changing this to 'Reproducibility in Crystallography' as a way of breaking down into one of several steps towards 'reliability' i.e. trust in a crystal structure. The other step being, after reproducing for oneself the calculations of a crystal structure and its publication from the deposited data, replicating with one's own study the results of the original study. These two terms are defined this way in an influential report from the U.S.A. National Academies of Sciences, Engineering, and Medicine in 2019 (see **https://doi.org/10.17226/25303**). Within the reproducibility stage the data of interest should follow the FAIR principles, namely that the data should be findable, accessible, interoperable (e.g. to different software packages) and thereby 'reusable'.

To open the session **Loes Kroon-Batenburg** from Utrecht University spoke on 'The role of archiving raw diffraction data in ensuring reproducibility in crystallography'. Loes is the Main Editor of a new section of the journal IUCrData named Raw Data Letters; the launch of this category of articles is described in the recent editorial: **https://iucrdata.iucr.org/x/issues/2022/09/00/**. The second speaker in the session was **Anthony Linden** from Zürich, who presented a talk entitled 'Reliability and reproducibility in small-molecule crystallography'. Tony had been a Main Editor of Acta Cryst. C from 2008 to 2017.

This journal, which had pioneered peer review of articles with their data, was introduced by Main Editor Sydney Hall from 1990 to 1999, and has been sustained through to the present day. The following talks, selected from the abstracts were: **Horst Borrmann** from Dresden, who spoke on 'The 'colouring' problem in the delafossite $PdRhO_2$ vanished?' i.e. as a case study; **Natalie Johnson** of the CCDC who spoke on 'Reproducibility and the CSD' and provided interesting statistics on multiple crystal structure determinations; and finally **Joanna Macnar** from Warsaw spoke on 'Analysis of common buffer molecules' conformations in ligand-protein complexes'.

There were two posters linked with the Microsymposium. **Charlie McMonagle's** (ESRF) presentation on 'Tensor of radiation expansivity – proposed measure of structural susceptibility to radiation damage' tackled the challenge of reproducibility and reliability of lattice parameters, a key concern for small molecule X-ray diffraction, for which a tensor approach was described. The poster I presented with **Genji Kurisu,** Director of the Protein Data Bank Japan (PDBj) and its own dedicated raw diffraction data archive XRDa, and **Loes Kroon-Batenburg,** was entitled 'CODATA, IUCr, PDBj collaboration for medical-protein crystal structure definitive versions of data files'.

My lecture in a Microsymposium on Teaching and Education

The microsymposium entitled 'New horizons in teaching crystallography in the 21st century' was chaired by **Annalisa Guerri** from Sesto Fiorentino, and Chair of the Gig3 Education, and **Santiago Garcia Granda** from Oviedo. I opened the session with my talk entitled 'How should we teach crystallography?'. As the opening lecture, I provided, in effect, a historical overview of the old through to the current horizons. I placed my slides at Zenodo: **https://zenodo.org/record/7027019#.Yw3Q03bMK00** and alerted colleagues via a tweet from my account **@HelliwellJohn**.

The second lecture, given by **Helen Maynard-Caseley** (ANSTO), was entitled 'Communicating crystallography to little people, the bragg your patterns project'. Details of this project, linked to IUCr2023 Melbourne, are at **https://braggyourpattern.com/** (see figure below).

The three talks selected from the abstracts were by **Berthold Stöger** from Vienna entitled 'An interactive tool to explore the two-dimensional Fourier transform'; **Maryia Fando** (Newcastle) on 'CCP4 Cloud as a system for crystallographic teaching'; **Nico Graw** from Göttingen on 'Ducks in space groups! Grasping arrangements of symmetry elements with 3D models'; this was detailed recently in his article **https://journals.iucr.org/j/issues/2022/01/00/gj5276/index.html** .

My pre–Conference Dinner talk as an ECA Past President, concerning the ECA/ECC 50th Anniversary

This double anniversary event was to celebrate the 50th year since the creation of the European Crystallographic Committee and its transition 25 years ago into the European Crystallographic Association. So, in a 45 minutes long ceremony, the past presidents of the ECA and one of the chairs of the ECC were to reminisce on their impressions of their time in office. My own time as President was 2007, when I was elected at the ECM in Leuven, Belgium, through to 2010 when I completed my term at ECM25 in Istanbul. In my three minutes allocated time, accompanied by a few slides including some of the Executive Committee members I had served with, I remarked on what an honour and privilege it felt to be able to make a British contribution to what in my view is a marvellous organisation promoting cooperation of crystallographers across Europe, Africa, and the Middle East. I commended the talented and conscientious individuals I had worked with on the Executive and in the ECM24 and ECM25 organising teams. As new initiatives I highlighted our launch, approved by ECA Council of course, of the ECA Scholarship Fund to complement the Bursary Fund for early career scientists, but to be for mid- and late-career scientists who needed financial support to attend an ECM. The session concluded with remarks by **Bill Clegg** (Newcastle), Chair of the Gig2 (Senior Crystallographers) and **Philipp Hans** from Austria, Chair of Gig1 (Young Crystallographers), as well as the current Past-President, **Udo Heinemann** from Germany and **Marijana Đaković**, from Croatia, the current President.

The ECA 25th and ECC 50th Celebration session at ECM33. [Courtesy of the ECM33 photographer, Laura Martin.] Left to right: Marijana Đaković (Croatia) the current President; John Helliwell (UK) President 2006-2009; Hartmut Fuess (Germany) President 2003-2006; Santiago Garcia-Granda (Spain) President 2009-2012; Paul Buerskens (The Netherlands) who represented the ECC and was its Secretary 1974 to 1997 (the first Chairman of the ECC was Andre Authier 1972-1975 (France); the second was Olga Kennard 1975-1981 (UK)); Claude Lecomte (France) President 2000-2003; Andre Roodt President 2012-2015; Alessia Bacchi (Italy) President 2015-2018; Philipp Hans (Austria) Chair of the Gig1 Young Crystallographers; Udo Heinemann (Germany) 2018-2021; Bill Clegg (UK) Chair of the Gig2 Senior Crystallographers. The complete list of the composition of past ECA Executive Committees can be found at http://ecanews.org/archive2019/composition-of-eca-executive-committees/

Judging the ECA Sig6 and Gig3 Poster Prizes

The ECA Sig6 Poster prize I had set up when I was ECA President, when the Vice Chairman of the Sig6 (Instruments and Experimental Techniques), Professor Jacek Grochowski, died in 2008 after a synchrotron experiment in DESY, Hamburg. I had got to know Jacek well when I was Sig 6 Chairman. He was such a fine and enthusiastic colleague on the Sig6. With funds from the SRS Daresbury and the University of Manchester (€1800), the ECA approved the Sig6 proposal for a poster prize in Jacek's memory. So, each ECM since has seen a Sig6 Jacek Grochowski memorial poster prize award. The judging panel was myself as Chair along with **Andrew Thompson** from the Soleil synchrotron Paris and **Michele Cianci** from Ancona. The winning poster was by **Emmanuel Wenger** from Lorraine on a unique diffractometer to explore the effect of electric fields on crystals. His subtitle was 'Volta crystallography'. [If you have the chance, I encourage you to visit the Volta Museum at Lake Como **https://www.comer-see-italien.com/en/gallery/volta-museeum-como_k66/**. More details on the life and scientific work of Alessandro Volta is at: **https://en.wikipedia.org/wiki/Alessandro_Volta**].

The Gig3 Education had two poster prizes. As Chair of the IUCr OUP Book Series, which has both a teaching books and a research monographs section, I organised the OUP to donate a teaching book as one of the Gig3 poster prizes. The judging panel was chaired by **Annalisa Guerri** from Florence, and members were **Teresa Duarte** from Lisbon, **Marta Morana** from Pavia, and myself. The winning poster was by Erhard Irmer from Göttingen, whose poster was entitled 'Expanding horizons – the use of crystallographic structures in high school chemistry classes'. His poster described both diffraction and interference of light waves from two slits as well as crystal structures from the CSD teaching subset. Erhard is exploring "what teachers dare to describe for their students in their chemistry classes" since "often teachers or students have little knowledge of crystallographic techniques". I made a visit to the OUP exhibit stand and consulted with **Sonke Adlung**, also my Book Series liaison at OUP, and selected 'Symmetry in Crystallography: Understanding the International Tables by Paolo Radaelli (see **https://academic.oup.com/book/2799**). I was impressed by the 'Bragg your patterns' project for schoolchildren in the talk of **Helen Maynard-Caseley** (see above) and this book's approach of "first examining simple patterns as found in architecture and art" provided a connection. But to hope for a connection in the schools to our international tables is maybe too much. We will see what Erhard Irmer makes of it in due course.

Erhard Irmer being presented with his poster prize by John Helliwell. Credit: Laura Martin

The Closing Ceremony

There were talks from **Sylvain Ravy** from the CNRS Laboratory of Solid State Physics at Orsay on behalf of the local organisers. As well as the statistics on the attendees (country of origin, gender split and overall numbers) we learnt that his son had designed the conference logo (see the cover of this issue). This had been inspired by the layout of the Versailles Palace Gardens. There were 15 poster prizes.

We had a presentation and look forward to ECM34 by **Gilberto Artioli.** It will be held in Padova, Italy in August 2024. Originally ECM34 was set to coincide with the 800th anniversary of Padova University but due to Covid-19 and postponements it will be the 802nd anniversary. The current ECA President **Marijana Đaković** closed ECM33 and orchestrated the thank you gifts for the local organisers (see figure below).

The closing ceremony at ECM33 had gift presentations to, from left to right, Sylvain Ravy, Jean-Paul Itié, Laure Della Giustina, Camille Godefroy and Andrew Thompson. Credit: Laura Martin

John R. Helliwell
University of Manchester

• • •

ECM33: A personal account

Attending ECM33 in Versailles was a very enjoyable and welcome experience after the two year dearth of 'in person' meetings. There is a huge difference between interacting with friends and colleagues face to face and just seeing panels of flat faces on a screen! Another major positive aspect was being able to renew contact with the many different companies and organisations exhibiting at the meeting.

Eurostar travel from St Pancras to Gare du Nord is fast, efficient and comfortable, but once arrived, a long and frustrating fight with a ticket machine finally resulted in a train ticket to Versailles (or so I thought). However, on arrival there I was fined €35 on-the-spot to be allowed out of the station, as I had purchased the wrong type of ticket: an inauspicious start but my only negative experience of the entire trip! I decided to walk everywhere from then on and also I made very sure I bought the right ticket for my return journey to Paris.

The conference venue was next door and to the left of the entrance to Versailles Palace, with many nearby convenient cafes and restaurants for chats and meetings with other delegates. Altogether a perfect arrangement! The 23rd August evening opening ceremony included a talk on the delights and symmetries of the gardens of Versailles Palace (see image on the cover) by the Chair of the local organising Committee, **Sylvain Ravy** (Orsay), which inspired me to make time to enjoy exploring them later in the week. This was followed by presentation of the 12th Max Perutz Prize to Bill Clegg, now Emeritus Professor of Newcastle University and well known small molecule crystallographer. He treated us to a whistle stop tour of his scientific life journey before refreshments in the Exhibition space which was spread over floors 0 and 2 of the venue.

Wednesday 24th August opened with a *tour de force* Plenary lecture given by **Joakim Esbjörnsson** from the Systems Virology group at Lund University. He gave a fascinating lecture on 'Fighting the enemy – understanding SARS-CoV-2 and its disease causing mechanisms', providing a comprehensive account of the origins and course of the pandemic. He pointed us to several reviews on the available vaccines and on the development of anti-viral drugs against the virus. He told us that a study of 12,333 bats in South America, Africa and Asia found that 9% of them carried in total 91 different coronaviruses, and that about 3,200 different types of coronaviruses can infect bats. He posed the question 'Can we stay ahead of the virus?': a very good and vital question!

As often at meetings with parallel sessions, the choice was difficult as on that first morning there were four on simultaneously that were of interest to me ('Infection and disease – hot structures', 'Crystallography in large scale facilities', 'What is inside the black box', and 'Time resolved diffraction and scattering techniques'). Opting for the first of these, chaired by **Kristina Djinović Carrugo** (EMBL, Grenoble) and **Andy Thompson** (SOLEIL), there was a range of talks on B_{12}-dependent radical enzymes (**Ahosna Benjdia,** Jouy-en-Jasas), the coronavirus structural taskforce (**Gianluca Santoni,** Grenoble), TraA, the relaxase from a gram-positive Type IV secretion system (**Walter Keller,** Graz), control of phosphodiesterase activity in RbdA (**Charlotte Cordery,** Southampton/Diamond Light Source DLS) and using crystallographic failures to identify artificial and endogenous inhibitors for plant growth and defence pathways (**Stefan Arold,** KAUST, Saudi Arabia).

At lunch time I cracked a boiled egg that I had taken from the hotel breakfast, only to find it was not hard boiled; it was raw and that I had a mess to clear up! That will teach me not to take more than I need for breakfast in future!

The first day concluded in the main lecture hall with a relaxing Baroque concert of music by Handel, Mozart, Rameau and Bach played by a select ensemble of musicians from 'Les Voyages Extraordinaires'.

Thursday morning's early Keynote was a fascinating lecture on 'Atomic resolution structure determination of

larger macromolecular complexes by cryo-EM and X-ray crystallography' given by **Holger Stark** (Göttingen). My five pages of notes on it are a testament to his comprehensive analysis of the factors that limit cryo-EM resolution, in which he started by pointing out that biochemical optimisation of sample preparation is pivotal to obtain the maximum biological knowledge. He stressed that attention should be paid to what occurs at air-water interfaces, especially for protein complexes that often fall apart. He recommended spraying the sample onto the grid and plunge freezing in 600 ms rather than blotting the grid preparation (as that takes 2 s). He then covered the resolution limitations imposed by aspects of the EM instrumentation, including optical effects which do not scale linearly with resolution and describing the specially designed EM in his laboratory.

'Structural Enzymology' chaired by **Ilme Schlichting** (Heidelberg) and **Allen Orville** (DLS) was my chosen morning parallel session. **Cathy Drennan** (MIT) talked about 'Capturing snapshots of metalloenzymes in action': since 50% of enzymes have metals of which 30% are transition metals, understanding their role is clearly very important. Cathy described their studies on carbon monoxide dehydrogenase which has a 4N-4Fe-S cluster. She was followed by **Chris Schofield** (Oxford) with a detailed account of 'Time resolved studies on oxygenase catalysis' using a wide range of methods to elucidate the mechanisms involved.

In the afternoon, after delivering my own Keynote Lecture for the next morning to the AV room, I attended an interesting talk in the 'Nucleic acids and their interaction' session on 'High resolution cryo-EM structure of a type II topoisomerase cleavage core complex with bound 18mer dsDNA' (**Shabir Najmudin,** Kings College, London).

Figure 1 Lukáš Gajdos and Ellen Fogh being awarded their EFLB prizes. Credit: Elspeth Garman

In the evening the 2022 Erwin Felix Lewy Bertault Prize of the ECA and European Neutron Scattering Association was awarded to **Lukáš Gajdos** (ILL) for his doctoral thesis work on the characterisation of lectins with sugars by neutron diffraction (see Figure 1), and he gave us a talk on his path to the results (which have now been published in Nature Comms). Lukáš is now a postdoc at the ILL and I have been part of his supervisory team since February 2021. It was a pleasure to finally meet him in person after 18 months of weekly virtual interactions! The 2021 EFLB Prize was also presented to Ellen Fogh (EPFL, Switzerland).

The next morning, Friday, I delivered my Keynote Lecture on 'Diversity in Crystallography: fact or fiction' but was sad not to be able to attend the parallel keynote by **Gisela Branden** (Göteborg) on 'XFEL- and synchrotron-based serial crystallography studies of the membrane-bound proton pump cytochrome c oxidase'.

Figure 2 Credit: Elspeth Garman

After having some individual meetings with different colleagues, I spent a really wonderful happy afternoon getting lost alone in the Versailles gardens (Figure 2) and was thrilled to see a red squirrel. I hadn't realised the hedges were at least 20 ft tall so it was very easy to completely lose a sense of direction.

The Conference Dinner for 450 people was on a Bateau Mouche travelling on the Seine through Paris (Figure 3) and was highly enjoyable with drinks on the deck in the sunset, and a delicious meal down below once it got dark.

Figure 3 Credit: Elspeth Garman

So in summary, thank you to all the ECM33 organisers for doing such a terrific job! Having been Co-Chair of ECM28 with Sandy Blake, I can well imagine what a lot of work and stress was involved to pull it off, especially with all the Covid-19 strictures and uncertainties.

Elspeth Garman
University of Oxford

General Interest Sessions at ECM33

As a member of the ECM33 Programme Committee representing the ECA Senior Crystallographers Group (GIG2), I combined forces with representatives of the Young Crystallographers (GIG1) and Crystallographic Education (GIG3) groups to propose microsymposia on educational and general interest topics. We were pleased to have a number of these in the programme, most of which I attended, and I will report mainly on these.

The opening ceremony on Tuesday was the usual succession of short welcome speeches by representatives of local government, education and research, and national and international organisations. Unusually, there were no musical or other cultural contributions except that **Sylvain Ravy** (Orsay), one of the conference organisers, spoke about aspects of symmetry to be found in the Palace of Versailles gardens (see the image on the cover), something we could explore at leisure during the week. I was honoured to give the opening Plenary lecture after this, in response to receiving the 12th Max Perutz Prize; I'll leave others to comment on that! A welcome reception followed.

On Wednesday I was the first speaker in the session 'What is inside the black box?' with a tutorial guide to some entries in International Tables Volume A, a requested shortened version of one I gave to the BCA YCG a few years ago. The aim of the session was to counter a 'black-box' automation mentality, and the other invited speaker **Petra Bombicz** (Budapest) discussed how much thought and care must be given to the interpretation of a crystal structure result once it is obtained, including aspects of intermolecular interactions, pseudo-symmetry, and solvent inclusion. **Cameron Hall** (Bristol) gave a mathematician's approach to identifying possible twin laws in an exhaustive but computationally efficient way. Another mathematical approach, the Crystal Isometry Principle, was presented by **Daniel Widdowson** (Liverpool), analysing geometric similarities and relationships among crystal structures; one consequence of this is the identification of possible errors (or even fraud) in some reported structures. Finally, in the context of recent advances in predicting protein structures with AlphaFold2, **Robert Oeffner** (Cambridge) encouraged a careful examination of the original diffraction data to avoid wrong assumptions that can be made when likelihood-based automatic procedures for solving crystal structures overlook factors such as non-crystallographic symmetry or twinning.

Undoubtedly the most frustrating aspect of this session was the small room allocated to it, with many of the would-be audience unable even to get near the door, a predictable problem encountered also for a similar session at the previous ECM in Vienna in 2019.

The afternoon educational session was entitled 'What should undergraduate students learn about crystallography?' **Christian Lehmann** (Mülheim) gave a chemist's viewpoint, with symmetry an essential component together with fundamentals of diffraction geometry, but also linking the theory with understanding and interpreting a typical short publication of a crystal structure – often this must be achieved in very limited available teaching time. **Marielle Yasmine Agbahoungbata** (Cotonou) described her approach in Benin, showing the importance of crystallography in various broader disciplines; here too the teaching of symmetry is a key component.

Jarosław Chojnacki (Gdańsk) gave an account of a Crystallographic Olympiad competition held four times so far in Poland, with entries at school and university levels; this seemed more of an encouragement through rewarded assessment of self-motivated learning rather than a teaching tool in itself, and provoked considerable discussion. **Ilaria Gimondi** (CCDC) showed how the Cambridge Structural Database (CSD) can be used in teaching, with particular reference to its freely available Teaching Subset and visualisation using Mercury to demonstrate topics such as isomerism and chirality. **Arun Royappa** (Pensacola) presented some other educational uses of the CSD in the context of a US undergraduate university without major research facilities. The session as a whole raised more questions rather than providing answers to the question of the title.

Thursday morning included another educational session, 'New horizons in teaching crystallography in the 21st century', though I would say it provided both old and new approaches. **John Helliwell** (Manchester) gave a personal reflection on 'How should we teach crystallography?', based on surveying the contents of a number of familiar textbooks and addressing in particular the question of whether symmetry should come before diffraction or vice versa – it seems opinion is divided on this. **Helen Maynard-Casely** (ANSTO) focused on communicating crystallography to younger children and their families, and described the 'Bragg your Pattern' project of Australia and New Zealand leading up to IUCr 2023. **Berthold Stöger** (Vienna) concentrated on Fourier transforms, with an interactive computing tool for the manipulation and display of two-dimensional FTs, applicable for demonstrating a range of crystallographic concepts including series termination effects and Patterson syntheses. **Maria Fando** (Newcastle) described educational use of the community-driven software suite CCP4 through its new front-end CCP4 Cloud, which is already in use in various International Schools and Workshops. The prize for transporting visual aids to ECM33 must surely go to **Nico Graw** (STFC) with his *ca* 50 cm models of some space groups produced by 3D printing and incorporating plastic ducks as the structural motif.

John Helliwell presenting his talk. Credit: Claude Sauter

Friday brought a session originally proposed as 'Reliability in crystallography' but revised to the more specific 'Reproducibility in crystallography' (perhaps future meetings will include microsymposia on the three other components of the FAIR principle). **Loes Kroon-Batenburg** (Utrecht) addressed what is perhaps the primary hot issue of the

desirability and practicalities of reliably archiving raw diffraction data in a retrievable way, together with all necessary metadata for completeness. **Tony Linden's** (Zürich) focus on small-molecule crystallography overlapped with this, but discussed also how we might assess the likely reproducibility of what is normally a one-off crystal structure result, standard validation procedures of course being part of this. **Horst Borrmann's** (Dresden) presentation on a class of mixed-metal oxides was much more specific, but problems of extreme crystal shape, high absorption, and severe extinction effects and potential substitutional disorder are commonly encountered in other compounds, if less dramatically. **Natalie Johnson** (CCDC) shared some of the concerns of the CSD in promoting reproducibility and reliability, which can be assessed to some extent from analysis of independently deposited versions of the same structure (REFCODE families). A similar consideration of the reproducibility of components of structures in the PDB was given by **Joanna Macnar** (Warsaw), well illustrated by an analysis of the conformations of common buffer molecules, some of which are clearly of poor quality.

Among plenary and keynote lectures were notably an account of crystallographic research on SARS-CoV-2 by **Joakim Esbjörnsson** (Lund), a discussion of structure-colour relationships in pigments by **Maguy Jaber** (Paris), a very personal view of diversity, mainly gender diversity, in crystallography by **Elspeth Garman** (Oxford), an account by **Delphine Cabaret** (Paris) of the life and work of René-Just Haüy 200 years after his death, and a presentation by **Philippe Dillmann** (Gif-sur-Yvette) on structural and archaeological considerations of the current restoration of Notre-Dame de Paris. Electron crystallography featured strongly throughout the meeting, both in scientific sessions and in the commercial exhibition.

I attended a number of formal business meetings (ECA Council and part of one of the Executive Committee meetings, and discussions of the three ECA GIGs, which are aiming to work more closely together). On the lighter side, there was an excellent Baroque concert one evening, a series of short semi-serious entertaining presentations on crystallographic topics in the 'Science Slam', and a magnificent conference dinner on a large floating restaurant on the River Seine in Paris, passing some of its famous landmarks. ECM-33 was certainly a memorable conference in both its location and its scientific content.

Bill Clegg
Newcastle University

• • •

Molecular crystals: from strength to strength at ECM33

The 33rd European Crystallographic Meeting was held in Versailles between the 23rd and 27th of August this year. The previous meeting took place in Vienna in 2019, before the pandemic disrupted all scientific (and other) gatherings, and the attendees were evidently quite pleased to be able to meet in person at long last (solid evidence for this in Figure 1!). Versailles is a particularly pertinent venue, given the French court's sponsorship of the sciences in pre-revolutionary times, as well as the city's proximity to Paris, which itself has a long history as a global scientific hub.

Figure 1 Finally an in-person meeting! Entry to the ECM33 venue. Credit: D-K. Bučar

The entire meeting was highly relevant to anyone with an interest in molecular crystals. The fields of organic solid-state chemistry, crystal engineering and chemical crystallography have been developing rapidly over the past two decades, but the three-year gap between Vienna and Versailles has served to highlight just how essential and commonplace techniques such as electron diffraction and facilities such as synchrotrons are becoming within our community's research programmes. I was also glad to see that the interest in molecular crystals did not appear to be limited to applied research, since so much of the literature over the last ten years has primarily emphasized applications. It was apparent that the community as a whole remains keenly interested in extending our understanding of the self-assembly processes that govern the formation of organic solid-state structures, to explore new methods for the crystallisation of functional organic solids, and to devise protocols for the formation of new crystal phases (or to recover elusive or disappearing crystal forms).

Indeed, it is very difficult to provide a complete and comprehensive summary of the meeting, since there was so much to interest a crystal engineer such as myself – and of course a lot of catching up with friends, colleagues and instrument vendors! I will not even attempt such a summary here. Instead, I will only highlight some of my own personal favourites amongst the many excellent microsymposia (MS) on molecular crystals and crystal engineering, while issuing the standard caveat that I have probably missed as many fantastic talks as I attended.

- **3D electron diffraction (MS24) and 3D electron diffraction for structure solution of organics and proteins (MS25)**

  This was an entirely engrossing session. As I am not an established practitioner or even an active user of electron diffraction (ED), the main take-home message for me was its emerging importance to crystal engineering, and indeed, to anyone interested in advancing the science of molecular crystals. Both sessions emphasised the maturity of 3D ED as a technique, the fact that it is becoming more accessible to non-expert users, and the myriad ways in which ED data is driving contemporary materials science and pharmaceutical research and development.

- **Navigating crystal forms in molecular and pharmaceutical materials (MS28)**

  The session showcased how time-resolved *in situ* diffraction measurements (and other types of analyses) can aid our understanding of crystallisation during mechanochemical reactions (**F. Emmerling**, Federal Institute for Materials Research and Testing, Berlin). It also featured a tale of serendipitous discovery: the fascinating and highly complex

structure of organic Frank-Kasper phases (**R. Montis,** University of Urbino) – see figure 2. There was also a particularly memorable demonstration of how quantum crystallography may be applied in the study of disappearing polymorphs (**M. Gryl,** Jagiellonian University).

Figure 2 Beautiful crystallography artwork shown in MS28 by R. Montis. Credit: D-K. Bučar

- **Crystal engineering: structural flexibility, phase transitions and non-standard manipulation of synthons (MS29)**

  This session highlighted the unpredictability of supramolecular synthons in molecular co-crystals (yours truly, UCL), and included a lively discussion on the role of metals as electron donors in sigma-hole interactions (**A. Frontera,** University of the Balearic Islands), a comprehensive study of how the structural flexibility (elasticity and plasticity) in metal-organic crystals can be tuned (**M. Đaković**, University of Zagreb), an overview of the manner in which non-covalent interactions dictate whether metal-organic compounds materialise as crystal or gel (**S. Bourne,** University of Cape Town), and a demonstration of how weak non-covalent interactions control the dynamic solid-state processes in peptoids (**C. Tedesco,** University of Salerno).

- **Unconventional interactions or symmetries for optimized and new properties, including chirality (MS31)**

  The session featured an in-depth consideration of non-covalent intermolecular bonds, including experimental studies of sigma-hole interactions (**G. Resnati,** Politecnico di Milano) and n→π* charge transfer interactions (**K. Molčanov,** Ruđer Bošković Institute). Also presented were a computational study of interactions involving aromatic moieties (**S. Žarić**, University of Belgrade), experimental findings on the interactions in substitutional solid solutions (**M. Lusi,** University of Limerick) and combined experimental and computational studies of lattice defects in molecular pigments (**M. Schmidt,** Goethe University Frankfurt).

- **Supramolecular recognitions (MS33)**

  This session consisted of a series of outstanding presentations, including one on how to identify and employ robust supramolecular synthons to create complex supramolecular structures in molecular crystals (**A. Lemmerer,** University of the Witwatersrand). Another highlight of the session was a talk on cutting-edge investigations of supramolecular recognition processes in solutions and pre-nucleation aggregation events in the context of co-crystal formation (**K. Edkins,** University of Manchester).

- **Structural characterisation of functional materials (MS13)**

  The session predominantly focused on functional perovskites, alongside insights into dynamic and adaptive molecular crystals (**P. Naumov,** New York University Abu Dhabi), and mechanically responsive coordination polymers (**M. Pisačić,** University of Zagreb).

I also managed to fit in a few excellent keynote lectures, including:

- **Configuring materials properties by crystal engineering (KN14)**

  Allesia Bacchi (University of Parma) gave a comprehensive talk on the utility of crystal engineering in the development of nutraceutical co-crystals that are liquid at ambient conditions, and of metal-organic frameworks for the controlled capture and release of components of natural essential oils. The work on metal-organic frameworks was particularly captivating from a crystallographic perspective.

- **Intermolecular interactions 'stabilising' a crystal structure – truth or wishful thinking (KN17)**

  Catherine Esterhuyson (Stellenbosch University) shared some intriguing and thought-provoking views on how to identify 'stabilising' interactions in a crystal structure and, more generally, on how non-covalent interactions should be analysed.

Finally (and this is usually the most enjoyable part of any scientific gathering) there were the poster sessions, providing a glimpse of the research currently being performed by the highly talented students and early-career researchers from across the crystallographic community. As always, there was an abundance of energy and enthusiasm in evidence at the poster stands, and this is something we can all take heart from: despite the many hardships and obstacles of the past couple of years, the next generation of solid-state scientists are eager and willing to advance our understanding of molecular solids. This bodes well not just for the future of the ECM, but for the field at large.

Dejan-Krešimir Bučar
University College London

• • •

Neutron scattering at ECM33

Amongst many other fascinating topics at ECM33, neutron scattering had a strong representation with several talks and posters every day. The following is only a small cross-section of the presentations containing neutron work, due to the fact that 6 microsymposia were running in parallel, but they caught my eye during the conference.

On the morning of day one, there were several talks in the microsymposium MS44 'Crystallography at large scale facilities'. I did not attend as I chose to attend other microsymposia (MS35 and MS-20). Neutron-related talks included those by **Claire Villevieille** (Grenoble) on 'Battery materials and diagnostics using advanced *operando* techniques' and by **Ruben De Barros** (Montpellier) on 'Structural complexity in the RP phase $La_2CoO_{4+\delta}$ explored by synchrotron X-ray Single Crystal Diffraction and Neutron Powder Diffraction'.

On the first day, **Paolo Mutti** from the Institut Laue Langevin (ILL) gave a fascinating insight into how recent developments in Artificial Intelligence and Machine Learning can both optimize data collection and improve data analysis. Indeed, drawing on examples from a Small Angle Neutron Scattering instrument and a triple-axis spectrometer, it was shown how deep learning can unleash on-the-fly analysis to guide modelling and data acquisition strategy and how a neural network model can optimize beamtime use by learning to recognize and subsequently focus the data collection on interesting region of reciprocal space.

Another first morning microsymposium (MS-20) talk focused on new work on a well-known Ruddlesden-Popper compound which has been the subject of intense research due to the wealth of complex phases it displays, related to a Van Hove singularity in its band structure and a topological Lifshitz transition which can be tuned by, for instance, magnetic field or uniaxial strain. **Alexandra Gibbs** from St Andrews University discussed tuning $Sr_3Ru_2O_7$ via light Ba-doping, and demonstrated the power of high resolution neutron diffraction in investigating subtle changes in structural distortions and how these affect its electronic properties.

Neutron diffuse scattering was also very well represented, with several talks in microsymposia such as MS-15 where **Kristoffer Stockler** from Aarhus described how combining X-ray and neutron diffuse scattering on the mineral bixbyite, $Fe_{2-x}Mn_xO_3$, afforded a unique insight into this material. Indeed, aside from an already suggested correlated disorder arising from epitaxial intergrowths of the mineral braunite, the different contrast between X-rays and neutrons allowed to show that the displacements of oxide ions are correlated with the substitutional disorder on the cation sites. Recent advances in analysing such complex diffuse scattering data and extracting local deviations from the average structure were brilliantly exposed by keynote speaker **Reinhard Neder** (Erlangen) on the second day. In particular, Reinhard gave a great overview on recent developments in 3D-ΔPDF technique which enables easier access to starting models and offers a good complementary approach and/or a starting point to more traditional quantitative data analysis based on reciprocal space data. The power of these methods is greatly enhanced by the advent of new neutron diffuse instruments such as CORELLI at the Spallation Neutron Source. This was illustrated perfectly by a talk in MS-38 by **Jonas Sandemann** from Aarhus who described how 3D-magnetic-ΔPDF was used to extract individual correlations in spinel $ZnFe_2O_4$ and, by considering exchange pathways, to get a detailed picture of magnetic exchange interactions. In yet another microsymposium session (MS-26), **Matthias Gutmann** (ISIS Neutron and Muon Source) showed how state-of-the-art neutron and synchrotron diffuse scattering data can be combined with *ab initio* phonon calculations to shed light on how low energy phonon modes are key to the thermoelectric properties of some materials, thereby offering a key for better materials design. On the software side, **Wojciech Sławiński** from Warsaw described the latest developments in RMCProfile7, which deals with both X-ray and neutron data and the possibility of combining them, such as in multi-phase refinement, multiple datasets, complex molecule moves….

A microsymposium dedicated to complex order in magnetic materials (MS22) strongly featured neutrons. **Claire Collin** (Grenoble) described single crystal neutron data under zero and applied magnetic field on nano-lamellar rare-earth based i-MAX phases where RKKY, exchange and crystal electric field effects on the 4f electrons combine to provide beautiful and complex magnetic structures, one of which requires a description in (3+2)D superspace. This was followed by a talk by **Ryuji Tamura** (Tokyo) on the observation, for the first time, of long range magnetic order (LRMO) in a real icosahedral quasicrystal for which Bragg peaks were observed in a neutron diffraction experiment. The study also highlighted the importance of the electron-per-atom (e/a) ratio in obtaining LRMO by showing previously synthesized icosahedral quasicrystals had their e/a ratio located in the strongly frustrated region.

In a parallel session, **Nick Funnell** (ISIS) described recent efforts on the PEARL beamline to obtain neutron total scattering measurement by carefully accounting for contributions from pressure transmitting media which possess their own local structures.

Neutrons were also strongly represented in prizes given during the conference. The Bertaut Prize was given to **Lukáš Gajdos** from the Institut Laue Langevin (see figure on page 16 in Elspeth Garman's report). Lukáš described the experimental difficulties that had to be overcome in order to pursue his research on the characterisation of the interaction of lectins with sugars by neutron diffraction, as well as reminding us the advantages that neutron diffraction brings in being able to locate hydrogen atoms.

The complementary of neutron and X-ray imaging for energy research was highlighted in an excellent talk in MS40 by **Sandrine Lyonnard** (Grenoble) who has studied silicon-graphite anodes using WAXS/SAXS to quantify lithiated phases formed at various stages as well as a combination of SAXS/WAXS, neutron imaging NeXT@ILL and XRD-Computed Tomography in graphite/$LiNiO_2$ cells.

One of the last symposia on the final day was dedicated to extreme conditions (MS27) and **Craig Bull** (ISIS) picked $BaTiO_3$ as an example of the type of neutron diffraction experiments that can be performed at high-pressure, showing how detailed information on the ferroelectric moment can be extracted from the neutron data collected through the various phases in the P-T phase diagram.

Pascal Manuel
ISIS Neutron and Muon Source

• • •

Personal Firsts at ECM33

Attending the ECM 2022 was a series of exciting personal firsts for me: my first international conference, my first visit to France, and even my first experience of travelling by Eurostar. After a long day of travelling, we arrived in Versailles on the opening day of the conference and after a short walk taking in the sights, we arrived at the conference centre. Being students of Newcastle University we were excited to witness **Professor Bill Clegg** (Newcastle University) receive the Max Perutz prize which was accompanied by a great talk (see image) through an impressive career in crystallography. I particularly enjoyed his humorous and entertaining ways of communicating science to children or those from non-scientific backgrounds.

Day 2 kicked off with plenary speaker **Joakim Esbjörnsson** (Lund University) delivering a talk relevant to everyone in attendance on how the scientific research community

worked to understand the structure and activity of SARS-CoV-2. We then spent the day attending talks that were helpfully arranged into microsymposia which allowed us to easily attend talks most aligned with our research interests. In the evening we attended the 'Science Slam' where those braver than myself gave short and entertaining presentations of their research, including a memorable 'cooking lesson' on pancake-bonded dimers by **Petra Stanić** (Zagreb).

The development of electron diffraction instruments and their applications had a strong presence at this year's conference. Like many crystallographers I had no prior experience with electron diffraction so this was a great opportunity for me personally to learn from experts to further my understanding of a field which has recently become relevant to my own research. It was particularly interesting see a live demonstration of electron diffraction in action by Rigaku at their vendor stall.

I then had the opportunity to present my own work in the form of a poster to a friendly and engaging crowd which was a great way to share ideas and make connections with other crystallographers. I'm incredibly grateful to the Arnold Beevers Bursary Fund to have provided me with the means to attend the ECM; I found the experience a great way to connect with crystallographers from around the world and get inspired by the new and exciting research presented at the conference.

Jake Weatherston
Newcastle University

• • •

Highlights from the Proceedings of the ECA Council Meetings at ECM33

The 2022 meeting of the Council of the European Crystallographic Association (ECA) took place over two lunchtimes on the 24th and 26th of August. ECA Council Meetings are attended by the ECA Executive Committee, the ECA national, individual, and corporate member representatives, and several attendees who are invited to discuss specific topics. The meetings are an opportunity to discuss matters concerning crystallography throughout the ECA region, with ECA national members coming from across Europe, the Middle East, and Africa. ECA Council meetings take place annually, normally during a European Crystallographic Meeting (ECM) or an IUCr Congress. This year's Council Meeting took place in person at the Palais de Congrès in Versailles during ECM33 and was the first fully in-person Council Meeting since 2019.

Due to the resignation of the previous Treasurer (Jacob Overgaard, Aarhus University, Denmark), it was necessary to elect a new Treasurer for the remainder of the 2021-2024 term. Antonia Neels (EMPA/University of Fribourg, Switzerland) has been elected to this role.

ECA Council Meetings are also used as an opportunity for the Councillors to receive updates on the planning of future European Crystallographic Meetings. Preparations are well underway for ECM34, which is scheduled to take place in Padova, Italy, from the 20th – 24th August 2024 (more information is available on the conference website: **https://www.ecm34.org/**). An update on the organisation of ECM35, which will take place in Lviv, Ukraine in 2025, was also provided.

The topic of Prizes of the ECA was also discussed in detail. The ECA awards a number of prizes at its meetings, including the Max Perutz Prize (awarded in recognition of meritorious achievements in any branch of crystallography), the Erwin Felix Lewy Bertaut Prize (awarded to a young scientist in recognition of notable experimental, methodological, or theoretical contributions to the investigation of matter using crystallographic or neutron scattering methods), and the Alajos Kálmán Prize (awarded by the Hungarian Chemical Society in recognition for outstanding scientific contributions in the field of structural sciences). At this year's ECM Bill Clegg won the Perutz prize, Lukáš Gajdos won the Bertaut prize, and Éric Collet won the Kálmán prize. Candidates must be nominated to be considered for these prizes, and more information is available online: **https://ecanews.org/prizes/**.

Finally, of interest to younger members of the crystallographic community, the ECA Council heard the report on the 7th European Crystallographic School (ECS7), which took place in person in Lisbon, Portugal, in July this year. European Crystallographic Schools combine lectures and hands-on tutorials to provide attendees with a fundamental understanding of the principles underpinning crystallography. Each school is unique, however, and offers a variety of topics to cater to a broad range of interests. ECS8 will take place during 2023 in Berlin, Germany, and a successful bid takes ECS9 to Nancy, France, in 2024. For further information on the ECS, please visit **https://ecanews.org/european-crystallography-school/**.

Suzanna Ward

Max Perutz Prize Symposium

18th January 2023 · Newcastle upon Tyne

Chemists at Newcastle University are organising a half-day symposium to celebrate the award of the ECA 12th Max Perutz Prize to Professor Bill Clegg. It will be held in the Bedson Building of Newcastle University from 12:50 (refreshments available from 12:00) to 17:00, followed by a drinks reception.

Guest speakers are Professor John Helliwell (Manchester), Professor Simon Parsons (Edinburgh) and Professor Steve Liddle (Manchester), together with Dr Mike Probert (Newcastle), and Bill will deliver the prize acceptance lecture he gave at ECM-33 in Versailles in August.

The event is open to all with no fee, but registration is requested to help with catering and other arrangements. Further information and a link for registration are available at **https://www.ncl.ac.uk/nes/news/events/event-items/european-crystallographic-association/**; you can also contact **andrew.houlton@ncl.ac.uk** as the main organiser.

Meeting Report

72nd Annual Meeting of the American Crystallographic Association (ACA)

THIS year the ACA Annual Meeting was held in a very hot and sunny Portland, Oregon, right on the banks of the Willamette River (see image), from 29th July-3rd August, 2022. As my first time at an ACA meeting (and in the U.S.A.), I was very excited – but a little nervous and more than a little jet-lagged!

The conference started with a full day of workshops, followed by an evening reception and an excellent keynote from **David Baker** (University of Washington) about the newest developments in *de novo* protein design and structure prediction.

The following four days covered a huge range of topics covering all aspects of structural science. Sessions ranged from homemade software and hardware to extreme condition crystallography.

Keeping up the structure prediction theme from the keynote, **Kathryn Tunyasuvunakool** (Deepmind) gave an insightful talk about best practices for structure prediction, how best to interpret the confidence estimates within AlphaFold, and the development of benchmarking sets for new applications of AlphaFold.

Particular personal highlights were the sessions on AI structure prediction, crystallography under physiological conditions, and time-resolved studies. The focus on structural dynamics was exciting and really highlighted many innovative techniques such as **Kara Zielinski's** (Cornell University) talk describing a new rapid mixing device and **Iris Young's** (Lawrence Berkeley National Laboratory) talk demonstrating a deconvolution technique to harness the full XFEL bandwidth and resolve both the structure and redox state of metalloproteins.

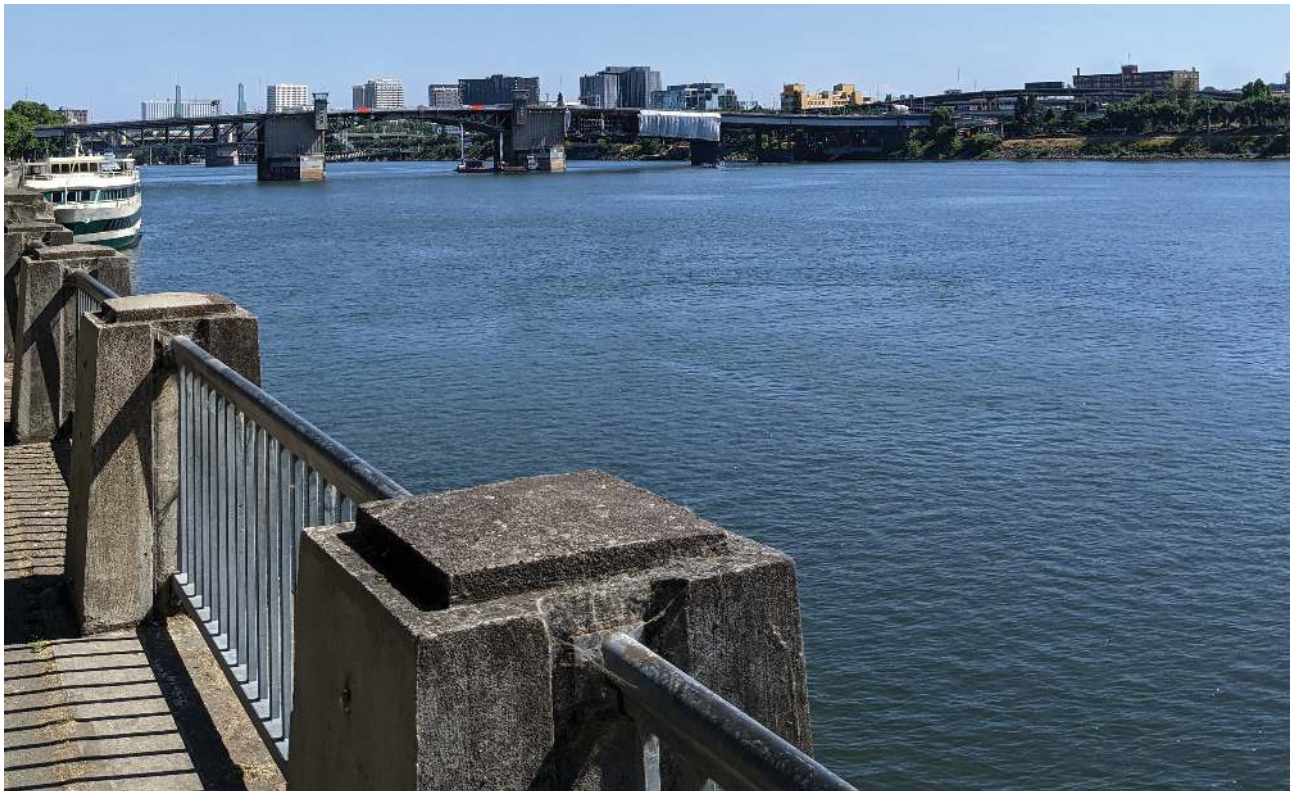
The Frankuchen Memorial Award was given to **David S. Goodsell** (Scripps Research), who delivered an excellent talk about his work communicating structural science and developing his characteristic style of visualising and illustrating molecules and cells. David produces his images by hand in watercolour but has worked to make programs like CellPaint and Illustrate so we can all achieve picture perfect results.

Airlie McCoy (University of Cambridge) received the Kenneth Trueblood award and gave a very entertaining Star Trek themed rundown of her work developing Phaser as well as some hints on what we can expect in the 'next generation' of the program.

It was great to be able to personally contribute to the three-minute thesis competition and a busy and engaging poster session. The Young Scientist Scientific Interest Group (YSIG) did an excellent job organising both academic and social events which were a great opportunity to meet other young scientists.

It is always great to see the welcoming atmosphere within the crystallography community and to leave full of new ideas and inspiration.

Jake Hill
University of Bradford



Meeting Reports
Isotope Special!

THE use of isotopes has enabled major advances in structural science, in particular – but certainly not limited to – deuteration. As there have been a number of meetings recently which either focussed on isotopic substitution or where much of the work reported used the technique, it seemed (to me at least) a good idea to put these meeting reports together as something of an 'isotope special'.

I hope you find some examples of the use of isotopes in these three reports of interest.

Deuteration for Neutron Scattering

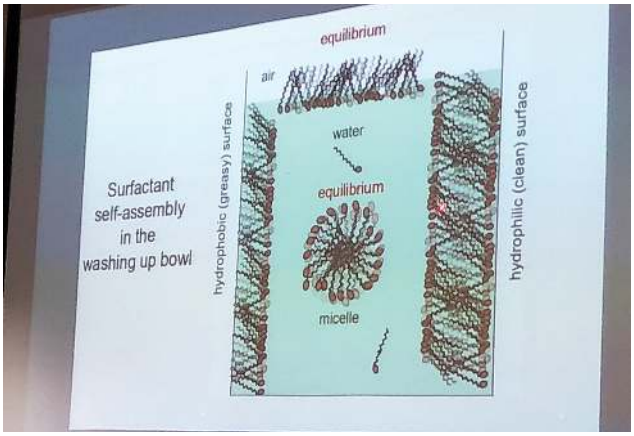
Milton Hill House, Abingdon 26th-27th September 2022

Selective deuteration is a major isotope substitution technique in the armoury of structural studies of complex systems. Whether it is used to make part of a system invisible to neutrons by matching the negative scattering factor of the proton with the positive scattering factor of the deuteron, or specific labelling of a component in order to focus on that component, its use has revolutionised our understanding of a range of multicomponent complex systems of physical, chemical and biological importance. As **Jeff Penfold** (ISIS Neutron and Muon Source) said in his opening talk on surfactant mixing, without deuteration this kind of work would just not have been possible.

Though a significant part of the meeting addressed structural studies of soft matter, it also looked at the use of deuteration in systems of biological interest, polymers, confined fluids and self assembly in a range of systems. What was also notable was the fact that many of the systems studied are of applied interest, including the development of better detergents, catalysis, corrosion, targeted drug delivery, memristors, tissue engineering, ion transport regulation, vaccine development, photoelectodes for water splitting, CO_2 capture and fuel cells. So it wasn't surprising that a significant amount of the work reported was in collaboration with industry.

The opening talks of each of the two days both tackled problems relating to multicomponent surfactant mixtures – appropriately given by **Jeff Penfold** and **Bob Thomas** (University of Oxford) who might justifiably be regarded as the fathers of the development of neutron reflectometry with isotope substitution. Jeff kicked off the day one proceedings by describing the thermodynamics of surfactant mixing, noting that the first specular neutron reflection work on surfactant structure at the air-water interface was published in 1989[1,2]. He went on to discuss much more complex mixtures (with up to *seven* different components!) such as incorporating biosurfactants to improve the biosustainability, biogdegradability and biocompatibility of the products, and the use of additives to improve tolerance to hard water, extreme pH and low temperature behaviour. A convincing demonstration that neutron reflectometry really has transformed our understanding of surfactant mixing.

A similar statement could also be made with respect to **Bob Thomas's** opening talk on day two, when he guided us through the surface behaviour of polyelectrolyte-surfactant mixtures. Although he had been pursuing this work for 25 years, he revealed that it's only in the last four years that he has begun to understand it! Focussing largely on *weak* polyelectrolyte-surfactant systems (important for the complex lipid mixtures used to transport mRNA vaccines, as well as relevant to the more mundane task of dishwashing), he explained how poor wetting capability can be changed to very good wetting by just adding salt. And also, perhaps somewhat surprisingly, why adding more of a minor component that at low concentrations improves a solution's performance can reduce its effectiveness, and that what actually happens at the *surface* is driven by what happens in the bulk solution (see image).



Bob Thomas's opening slide!

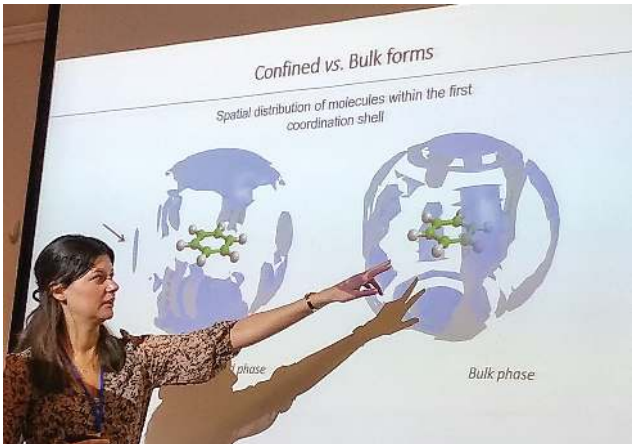
Jeff's day one talk was followed by a number of further presentations on soft matter. Among other problems, **Stuart Clark** (University of Cambridge) told us how, by judicial contrast matching, a dissolving surface can be followed, with the ability to observe much smaller amounts of corrosion than is possible using other methods. His wide-ranging talk also touched on the two-dimensional self-assembly of light-harvesting molecules, studies on the dynamics as well as the structure of adsorbed layers and the effects of ion association in the reduction of conductivity in supercapacitor electrolytes. In a talk that concentrated on the use of neutron scattering and reflectivity for industrial applications (mentioning specifically detergency, ice cream, SARS-CoV-2 disinfectant and emulsion paints), **Joran Petkov** (Arxara UK) told us about Colgate-Palmolive's interest in the effect of hard water on the solubilisation of SLES (sodium lauryl ether sulphate), and also how difficult it can be to really clean a surface. At the top of his list of what is needed in order to dig deeper into what surfactants can and cannot do came the Wheatsheaf Inn near ISIS and strong ristrettos – though he didn't ignore the importance of ingenious and enthusiastic collaborators and the use of the cutting edge techniques of neutron scattering and reflectivity...

The talk by **Benedetta Rosi** (Jülich Centre for Neutron Science, Germany) on structural transformations in homo- and block copolymers (relevant to, for example, drug delivery, tissue engineering and ion transport regulation) took me back to earlier work I had been involved in[3] on the so-called dynamical transition first noted[4] in proteins by Steve Cusack at EMBL Grenoble. Using inelastic incoherent neutron scattering, Benedetta's work focussed on the similar behaviour found in polystyrene-poly(N-isopropyl-acrylamide) (PNIPAM) block copolymers. She used partial deuteration to focus on the 'source' of the transition, and the very different effect on the transition temperature of adding the 'stabilisers' glucose and glycerol.

Several other talks also had significant biological relevance. For example, **Jian Lu** (University of Manchester) discussed biointerfacial interactions such as that between antimicrobial peptides and membranes, looking at the interfacial structure of DPPC[5] and DPPG[5] lipids before and after peptide addition. **Jürgen Allgaier** (Jülich Centre for Neutron Science, Germany) discussed his studies on membrane translocation while **Kunlung Hong** (Oak Ridge National Laboratory, USA) talked about mimicking lipid membranes for memristors. **Wuge Briscoe** (University of Bristol) reported his work on the self-assembly and interactions of bacterial lipids, using small angle neutron scattering (SANS) to explore the effects of molecular architecture and temperature on the self-assembly of lipopolysaccharides, while **Najet Mahmoudi** (ISIS Neutron and Muon Source) completed the soft matter presentations by examining the structural details of biological complexes in the context of developing an antiviral for the Hepatitis B virus.

Moving away from soft matter brought us initially to two talks on structural changes in deep eutectic solvents (DES). Working with the surfactant sodium dodecyl sulphate (SDS) and the choline chloride-urea system, **Andrew Jackson** (European Spallation Source) probed the self-assembly process as a function of concentration, concluding that the interaction between the headgroup and the solvent allows the structure to be tuned – for example to produce worm-like micelles. He also argued for the existence of long-range electrostatic interactions in the DES, despite the high ionic strength. Noting its potential as a photoelectrode material for water splitting, again using the choline chloride-urea solvent **Daniel Bowron** (ISIS Neutron and Muon Source) showed that, by controlling the amount of added water, the structure of precipitating Fe_2O_3 nanoparticles can be varied – of interest as the structure of the nanoparticles can affect the current performance. In addition to using neutron diffraction, SANS and SAXS, EXAFS results confirmed the local atomic level structure, as well as giving information on the kinetics. Finally, TEM was used to confirm the nanoparticle form – all-in-all demonstrating the value of using multiple techniques to pin down a complex problem.

Under the heading of Disordered Materials, the final morning saw two talks on neutron scattering studies of structure in confined fluids. Taking data on the NIMROD instrument at ISIS – which enables the probing of structure at the atomic and mesoscopic scales in the same experiment – **Marta Falkowska** (University of Manchester) looked at the structure of toluene in MCM-41, which has mesopores with diameters of 2 to 6.5nm, while following the pore-filling process. Her work on confined benzene showed that the liquid structure in confinement is different from that in the bulk liquid, and that the geometry of benzene-benzene first neighbour interactions changes as the distance from the pore surface increases. Marta's work also showed it was possible to follow the filling process of gases in mesoporous materials, examining the structures of the layers as they build up from 1-2 layers through capillary condensation to saturation. She proposes further work to try to understand confinement effects on phase separation and on more complex multicomponent confined systems.



Marta Falkowska demonstrating the difference in the spatial distribution function of liquid benzene molecules between confinement and in the bulk liquid.

In the final neutron scattering paper – again on confined fluids using NIMROD – **Terri-Louise Hughes** (ISIS Neutron and Muon Source) followed the catalytic conversion of benzene to cyclohexane in MCM-41 with a Pt catalyst. The reaction took place on beam in real time, with a time resolution of five minutes, in parallel with NMR to monitor the progress of the reaction. Atomic-level structural detail, including the relative intermolecular orientations throughout the process, was extracted from the neutron data. In some ways, this was a demonstration experiment to show how the combination of NMR and neutron scattering can be used to study heterogeneous catalytic systems *in situ*, and should lead to the study of more complex reacting systems using NMR to inform on chemical composition while neutron scattering simultaneously probes the structure as the reaction progresses.

Though deuteration is only one aspect of the use of isotopic substitution in the study of structure – and dynamics – of complex non-crystalline systems, the wide range of systems looked at during the meeting was impressive. As Daniel Bowron said in his concluding remarks: deuteration is an essential tool in learning about these systems of increasing complexity. It was also good to see that much of the work reported related to systems of significant applied relevance – often done in collaboration with relevant industry.

To re-echo Jeff Penfold's opening comments, none of this would have been possible without deuteration (and of course neutrons). As one speaker put it, neutron scattering combined with deuteration is a silver bullet. Or if you prefer Arthurian legend – Excalibur!

John Finney
UCL

References and footnotes

[1] E.M. Lee, R.K. Thomas, J. Penfold and R.C. Ward. *J. Phys. Chem.* **93,** 381 (1989).

[2] On a personal note, this mention took me back to my time at ISIS in its early days, when this was one of the flagship experiments that I frequently used in talks on the new science that ISIS was developing.

[3] R.M. Daniel *et al. Biophys J.* **75,** 2504 (1998).

[4] W. Doster, S.C. Cusack and W. Petry. *Nature* **337,** 754 (1989).

[5] DPPC: Dipalmitoyl-phosphatidyl-choline; DPPG: Dipalmitoyl-phosphatidyl-glycerol.

Disordered Materials User Group Meeting

Cosener's House, Abingdon 14-15 June 2022

Some 40 years ago, in the early days of the UK's pulsed spallation neutron source ISIS, 'disordered materials' meant simply liquids and glasses. With the developments that have taken place over the life of the facility – the source, the instrumentation, the sample environment, and not forgetting the power of isotope substitution when neutrons are used – the diversity of the systems accessible to structure analysis has increased dramatically. This diversity was demonstrated by the Disordered Materials Group Leader **Daniel Bowron** (ISIS Neutron and Muon Source) in a slide (figure 1) that showed not only the areas of science being targeted in the latest round of beamtime applications, but also the relevance of many of them to real-world applications. It also set the scene for the feast of fascinating science talks that were presented by users (from Ph.D. students to distinguished professors) during this first in-person user group meeting since the start of the pandemic.

One of the drivers of the increased diversity of disordered material science at ISIS has been the increased ability to look on the same instrument at structures over a very wide range of length scales, opening up the Pandora's box of not only biomolecules themselves but also of assemblies of them. This was highlighted in the first science talk by **Lorna Dougan** (University of Leeds), who introduced us to her group's work exploring proteins as biomaterial building blocks, with the aim of creating biomaterials with programmable structure and dynamics (reminding me of Ned Seaman's pioneering work on programmable DNA nanostructures and nanomachines – see my comments in Crystallography News June 2022 page 4). Perhaps Lorna's introductory slide (figure 2 – including remote Lorna!) summarises the vision of her group's work. She concluded her talk by looking at the hydration of protein hairpins, specifically targeting the solvent structure around Pro-Gly-Pro and the effect of it of urea – often considered to be a structure destabiliser.

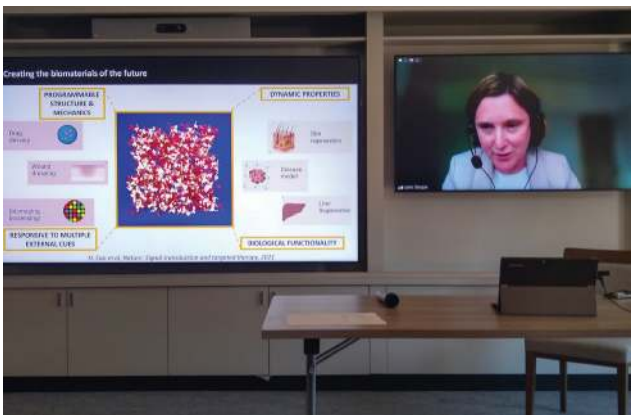


Figure 2

Indeed, the perturbation of structures (of both biomolecules and their solvent) by so-called 'structure makers' and 'structure breakers' has been an active – and often controversial – area of liquid structure research for many years, with reference, for example, to protein structure (de) stabilisation and protection under conditions of e.g. cold, heat or high salt. So it was not unexpected that several of the other papers addressed this important issue in a range of systems. For example, **Harrison Laurent** (also from Leeds) talked to us about deep marine organisms and how they might overcome the destabilising effects of pressure on proteins, DNA and lipids. How they are able to do this is thought to relate to the ability of trimethylamine N-oxide (TMAO) to restabilise the biomolecules. The conventional wisdom has been that TMAO is preferentially excluded from the biomolecular surface, with the effect being indirect and related to the effect of the TMAO on the water structure. Looking at the TMAO/water system under pressure, he concluded that indeed TMAO did resist the pressure-induced structural change, but that the effect was smaller than expected. He concluded that while pressure weakens bulk water hydrogen bonding, TMAO additions enhances it, the calculated balance between the two effects being in good agreement with the measured data.

Solvent structure perturbation was also implicated in John Holbrey's (Queen's University Belfast) talk on sodium acetate trihydrate/urea, a system used in heat storage and release

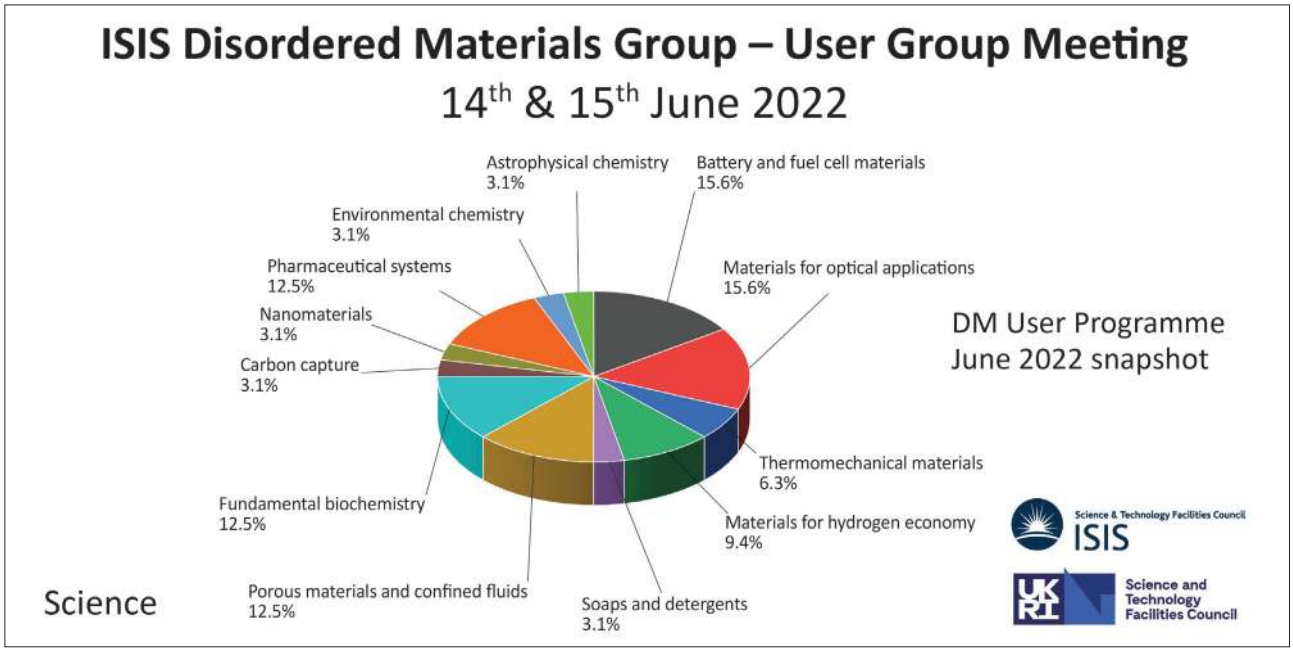


Figure 1

devices such as hand warming pads and building insulation. One of this system's problems is that it supercools easily, so John was interested in understanding the structure in order to try to reduce the supercooling tendency. Looking at the detailed three-dimensional structure, with particular reference to the ways in which the different urea hydrogens interacted, he concluded that the urea was acting as a disruptor of the structure.

Two other papers also looked at differences in water structures and/or water-related hydrogen bonding. In the first of these on a structural analysis of potassium borate solutions, **Zhu Fayan** (Qinghai Institute of the Salt Lakes, China) argued that the hydrogen bond between $B(OH)_4^-$ and water is stronger than that between water molecules in the hydration layer. In the second on water in cement, **Zhanar Zhakiyeva** (ILL) considered the cement structure across a wide length scale range, looking at water between silicate layers, at cement grain interfaces and within pores. Using both neutron diffraction and inelastic neutron scattering, she concluded that the interfacial and interlayer water demonstrated both structural and dynamical properties that are distinct from bulk water. In exploring the solvent in cements whose manufacture releases less CO_2 – so a material that is of obvious interest in the context of mitigating global warming – Zhanar said that the results were similar.

Putting on my sceptical hat (though some colleagues think it's a permanent part of my head gear…), discussions of structure disruption/enhancement in liquids can be problematical as we don't – unlike in a crystal – have a clear idea of what it means to increase or decrease the structure of an inherently disordered system such as a liquid or glass. So I found the paper by **Luis Carlos Pardo Soto** (Universitat Politècnica de Catalunya) that presented a possible way of quantifying changes in disorder particularly interesting. He looked at the hydration of adamantane, which he analysed using software he has developed to visualise the orientational correlations in liquid systems. Approaching the quantification of order/disorder through the concept of Shannon entropy[1] from information theory, he obtained Shannon entropy values for the adamantane-water system that were clearly different from that for bulk water. We may argue about the relationship between Shannon entropy and structural disorder, but – again on a personal note – Soto's approach is a considerable advance on my attempts as a Ph.D. student to estimate using a similar approach the entropy of of Bernal's model of an ideal liquid[2].

Not only can neutrons look at structural perturbations in liquids as addressed in these presentations, but they can also look at changes in the structure of a liquid or solution prior to crystal nucleation, a field pioneered at ISIS some ten or so years ago by Roger Davey[3] in Manchester. It was therefore perhaps particularly appropriate that we had a paper from **Kathi Edkins** from Manchester on how the solution structure of the drug cimetidine influenced the form of the crystalline hydrate. Considering that there are six cimetidine tautomers, interpreting the data from the NIMROD instrument was quite a challenge for the developing *Dissolve* software, but the results indeed threw very interesting light on the changes occurring to the water interactions in different parts of the molecule – and the difference of these in the different tautomers. Overall, the results implied that the main solvent interactions in the crystal survive in the solution. Moving away from water-containing systems, the paper by **Huang Shi** (University of Hull) discussed structural changes during the amorphous to crystalline transition in multicomponent Al-based alloys. Looked at in terms of the local polyhedral structures, as the system cooled, there was a movement from vertex sharing, through edge sharing to face sharing of the polyhedra. Also from the Hull team, **Jiawei Mi** looked at pre-nucleation structures in liquid and amorphous metals, as well as changes in atomic structure during stress fracture.

In all, there were 35 presentations covering not only a wide range of science, but also developments in software and user facilities by colleagues from ISIS. For example, **Tristan Youngs** discussed progress on *Dissolve* as the successor to EPSR for obtaining non-crystalline structure from diffraction – and increasingly other – data; **Bindu Kolli** took us through the possibility of coarse graining to handle even larger systems, and **Sarah Youngs** updated us on the Deuteration Laboratory that's essential to those of us using H/D substitution. Other science presentations covered short and medium-range structures of liquid and amorphous systems (both organic and inorganic), as well as 'mesoscopic' systems such as gas adsorption in fluids and porous solids, including amorphous ice and its relevance to star formation, and glass/metal-organic framework composites.

It's obviously impossible to cover all the 35 presentations in the space the editor has given me (!!), but there is one other paper that I think will be of particular interest to crystallographers generally – and that was presented by 'our own' **Helen Playford** (ISIS).

Entitled challengingly 'How fast can we go', Helen cheekily implied that we may be taking more data than we really need to – and so eating up more expensive beam time than we need to. Taking total scattering data on the POLARIS instrument, she compared what we could learn from 10 minutes of data collection compared to four hours – a counting time difference of a factor of 24! Moving up from crystalline gallium phosphate (which has a quartz structure) through amorphous and disordered crystalline systems to a molecular crystal, she demonstrated that the shorter data collection time was very often perfectly sufficient to obtain the structural information required. But perhaps not always, suggesting that 'subtle molecular interactions' might be 'the point of failure'.

Thanks to ISIS for enabling user meetings such as this – not only in providing an excellent venue but, by covering costs, making it easy for young scientists to participate.

John Finney
UCL

References

[1] C.E. Shannon. *Bell System Technical Journal* **27,** 379 (1948).
[2] J.L.Finney. *Proc. Roy. Soc. Lond. A* **319,** 495 (1970).
[3] R.C. Burton *et al. J. Phys. Chem. B* **114,** 8807 (2010).

SANS Group Meeting

Much of the work discussed in the Deuteration Meeting used small angle neutron scattering techniques. The ISIS Small Angle Neutron Scattering (SANS) group will be hosting its first User Meeting 30-31 January 2023. This will be a great opportunity, not only for users to meet in person and share their recent scientific findings, but also for anyone who may be interested in the kind of work discussed at the Deuteration Meeting to learn more about the possibilities.

Further details about the meeting will be found at **https://www.isis.stfc.ac.uk/Pages/SANSgroup.aspx**

John Enderby and his Contributions to Science

University of Bristol
5-6 September 2022

Within an issue exampling the use of isotopes in structure determination, it would be highly amiss not to say something about the person who started the whole idea of neutron scattering with isotopic substitution[1] which has advanced fundamental understanding of the structure of multicomponent liquids – including water and aqueous solutions, liquid alloys, glasses, liquid semiconductors and molten salts. Sadly, Sir John Enderby FRS died in 2021, so a memorial meeting under the joint auspices of the Institute of Physics Liquids and Complex Fluids and Neutron Scattering Groups was organised by the Bristol Physics Department on September 5th and 6th 2022.

The first session consisted of presentations from five of John's scientific 'children'. **Phil Salmon** (University of Bath) kicked off the proceedings by taking us through John's career from his time as a schoolteacher and through his part-time undergraduate degree at Birkbeck[2]. Following his Ph.D. there under Norman Cusack, he lectured in Huddersfield from 1957-1960, then moved on to Sheffield and Leicester. He finally accepted a chair in Bristol Physics Department in 1976, taking leave from 1985 to 1988 to be Directeur-Adjoint at the Institut Laue-Langevin in Grenoble, the world's premier reactor neutron beam facility. **George Neilson** (University of Bristol) followed on from Phil, focussing on the ground-breaking work on aqueous ionic solutions using nickel and chlorine isotopes, work which was to develop to sweep away much of the previous 'conventional chemical wisdom' on ion hydration.

Alan Soper (ISIS Neutron and Muon Source), after commenting on how stimulating John's undergraduate lectures were at Leicester, told us how the original idea of taking a first difference between the scattering data from two different isotopic systems could remove the inelasticity droop in the measured structure factor. It was a fitting judgement on John's experimental work that even the data taken some forty years ago on, for example, HCl, has stood the test of time. **Bob Newport** (University of Kent) stressed how John had supported his career, and with examples underlined the importance John put on constructive scepticism, professional ethics and integrity, while **Adrian Barnes** (University of Bristol), as the last of John's scientific 'children', discussed their work on liquid metals and alloys. I had the honour of rounding off this section of the programme with examples of how John's ideas on determining liquid structures had influenced the work of my group, and how his simple but brilliant idea on isotopic substitution was now being used to understand structure and function in a wide range of not only chemical, but also biological systems. This active field of 'Liquid State Crystallography' using isotopic substitution was made possible by John's insight.

The second day was focussed on specific scientific problems, generally given by younger scientists (John's scientific 'grandchildren'), and demonstrated the extremely wide application of isotope substitution in studying the structure and dynamics of glasses and liquid systems of a range of complexity. **James Drewitt** (University of Bristol) discussed liquid studies under extreme conditions, focussing on levitated samples. **Tom Headen** (ISIS Neutron and Muon Source) took us on a journey from the molecular structures of liquids of simple aromatic systems such as benzene, where the structure results from a very delicate balance between different kinds of forces, to recent work exploring the aggregation of the more complex asphaltines – one of the oil refining industry's *bète noirs* that foul refinery equipment. The final talk relating to isotopic substitution by **Hesameddin Mohammadi** (University of Bath) looked at the structures of the magnesium aluminium silicate glasses that are widely used in mobile phones in order to probe the structural reasons for their high strength and crack resistance.

Late hangers on at lunch at the end of the meeting outside the Bristol Mathematics School Fry Building. Bob Evans who set up the meeting is in the foreground on the right. The sculpture representing a Voronoi tessellation of a two-dimensional disordered system seemed a highly appropriate backdrop (though one of the vertices bothers me – perhaps a question for a future 'Puzzle Corner'?).

It was a great two days, and really good to see many old friends. Three statements made during the meeting about John remain in my mind. "He was an inspirer as well as a performer of outstanding work." "His wise counsel has helped many of us in this room." And recognising the revolution in liquid structure studies that have been made possible by his development of isotopic substitution methods with neutron scattering: "Nobel prizes have been awarded for less".

John Finney
UCL

Footnotes

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

[2] Phil told an interesting story about John's time as an undergraduate at Birkbeck. The Head of Department J.D. Bernal (see Crystallography News, September 2021) was sufficiently impressed by John's performance in his exams that he wrote to the headmaster of Penge Secondary Modern School where John was teaching, asking that John be released from his teaching responsibilities for two terms. The request was accompanied by a statement that if the headmaster refused, questions would be asked in Parliament (!). John was given the time off and duly ended up with First Class Honours.

News from the Cambridge Crystallographic Data Centre

CCDC's Computation-Ready MOFs Collection is 17% Bigger!

The CSD MOF collection that contains the crystal structure data of MOFs which is curated, prepared, and ready for computational analyses, has been updated and is now 17% bigger. This resource is free of charge for academic research.

In March 2021 the Cambridge Crystallographic Data Centre released the CSD MOF collection. This resource included over 10,600 3D MOF crystal structures, with significant void space, all prepared and ready for high-throughput computational analysis.

The dataset was prepared from the Cambridge Structural Database, or CSD, the world's database of small-molecule organic and metal-organic crystal structures. All structures are from experimental results, collated from the published scientific literature, and by direct deposit from scientists around the world. Each is then curated and annotated by experts to make it more findable and accessible to humans and machines, for example by adding common names, 2D diagram representations and more.

The dataset has now been updated, and now stands at 12,505 structures — a 17% increase.

For commercial users, or those who want even more, the full CSD database **www.ccdc.cam.ac.uk/solutions/csd-core/components/csd/** contains over 100,000 MOF-like frameworks, including some more diverse structures such as 1D and 2D frameworks, or disordered structures.

Learn more and get the dataset here: **www.ccdc.cam.ac.uk/Community/csd-community/csd-mof-collection/**

Glossary of CSD Terms available online

What is a CSD refcode? What is a CSD deposition number? What's the difference between a CIF and a GCD file?

Our recent article defines many technical terms and acronyms used when talking about the Cambridge Structural Database (CSD). It's an ideal resource for new or experienced crystallographers.

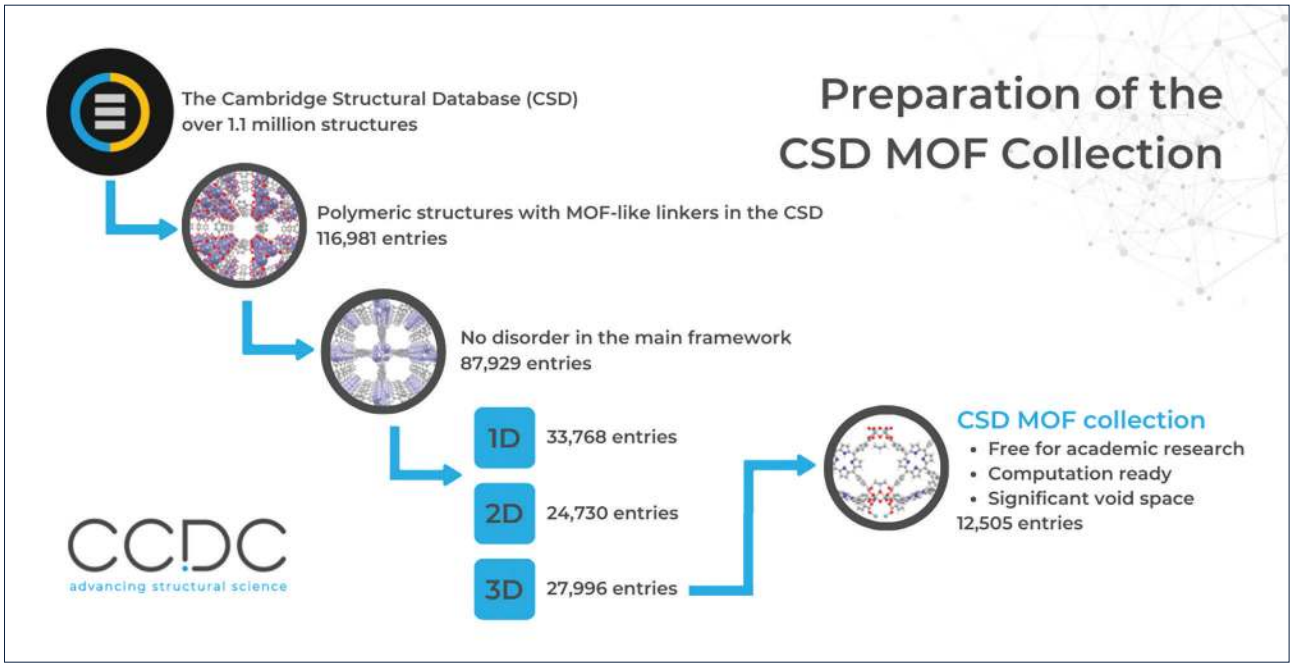
Thought of more terms we've missed? Email us on **hello@ccdc.cam.ac.uk** and we'll keep growing this resource.

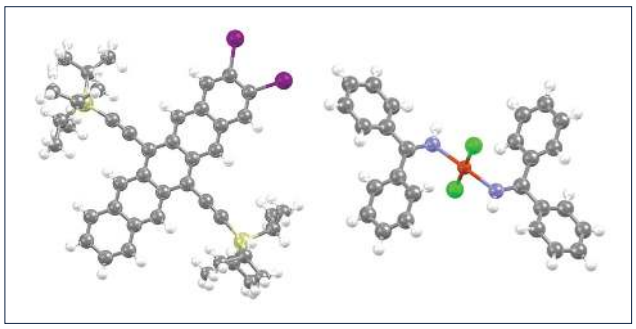
The CSD technical terms glossary is at **www.ccdc.cam.ac.uk/Community/blog/csd-terms-glossary/**

Conclusions of the 7th Crystal Structure Prediction (CSP) Blind Test

In the 7th CSP Blind Test that ran from October 2020 to September 2022, seven structures of 2D systems that had been experimentally analysed but not published ('blind') were released to participants along with some experimental conditions.

Other structures included one of the most challenging systems in CSP Blind Test history – a large, highly polymorphic, pharmaceutical drug candidate – along with agrochemicals and a food flavouring. More experimental data was released over the course of the test to simulate real world conditions.





Target systems included an optoelectronic system containing silicon (left) and a metal-organic system containing copper (right)

Participants included groups from both industry and academia, and all compounds successfully had their experimentally observed crystal structures predicted by at least one group from landscapes of 1K+ potential structures.

CSP is an ever-evolving discipline and the 7th Blind Test identified future challenges. These include disorder prediction that had previously been disregarded owing to its complexity but is now more industrially relevant to solve as bigger molecules with more flexible groups are being seen in drug development; more challenges that reflect industrial reality; and continued broadening beyond pharmaceuticals to solid-state devices.

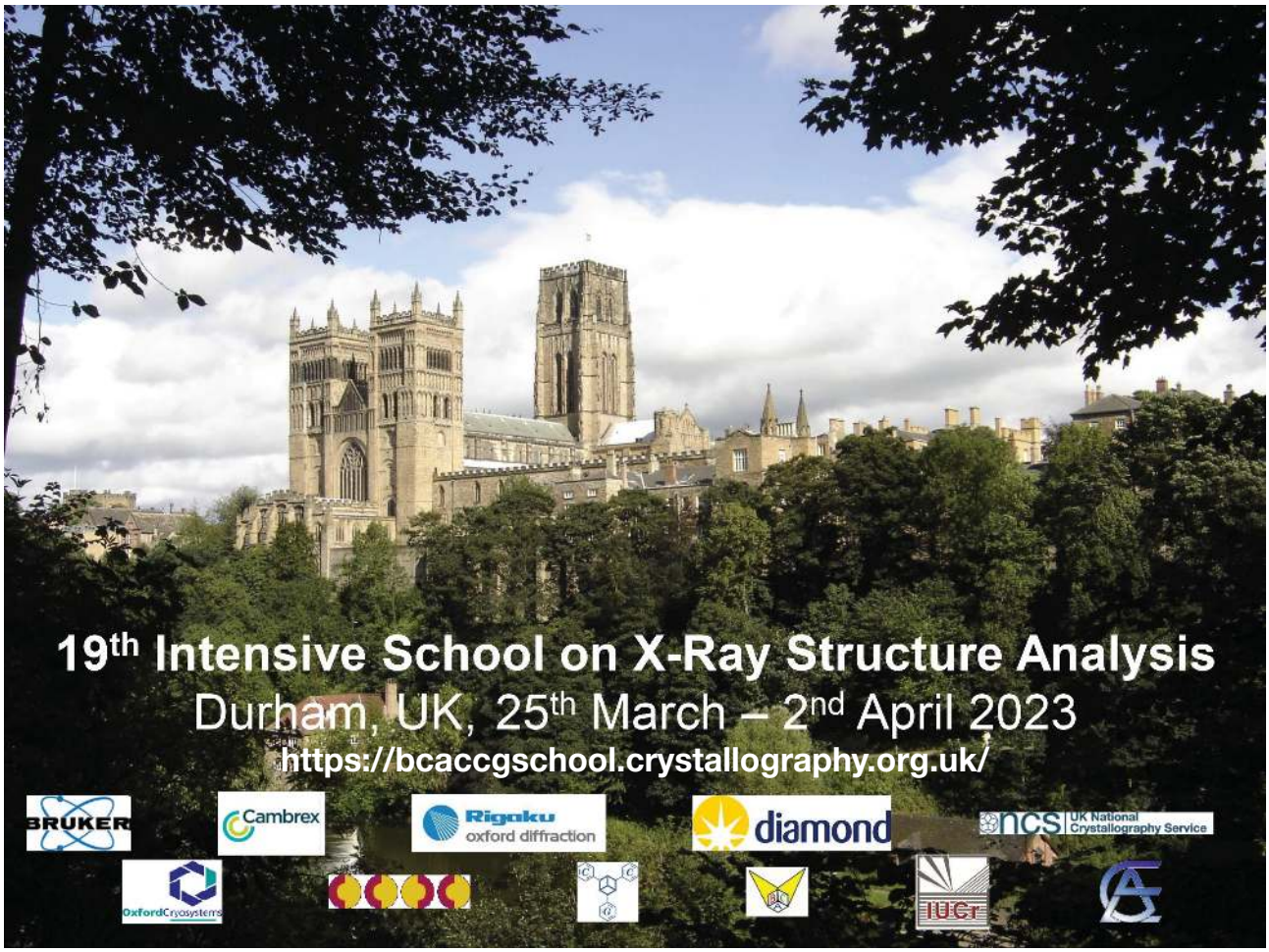
The seven 2D structures included Cu- and Si-containing systems which pushed the boundaries of CSP beyond the pharmaceutical sector to areas such as electronics and photonics.

A scientific paper with full results will be submitted for publication in 2023. Preliminary detailed results, including how many groups correctly predicted each target, the lowest rankings, CPU time used and details of methodologies are available by emailing **hello@ccdc.cam.ac.uk**.

On-line training, events and webinars

CCDC is planning more webinars and Workshops for 2023 so do check our events page at **www.ccdc.cam.ac.uk/News/Events/** for more details on dates and topics. If you would like to suggest topics for our sessions in 2023 you can email us on **hello@ccdc.cam.ac.uk**.

If you can't wait until 2023 we also have five free online courses where you can learn about structural chemistry and the CSD. Find out more at **www.ccdc.cam.ac.uk/Community/educationalresources/CSDU/** .



Meetings of interest

With a little less concern about the virus, the conference scene seems to have been strongly revitalised, with a lot of new meetings being organised – so you might well find something new and interesting in this list. Most meetings are in-person ones, though some remain online or hybrid. Further information may be obtained from the websites given. Assistance from the IUCr website is gratefully acknowledged.

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

6th Dec 2022 - 10th Dec 2022
IUCr High Pressure workshop
'Advanced High Pressure Crystallography'
Chicago, IL, U.S.A.
https://gsecars.uchicago.edu/education-and-outreach/2022-iucr-high-pressure-workshop-advanced-high-pressure-crystallography/

8th Dec 2022 - 9th Dec 2022
7th International Conference of the Bangladesh Crystallographic Association
Dhaka, Bangladesh.
https://bangladeshcrystallographicassociation.org/7th-bca-conference-2022/

11th Dec 2022 - 14th Dec 2022
2022 MicroED Workshop
UCLA, California, U.S.A.
https://cryoem.ucla.edu/course-2022

11th Dec 2022 - 16th Dec 2022
5th International Conference on Soft Materials
Jaipur, India.
https://www.smrsi.org/icsm2022/index

17th Jan 2023 - 21st Jan 2023
Pan African Conference on Crystallography (PCCr3)
Nairobi, Kenya.
https://www.pccr3africa.org/

8th Feb 2023 - 11th Feb 2023
EMBO Workshop on *in situ* Structural Biology
Heidelberg, Germany.
https://www.embl.org/about/info/course-and-conference-office/events/iss23-01/

12th Feb 2023 - 24th Feb 2023
2nd International School on Crystallography for Space Sciences
Addis Ababa, Ethiopia.
https://crystallopia.essti.gov.et/

23rd Feb 2023 - 2nd March 2023
MC2023. Microscopy Conference
Darmstadt, Germany.
https://www.microscopy-conference.de/

19th Mar 2023 - 23rd Mar 2023
Neutron and X-ray Scattering in Materials Science (TMS Annual Meeting)
San Diego, CA, U.S.A.
https://www.tms.org/AnnualMeeting/TMS2023

20th Mar 2023 - 23rd Mar 2023
European Conference on Neutron Scattering (ECNS 2023)
Garching, Germany.
https://ecns2023.eu

26th Mar 2023 - 30th Mar 2023
Frontiers of Structural Biology in Complex Environments
Indianapolis, IN, U.S.A and hybrid.
https://www.acs.org/content/acs/en/meetings/acs-meetings/spring-2023.html

27th Mar 2023 - 30th Mar 2023
Physics of Life 2023
Harrogate, U.K.
https://www.physicsoflife.org.uk/physics-of-life-2023.html

27th Mar 2023 - 30th Mar 2023
31st Annual Meeting of the German Crystallographic Society
Frankfurt am Main, Germany.
https://dgk-conference.de/

3rd Apr 2023 - 5th Apr 2023
Annual Meeting of the British Zeolite Association
Manchester, U.K.
A.M.Doyle@mmu.ac.uk

12th Apr 2023 - 14th Apr 2023
Harnessing Non-covalent Interactions for Synthesis and Catalysis (Faraday Discussion)
York, U.K.
https://www.rsc.org/events/detail/48165/

16th Apr 2023 - 21st Apr 2023
Experimental Advances in Macromolecular Crystallography
Dubrovnik, Croatia.
https://htcc5.org/

12th Jun 2023 - 16th Jun 2023
Summer School on Mathematical Crystallography
Nancy, France.
http://www.crystallography.fr/mathcryst/nancy2023.php

18th Jun 2023 - 24th Jun 2023
8th European Crystallography School
Berlin, Germany.
https://ecs8.ecanews.org

3rd Jul 2023 - 6th Jul 2023
16th International Conference on Materials Chemistry
Dublin, Ireland.
https://www.rsc.org/events/detail/72840/

7th Jul 2023 - 11th Jul 2023
73rd ACA Annual Meeting
Baltimore, MD, U.S.A.
https://www.amercrystalassn.org/future-meetings

22nd Aug 2023 - 29th Aug 2023
26th Congress and General Assembly of the IUCr
Melbourne, Australia.
https://iucr2023.org/

4th Sep 2023 - 8th Sep 2023
CMD30 (Condensed Matter Division of the European Physical Society)
Milano, Italy.
https://eventi.cnism.it/cmd30-fismat

4th Sep 2023 - 8th Sep 2023
25th Conference on Organometallic Chemistry (EuCOMC XXV)
Alcalá de Henares, Spain.
https://congresosalcala.fgua.es/eucomc2023/

OXFORD CRYOSYSTEMS

CRYOSTREAM 1000

Precise Cryogenic Sample Cooling Made Simple

Introducing the latest in cryogenic sample cooling

Available in Standard (80K – 400K), Plus or Compact (80-500K) variants, the Cryostream 1000 is a revolutionary edition of the world's leading cryo-cooler. All new electronics and firmware are incorporated into an elegant, compact design with a focus on reliability, simplicity and an enhanced user experience.

KEY FEATURES

X-ray Transparent Nozzle: An optional attachment for the coldhead nozzle, the X-ray transparent extension is made from a durable and low-temperature compatible material that minimises shadowing on the X-ray detector, increasing the amount of useful diffraction data collected without compromising cooling performance. This can either reduce the duration of experiments or improve the signal-to-noise ratio and overall data quality.

LED Status Indicator: The coldhead now provides the user with immediate visual feedback on the Cryostream's operational status without the need to refer to the control screen.

Gas Supply Module: Combines the Nitrogen pump, dry-air supply and touch screen controller into a single, compact and portable enclosure that reduces cabling, simplifies installation and improves the user experience.

Remote Annealing: Controlled and programmable interruption of the gas flow over the sample for annealing without physical manipulation (also available via an open network protocol).

Intelligent Diagnostics: An integrated real-time clock now tracks the use of the system, notifying the user of upcoming service requirements, helping to eliminate unscheduled downtime.

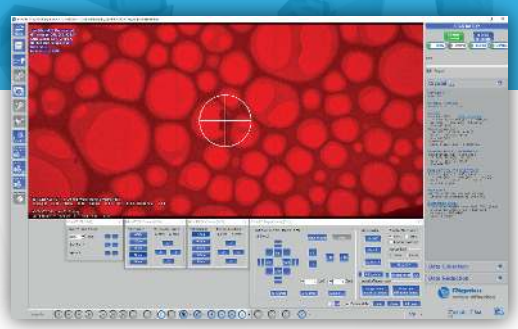
2 Year Standard Warranty: All Cryostream 1000 systems ship with a two year warranty as standard.

For more information, visit our website or contact info@oxcryo.com.

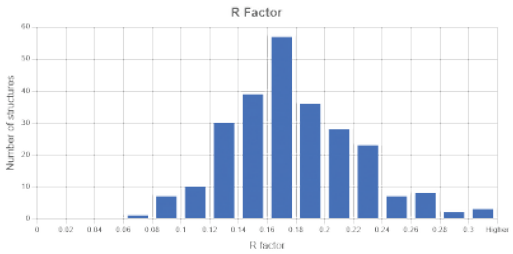
www.oxcryo.com

THE MOST PRODUCTIVE ELECTRON DIFFRACTOMETER:
XtaLAB Synergy-ED

- HyPix technology inside
- CrysAlis^{Pro} for easy instrument control and data processing
- Study submicron samples with ease



Fully controllable from CrysAlis^{Pro}. Find, center and collect data on samples with our intuitive control and data processing software.



Features a Rigaku HyPix detector for high-quality electron diffraction data.

With over 250 unique structures collected by just one XtaLAB Synergy-ED instrument since its launch and multiple installations completed or underway, the XtaLAB Synergy-ED is the world's most productive electron diffractometer. We wanted to lower the barrier to entry to the emerging field of single-crystal electron diffraction, so we joined forces with JEOL to combine the expertise of both companies into one fantastic product. With JEOL's expertise in the generation and control of electron beams and Rigaku's expertise in HPC detectors and crystallographic software, we bring you our electron diffractometer, the XtaLAB Synergy-ED.

Rigaku
POWERING NEW PERSPECTIVES

Rigaku Europe SE | Hugenottenallee 167 | 63263 Neu-Isenburg | Germany | rigaku.com | info@rigaku.com