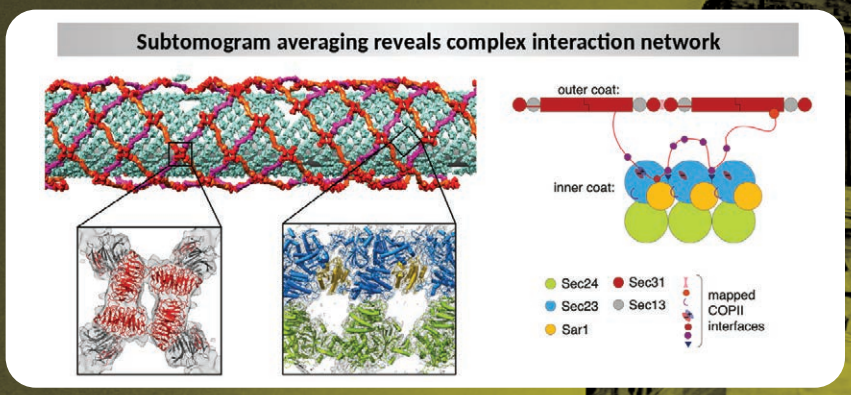
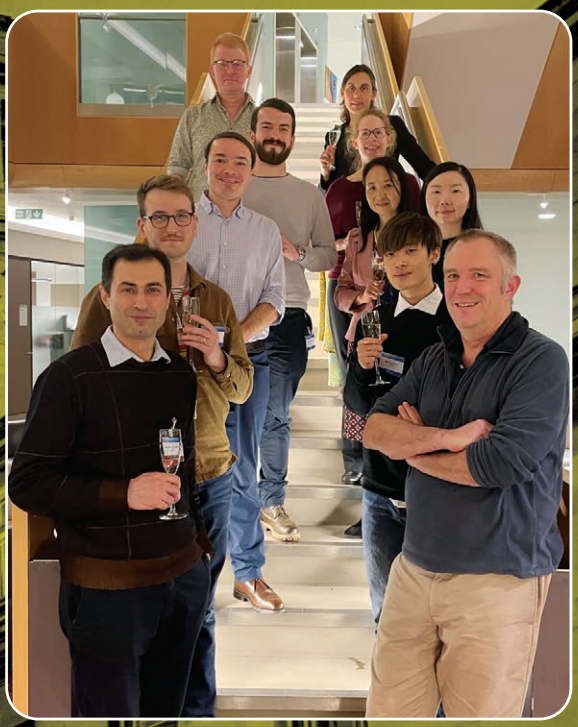
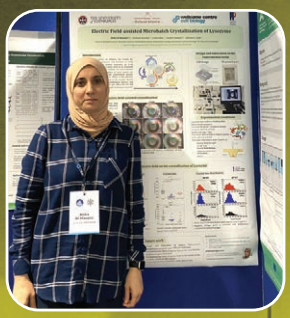
# Crystallography News

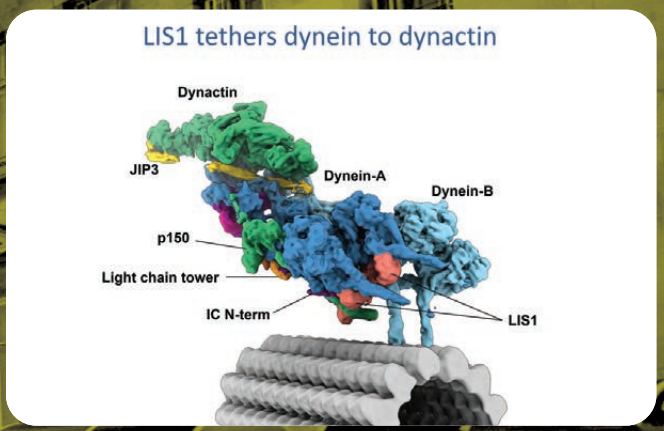
## British Crystallographic Association

Issue No. 168 March 2024
ISSI 1467-2790








## Slides and scenes from recent industrial and biological structures group meetings


| | | | |
|---|---|---|---|
| BCA Spring Meeting 2024 | 6 | British X-ray Crystallographers | 18 |
| IG Autumn Meeting | 12 | News from CCDC | 21 |
| BSG Winter Meeting | 13 | Historical Reflections | 22 |
| ISIC 2023 | 16 | CCP4-BCA Summer School | 25 |
| ECA Council | 17 | Meetings of Interest | 26 |

# A revolution in structural analysis: XtaLAB Synergy-ED and XtaLAB Synergy-DW VHF

XtaLAB Synergy-DW VHF:
The ultimate X-ray diffractometer with a powerful rotating anode source and two selectable wavelengths. Now, with iOptiX for peak performance at the push of a button.


XtaLAB Synergy-ED:
The world's first electron diffractometer designed to be used by crystallographers.

## The combination of X-ray diffraction and electron diffraction broadens the range of single crystal sample size from nanometers to microns

Every working lab faces challenging crystal samples. With the XtaLAB Synergy-DW VHF with iOptiX, it has never been easier to achieve consistently excellent X-ray crystallography results. For those times where your sample doesn't want to form large enough crystals, we offer you the XtaLAB Synergy-ED, a high-performance electron diffractometer built with crystallographers in mind. With intelligent automation built in, it's never been easier to push the boundaries of science. Join the revolution today.

Rigaku oxford diffraction

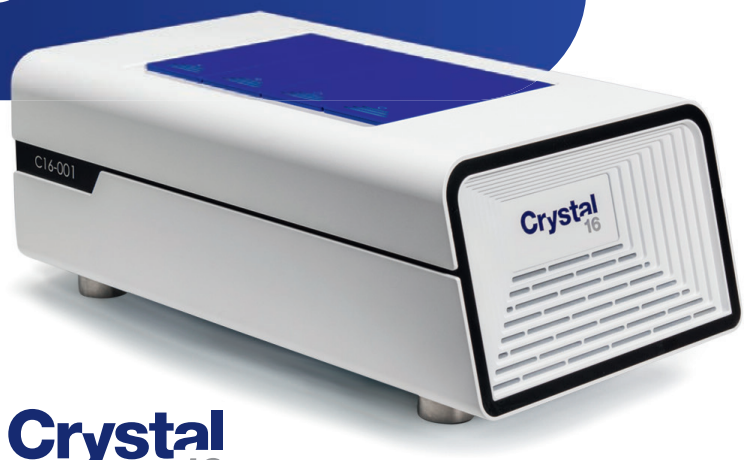
CrysAlis Pro

*"Invaluable instrument in pharmaceutical process development"*

*Principal Scientist MSD,*
*Lead of Crystallization Lab.*

# THE NEW INDUSTRY STANDARD

**BOOK YOUR DEMO NOW**




Crystal 16

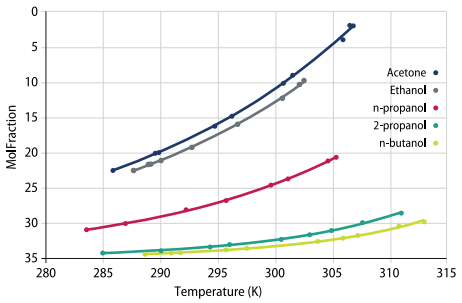
## A powerful system for polymorph, salt & co-crystallization research

Designed by scientists, for scientists, the Crystal16® parallel crystallizer is a multiple reactor station providing a screening solution for temperature dependent solubility determination and solid-state research.

### Benefits

- Obtain 4 temperature dependent solubility curves in 4 hours with as little as 100 mg API
- Determining solubility curves and MSZW has never been easier
- Easily calculate nucleation rates from induction times with built-in software and make use of the feedback control feature
- Run 16 experiments simultaneously at 1mL scale

### Solubility curves in different solvents




**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

# BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
- 10% discount on exhibition stands at the annual BCA Spring meeting.
- Two free registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly Crystallography News.
- Corporate Members will be listed in every Crystallography News and on the BCA website with clickable links to your organisation's website.

Corporate Membership is currently **£850** for one year.

*Corporate Members:*

Bruker: **https://www.bruker.com/**

Douglas Instruments: **https://www.douglas.co.uk/**

International Centre for Diffraction Data (ICDD): **https://www.icdd.com/**

Molecular Dimensions: **https://www.moleculardimensions.com/**

Oxford Cryosystems: **https://www.oxcryo.com/**

Photonic Science: **https://photonicscience.com/**

Rigaku: **https://www.rigaku.com/**

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

### Benefits of Individual BCA Membership:

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

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

# Conference Bursaries 2024

Bursaries are available for BCA members to attend national/international crystallographic meetings in 2024.

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 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/**

# Contents


| | |
|---|---|
| From the President | 2 |
| BCA Council 2024 | 3 |
| From the Editor | 4 |
| Puzzle Corner | 5 |
| BCA Spring Meeting 2024 | 6 |
| BCA AGM Minutes 2023 | 10 |
| Meeting Reports | 12 |
| Bursary Winner Reports | 16 |
| Highlights from the Proceedings of the ECA Council Meetings 2023 | 17 |
| British X-ray Crystallographers | 18 |
| BCA Spring Meeting 2023, CCG Session Report | 20 |
| News from CCDC | 21 |
| Historical Reflections on X-ray Crystallography | 22 |
| Down Memory Lane | 24 |
| CCP4-BCA Summer School 2023 | 25 |
| Meetings of Interest | 26 |


## *This month's cover:*

*Slides and scenes from recent industrial and biological structures group meetings.*


**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 June 2024 issue are sent to the Editor to arrive before 25 April 2024.

Editor: Jon Cooper
University College London,
Gower Street, WC1E 6BT
e-mail: jon.cooper@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 Northwolds Richardson Group Ltd
83 Halifax Way, Pocklington Industrial Estate,
Pocklington, York, YO42 1NR
Tel: 01759 303944
Web: www.nrgprint.co.uk

# From the President

**WELCOME to the March 2024 *Crystallography News*. Advance warning: it's the final President's column before I reach the end of my term, so expect some reflection – no crystallography pun intended.**

The governance of the BCA since 2021 has been significantly less stressful than the preceding 3 years which included the cancellation of the 2020 Spring Meeting and the organisation of the 2021 Spring Meeting online. Perhaps one beneficial side-effect of the latter contingency was that you have only had to endure two conference dinner speeches from me.

Looking back across any period of time or project, it can often seem that things not yet achieved loom large, while it's easy to lose sight of everything that 'just worked', and bits of steady progress made towards projects that have not yet fully crystallized.

There was a recognition three years ago that there were some advantages to running online meetings. Despite regularly exploring possibilities, we still haven't found a cost-effective way to organise hybrid BCA Spring Meetings, but many groups of the Association have adopted online-only one-day meetings, and, on the administrative side, nearly all meetings of BCA Council and Group committees are carried out remotely or in hybrid form, saving travel time, costs and carbon.

Some small but significant additions have been made to our organisational processes over the last couple of years. Firstly, a code of conduct for meetings is now in place. It seems like the last thing a generally well-behaved bunch of crystallographers should need. However, as well as setting expected behaviour from meeting attendees, it sets out processes for handling any incidents. Secondly, as we continue to monitor gender balance at our Spring Meetings, we have updated how we collect EDI data in order to reflect current approaches. In addition, we have introduced an option for Spring Meeting delegates to display their preferred personal pronouns on their lanyard badges if they wish.

Since 1st January, the BCA has a new membership category available: the Fellow category recognises those with an established career in crystallographic teaching or research and provides a way to support the organisation through the membership subscription. A good number of members have already applied for this membership and we hope that this strengthening of membership income will allow us to continue to underwrite and support our annual Spring meetings, support attendance at these and other crystallographic meetings and schools through bursaries to members, and support small outreach and engagement projects as they arise. Members can normally qualify for fellowship membership by having at least five years continuous membership of the Association, although straightforward exceptions can be made for members who have established a career outside the UK, or who have taken career breaks. If you had intended to apply for Fellow membership, but didn't get around to it before renewal, you can apply now by sending a message to bca@hg3.co.uk.

A slightly delayed project will shortly see the publication of short personal profiles of our corporate members and exhibitors in *Crystallography News* and on our website. We hope these introductions might act as ice-breakers for readers who have yet to meet the teams sponsoring and attending meetings. We intend to run the profiles in a random order and will ensure that the all organisations are offered a chance for a profile before we finish the series.

The BCA Spring Meeting will be held later this month in Leeds (25th – 28th March 2024). As always, I would like to record my heartfelt thanks to the chairs of the scientific programme committee, **Hanna Kwon** and **Peter Moody** (Leicester), and to everyone on that programme committee for pulling together another fantastic programme with an overarching theme of *'Breaking Barriers'*. The programme appears elsewhere in this issue, and it's always worth checking the meeting website for last minute additions. The current draft has too many excellent and exciting speakers to single any out. I can genuinely say that there is something of interest in every session, and sometimes a difficult choice of which parallel session to attend: I maintain that this is a sign of a high-quality, densely packed scientific programme. Crystallography is a subject at the interface of a great number of scientific areas and this is evident in the diverse range of topics, including synthesis of framework and pharmaceutical materials, AI in structural biology, and electron crystallography. Thanks to Hg3 for organising so many aspects of the Spring Meeting from the initial planning and contract negotiation, all the way through to on-site support during the meeting. Thank you also to our exhibitors and sponsors of prizes – please do have a chat with them at the meeting. If you want to be involved in the programme committee or suggest ideas for sessions at the 2025 meeting, please get in touch with me or with your BCA Group committee. Planning begins straight after this year's BCA Spring Meeting.

Finally, thank you all for this wonderful opportunity to serve as BCA President and for your continued support – I have genuinely loved nearly all aspects of the role. If there is one downside, it is having to write this column every three months – the deadline is today as I write this, of course. Thanks **Jon Cooper** and previously **John Finney** for ensuring I hit all those deadlines. Writing aside, the job is made significantly easier by support and great input from the rest of the BCA Council – thank you to everyone who has been involved, and I will be forever grateful to the rest of the officers: my immediate predecessor **Simon Phillips** for ensuring a smooth handover, **Alex Stanley** and **Lauren Hatcher** in the role of Secretary have ensured that important documents have been signed and sent out on time; **Simon Parsons** and **Suzanna Ward** as Vice-presidents – have, amongst other things, been the vital connection between the Spring Meeting programme committee and Council; and **Claire Naylor** as Treasurer: none of this could work without her attention to detail and oversight of the not insignificantly complicated and intertwined BCA and Group finances.

I am delighted to hand over responsibility to **Alex Gibbs**, to whom I offer any support that is asked for, and wish her a successful term with as few surprises as possible.

**Richard Cooper**
Oxford

# BCA Council 2024

## 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 (2026)***
**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 Briony Yorke (2026)**
School of Chemistry, University of Leeds, Woodhouse Lane, Leeds, LS2 9JT
B.A.Yorke@leeds.ac.uk

## EDUCATION & OUTREACH

**Dr Ilaria Gimondi (2024)**
CCDC, 12 Union Road, Cambridge, CB2 1EZ

## GROUP REPRESENTATIVES

***Biological Structures***
**Dr Mark Montgomery**
Syngenta
Jealott's Hill International Research Centre, Bracknell, Berkshire RG42 6EY, UK.
mark.montgomery@syngenta.com

***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

***Early Stage Crystallographers***
**Dr Anthony Carter**
Pharmaron Hoddesdon, West Hill Innovation Park, Hereford 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

***Programme Chair (2024)***
**Prof Peter Moody**
Department of Molecular Cell Biology,
The University of Leicester, University Road,
Leicester, LE1 7RH
peter.moody@le.ac.uk

## 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***
**Luca Russo**
GSK Medicines Research Centre, Gunnels Wood Road, Stevenage, Hertfordshire, SG1 2NY, UK
luca.x.russo@gsk.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, Hereford Road, Hoddesdon, EN11 9FH
Anthony.Carter@pharmaron-uk.com

## EX-OFFICIO MEMBERS

***BCA Administrative Officer***
**Nicola Hardaker**
Hg3 Ltd
4 Dragon Road, Harrogate, HG1 5DF
bca@hg3.co.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 Jon Cooper**
University College London, Gower Street, London, WC1E 6BT
jon.cooper@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

**IT is a great pleasure to bring you the March 2024 issue of *Crystallography News*. There is something eye-catching about that number (2024) which seems, at first glance anyway, to be rich in factors of 2. Indeed it reminds me of the game 2048 that is based on a 4 x 4 pattern of squares in which the number 2 appears initially in a few random squares. When the player slides the pattern left, right, up or down, identical numbers add together. The aim is to reach a grand total of 2048 but after playing the game in my odd moments for about a year, I managed to reach 1024 – not a victory but a success of sorts. After that, my performance has improved to the point where I can now reach 1024 about once a week, so after 3 years I can get half way to winning score on a regular basis. What has this got to do with crystallography? Well, it's a game set in a square pattern (yes, plane groups feature prominently in this issue – see the answer to the quiz question we posed in the last issue) and it relies on symmetry in the sense that it is only identical numbers which combine into one. Beyond that, I am struggling a bit, but fear not for I will have no trouble in convincing you of the relevance of the rest of this issue. For instance, we have a report on the 2023 Industrial Group Autumn meeting held at Pharmaron and an account of the Biological Structures Group Winter Meeting held in Oxford in December. We then have a bursary awardee report on the International Conference on Industrial Crystallization which was held in Glasgow last September. Highlights from the Proceedings of the ECA Council Meetings held at the IUCr in Melbourne last year are covered as are the events of a meeting of the Royal Society of Chemistry (RSC) Historical Section on "British X-ray Crystallographers." We then wrap up one or two outstanding session reports from the 2023 Spring Meeting and hear from one the BCA's founder members on some of the BCA's own history, before taking another stroll Down Memory Lane and looking at an electron diffractionist whose exploits in another realm have, I think, largely gone unnoticed in the crystallographic sphere. Most importantly of all, we begin with the up-to-date programme for this year's up-coming Spring Meeting in Leeds which promises to be truly outstanding. Finally, we report on the 2023 BCA-CCP4 Summer School in York.**

Having blotted my copybook by discussing anomalous phenomena in recent issues, I thought I would return to orthodox scientific research and study a couple of fairly recent publications in refereed journals which might be of interest to members. The first is an opinion paper by Chen *et al.*, in *PNAS* entitled "Protein folds vs. protein folding: differing questions, different challenges"[1] which begins by outlining the well-known strengths of AI in predicting protein structure. However, the authors then state: "But this is not folding prediction. Patterns extracted from proteins in the Protein Data Bank (PDB) provide a ready "parts list," circumventing the folding process entirely. These patterns are fully baked." The reason for this statement is that the authors are interested in protein folding pathways and mechanisms *i.e.* exactly how the polypeptide folds to reach the final functional conformation that we see in X-ray, NMR or cryo-EM structures. Biological readers will be well versed in the classical protein folding experiments on ribonuclease by Christian Anfinsen who demonstrated that the process is reversible and that all the requisite information is present in the amino acid sequence. For this work Anfinsen was awarded the 1972 Nobel Prize for Chemistry. The only slight variation on this theme is that some larger proteins require assistant molecules, or chaperones, to prevent them becoming trapped in false minima encountered on their folding pathways. The authors compare the ability of AI to spot the patterns relating protein sequence to structure with the work of Dmitri Mendeleev in compiling the periodic table of elements. That was the pattern recognition phase of chemistry and now theoreticians have a detailed model (quantum mechanics) which allows chemists to understand a large chunk of their discipline. Write to me if you disagree! The authors continue: "How does the relevant physical chemistry select the native structure from a protein's amino acid sequence?" This is a time-honoured question and the current lack of a clear answer does leave one with the impression that AI has perhaps beaten physical chemistry at solving the protein folding problem. I do not fully understand another sentence in the paper which says "A natural direction is physics-informed AI in which existing physical models can be transformed into descriptors within a machine learning framework" but this sort of thing could very well form some interesting sessions at BCA meetings. The authors close by saying: "In short, it seems likely that a physical–chemical theory of protein folding, one that covers the full spectrum of inquiry… is within our grasp."

Another paper by Terwilliger *et al.*, entitled "AlphaFold predictions are valuable hypotheses and accelerate but do not replace experimental structure determination"[2] reaffirms my faith that crystallography will continue to contribute very significantly in biological research. The authors report that for matching pairs of structures in the PDB crystallised in different space groups, the Cα RMS deviation was approximately half that obtained when fitting AlphaFold predictions to high-resolution X-ray structures. The authors describe how the AI approach struggles to predict side chain conformations although they claim that AI structures make good MR models, as indeed many have found. In summary, the authors conclude that experimental structure determination is still very much needed, at least for the foreseeable future.

*Crystallographic Forteana* will return in a future issue.

**Jon Cooper**
UCL

**References:**

1. Chen, S. J. *et al.*, (2023). Opinion: Protein folds vs. protein folding: Differing questions, different challenges. *Proc. Natl. Acad. Sci.* USA. **120**, e2214423119. https://www.pnas.org/doi/10.1073/pnas.2214423119.
2. Terwilliger, T. C. *et al.*, (2024). AlphaFold predictions are valuable hypotheses, and accelerate but do not replace experimental structure determination. *Nature Methods* **21**, 110–116. https://doi.org/10.1038/s41592-023-02087-4.

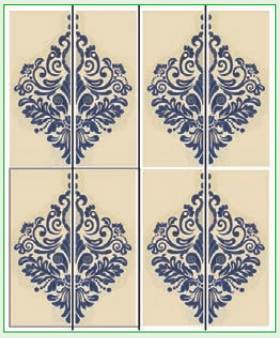
# Last issue's puzzle

The challenge was to identify the plane group of each of the following wallpaper patterns which were photographed in a Venice hotel by **John Lisgarten** (London).

(a)

(b)

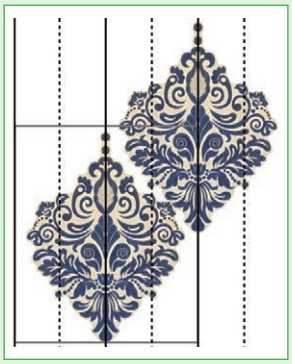
I am not an expert on plane groups but it was fairly clear to me that both patterns were of the same symmetry. The only answer received by the editor was from **Philip Bradfield** (Edinburgh) who is to be congratulated for being a stalwart contributor to this section. Philip's answer is as follows: "I offer (rectangular) *cl* [**cm*] (or equivalently cg) for each of the two plane patterns (vide "An Introduction to Crystallography" (1971) by F. C. Phillips. 4th ed. fig 441 p. 247). *Phillips interestingly uses *cl* rather than *cm*." To the editor, Philip's answer looks absolutely correct with *cm* appearing as plane group number 5 in the International Tables Vol. 1 (1969) having equivalent positions of ($x$, $y$), ($-x$, $y$), ($\frac{1}{2}+x$, $\frac{1}{2}+y$), ($\frac{1}{2}-x$, $\frac{1}{2}+y$). It is interesting that this question has so many correct answers – perhaps a puzzler's dream, as the chance of getting the right answer couldn't be better if several answers are actually correct! Oh well, let's take it back to fundamentals and redraw some of the diagrams in the Phillips book with one of the wallpaper patterns and start from first principles. Fig. 1 below shows the plane group *pm* (although Phillips calls this *pl*) with the mirror lines (shown solid) running vertically and one unit cell shown as a grey box on the lower left.



This certainly has some elements of the actual wallpaper pattern but there's definitely something missing *i.e.* about half of the pattern! So let's try the next point group which Phillips describes. This is *pg* with vertical glide reflection lines rather than mirror lines, giving us the pattern shown in Fig. 2 below. Remember that a glide is a reflection plus a half unit cell translation parallel with the mirror.

Again, not the complete pattern, but we have the potential to create an interesting zig-zag effect, remembering that the unit cell translations will fill in some of the gaps, as shown below. Still our pattern is nowhere near as tightly packed as it should be.

The point about the patterns given in the quiz is that they are centred. As explained in the book by F. C. Phillips, when you add a lattice centre to *pm* (aka *pl*) or *pg*, they boil down to the same plane group which is *cm*, although Phillips mentions that *cl* and *cg* are equivalent alternative notations. In this point group, the glide plains are now half-way between the mirror planes and are shown dashed below.



In this figure we have only shown the action of the central glide line and the two adjacent mirror lines.The remainder of the pattern is generated by unit cell translations or by applying the other symmetry elements.

I am hoping the quiz will return in the next issue.

**Jon Cooper**
UCL

# BCA Spring Meeting 2024


## Monday 25 March 2024

### ESCG Early Career Satellite Meeting

#### Early Stage Crystallographers Group (ESCG)

**13:00 – 21:00**

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

**13:00 – 13:30**

#### ESCG Opening Plenary:

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

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

**13:30 – 17:15**

#### ESCG Research Sessions

Contributed talks from the ESCG community.

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

**17:15 – 17:45**

#### ESCG Annual General Meeting

**18:30 – 21:00**

#### Flash Poster Presentations

Session Chairs: **Phillippa Partridge** (University of Edinburgh) and **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

## Tuesday 26 March 2024

**09:00 – 09:30**

#### Parkin Lecture

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

**09:30 – 10:30**

#### Session 4

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

**10:30 – 11:00**

#### Closing Plenary

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

***Teasing out the secrets of subtle protein dynamics***

### MAIN MEETING

**11:30 – 12:15**

#### Lonsdale Lecture

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

***Thermally Responsive Molecules and Materials***

13:00 – 13:45

## CCG Plenary

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

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

14:00 – 15:30

## Parallel Sessions

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

***Precision, power, and progress: Mastering synchrotron experiments***

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

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

***From Mechanochromism of Organometallic Crystals to Mechanochemical Organic Synthesis***

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

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

***Advances in Processing and Analysis of Bragg Coherent Diffraction Imaging Data***

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

16:15 – 17:45

## Parallel Sessions

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

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

**CCG: Mechanochemistry**
Session Chair: **Guilio Lampronti** (University of Cambridge)
Keynote: **Stuart James** (Queen's University Belfast)

***Mechanochemistry: from curiosity to commercialisation***

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

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

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

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

18:00 – 18:45

## BSG Plenary

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

***When structural data gets messy: insights from molecular simulations***

19:00 – 21:00

## Poster Session with Dinner and Wine

## Wednesday 27 March 2024

09:00 – 09:45

### IG Plenary

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

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

10:15 – 11:45

### Parallel Sessions

**CCG: Framework materials**
Session Chair: **Georgia Orton** (University of Birmingham)
Keynote: **Ross Forgan** (University of Glasgow)

***Probing Physical Properties of Metal-Organic Frameworks by High Pressure Single Crystal X-Ray Diffraction***

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

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

***Synergising Diffraction Sciences – an Industrial Perspective***

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

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

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

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

11:45 – 12:15

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

13:00 – 14:30

### Early Career Prize Lectures

**Biological Structures Group Early Career Prize**

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

**Chemical Crystallography Group Prize for Younger Scientists**

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

**Physical Crystallography Group Early Career Prize**

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

14:30 – 14:45

### Exhibitor Forum

15:15 – 16:45

### Parallel Sessions

**BSG: Artificial intelligence in structural biology**
Session Chair: **Georgina Menzies** (Cardiff University)
Keynote: **Isabel Moraes** (Google Deepmind)

***Integrative Structural Biology with AI***

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

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

***Under Pressure: Rational Design of Complex Mechanical Phenomena in Molecular Crystals***

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

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

***Operando Studies of Local Structure in Battery Materials***

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

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

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

***The future of macromolecular crystallography in the age of machine learning***

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

18:00 – 19:00
## BCA Annual General Meeting

19:30 – 01:00
## Conference Dinner & Ceilidh

# Thursday 28 March 2024

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

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

10:15 – 11:45
## Parallel Sessions

**BSG: Breaking barriers with emerging technology in structural biology**
Session Chair: **Hanna Kwon** (University of Leicester)
Keynote: **Dr Pedro Nunes** (Diamond Light Source)

***The High-energy Electron Xtallography Instrument: a new tool for macromolecular structure determination***

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

**CCG: Molecular interactions and Supramolecular chemistry**
Session Chair: **Krešo Bucar** (University College London)
Keynote: **Katharina Edkins** (University of Strathclyde)

***Drug/co-former assembly in solution and the solid – from predicting co-crystallisation to taste masking***

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

**PCG/IG: Energy & Sustainability**
Session Chairs: **Glen Hebberd** (Durham University) and **Tony Bell** (Sheffield Hallam University)
Keynote: **Beth Johnston** (University of Sheffield)

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

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

12:15 – 13:45
## Parallel Sessions

**BSG: Open Session**
Session Chairs: **Georgia Isom** (University of Oxford) and **Benjamin Cooper** (University of Oxford)
Keynote: **Tanmay Bharat** (MRC Laboratory of Molecular Biology)

***Solving Structures of Crystals in Cells using Electron Tomography***

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

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

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

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

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

## CLOSE OF CONFERENCE

# BCA AGM 2023 Minutes

## Draft minutes of the 2023 Annual General Meeting of the British Crystallographic Association

High Tor 1 The Edge, University of Sheffield at 18:00 on Wednesday, 5th April, 2023.

1) **Approval of Agenda**

The agenda was approved; proposer: Elspeth Garman, seconder: Bill Clegg

2) **Apologies for Absence**

Apologies were received from Simon Phillips, Judith Howard and Lauren Hatcher.

3) **Minutes of last AGM**

The minutes were published in the March 2023 issue of Crystallography News, and a link was included with the email containing the AGM agenda.

The minutes were approved; proposer: Mike Glazer, seconder: Charlie McMonagle

4) **President's Report**

The president, Richard Cooper, noted the sad loss of one of our Founder members, Olga Kennard, and also from CCDC, David G. Watson. Thanks were recorded to all those who played a role in organising the current meeting: Helen Playford (program committee chair), Suzanna Ward (as VP, representing BCA officers), all the volunteers on the programme committee, Hg3 and the Sheffield Conferences team, and all of our meeting sponsors and exhibitors.

The next BCA Spring Meeting will be held at the University of Leeds, 25th to the 28th of March, but in a different lecture and exhibition space than the 2022 meeting. The president reported that Council were keen to establish a long-term relationship with one or two conference venues, including Leeds, in order to simplify meeting planning. Members with ideas for the 2024 program were encouraged to pass them on to group reps who would be attending the first planning meeting at 8am on Thursday. The 2024 Bragg lecturer has been announced as Prof Arwen Pearson, and the lecture will be hosted during the 2024 Spring Meeting.

The president thanked the BCA Council, especially outgoing Crystallography News editor John Finney, and outgoing members Hazel Sparkes and Christine Beavers, and welcomed Ilaria Gimondi who has been co-opted as Education and Outreach Coordinator.

5) **Secretary's Report**

In the absence of the secretary, Lauren Hatcher, her report was presented to the meeting by the president.

The secretary has kept the IUCr and the ECA up to date with the composition of BCA Council. We have held two council meetings this year. We have retained the practice of having the Autumn Council meeting online, because it reduces travel costs and means everyone doesn't have to spend a day travelling. This year the Spring Council meeting was in a hybrid format, which meant that people who were not here on the Monday night could join. That worked very well. Nominations for the council elections last year were received on time. The secretary notes her thanks to the Nominating Committee for their hard work in selecting candidates.

No questions were raised.

6) **Hg3 Report**

In the absence of a representative of Hg3, the President presented the current membership data. Our membership stands at 487 members versus 494 last year. Our corporate members are Bruker, CCDC, Douglas Instruments, ICDD, Molecular Dimensions and Oxford Cryosystems. There are a couple of big names missing off that list and they are currently being chased up.

Our main advertisers in Crystallography News are Bruker UK, Oxford Cryosystems Limited, Rigaku and Technobis.

The total number of attendees at the current meeting is 206, which up by five on last year. The list of our exhibitors is Rigaku Europe SE, STOE & Cie GmbH, Anton Paar, Douglas Instruments, Formulatrix Inc, Constant Systems Limited, Oxford Cryosystems, Bruker UK Ltd, CCDC, Malvern Panalytical and Molecular Dimensions. Meeting sponsors are Royal Society of Chemistry (CrystEngComm), STOE & Cie GmbH, ACA AIPP, Faraday Institution, IUCr, Malvern Panalytical, Rigaku Europe SE and poster prizes have been sponsored by IUCr (3), AIPP/ACA (1), Faraday Institute (1), CrystEngComm (2), Rigaku (2).

No questions were raised.

7) **Report of the Treasurer to include Presentation of the Accounts for 2022 and the Examining Accountant's Report**

The treasurer, Claire Naylor, presented the Accounts for 2022. Final copies are available on the Charity Commission website when they are finalized. In summary it was a successful year financially. Grants and sponsorships are significant this year thanks to a very generous gift from Carl Schwalbe in his will of nearly £11,000, and thanks to the IG group for a £5,000 donation to the ABBF, and for setting up a new IG bursary fund with an additional £5000. Crystallography News continues to generate significant income.

We continue to try and keep down expenses – moving one of the council meetings online in the autumn is a significant saving, which enables us to direct more funds to our charitable activities. Market conditions have been difficult, so we did make some losses on our investments, but those have already recovered this year. Our main income each year is the income from the membership – please encourage people to become members.

The treasurer thanked Hg3, council members, BCA group treasurers, and our investment manager Charles Stanley and the UHY Hacker Young accountants.

A question was raised as to why the admin fee was higher in 2022 than in 2021. The treasurer responded that the online meeting in 2021 removed some admin expenses for Hg3.

A question was raised as to why the membership subs dropped by nearly £3000 in 2022 compared to 2021. After a short investigation, the treasurer reported that the number of corporate members had dropped by 3 in that year, and that efforts were being made to grow the corporate membership again.

Acceptance of the accounts; proposed: Elspeth Garman, seconded: Andy Maloney.

**8) Appointment of Examining Accountant for 2023**

The treasurer recommended reappointing UHY Hacker Young due to their familiarity with the somewhat complex arrangements of the Association.

Appointment of Examining Accountant for 2023; proposed: Helen Playford, seconded: John Helliwell.

**9) Elections to Council**

Elections are now held online in January. Briony Yorke was elected as an Ordinary Member of BCA Council for the term 2023-2026. The president noted that three posts would be open for election in 2024: Education and Outreach Coordinator; Ordinary Member; President. He thanked the BCA Nominating Committee for their work in securing nomination for these posts, particularly Elspeth Garman who has served a six-year term on the committee. The current committee is Jon Agirre, Simon Phillips, Paz Vaqueiro, Claire Wilson and Chris Frampton.

**10) Honorary Members**

No nominations for honorary members were received by the 2022 deadline. Nominations for 2023 should be sent to the President by August 31st 2023.

**11) Proposal to modify the Statutes to introduce a Fellowship class of membership**

Following discussion at the 2022 AGM, the Council brought a proposal to update the statutes to introduce a new class of Fellow membership to the BCA. The wording specifies a new class of membership normally requiring five years of membership, and including a discretionary waiver of this for exceptional circumstances.

A question was raised about whether Fellow members could use letters after their name (e.g. FBCA). Council will look into this option in the future.

A question was raised about what the new membership class signified given that five years of membership is not a guarantee of expertise. The view of Council is that the simple requirements are pragmatic and will generally indicate commitment to the organisation and subject.

Proposal to modify the Statutes; proposed Richard Cooper – vote of the AGM: 33 in favour, 4 against.

**12) Membership, annual subscriptions and subventions**

No change of membership fees recommended by Council. Fees for Fellow members set at double the normal category for this member.

It was noted that this left Honorary members with a zero rate for Fellow membership – however the statutes require further updates if the AGM wishes to allow a non-zero rate for Honorary members.

Acceptance of proposed membership fees; proposed Mike Probert, seconded Claire Naylor.

**13) Equality, Diversity and Inclusivity report**

The AGM was reminded of our current Conference and Speaker Invitation policies. Statistics are available on the BCA website and are presented as % women in each class. The president noted that this categorisation does not allow us to report rates of non-binary identities as we do not collect or hold this information for meeting organisers or speakers. The overall statistics for 2022 and 2023 are reported to the nearest 5%. The YCG meeting reported 50% women speakers, chairs and plenary speakers. The main meeting could improve numbers of women chairs and speakers – currently the numbers approximately reflect the distribution in our membership, but our aspiration is that this distribution should reflect the general population.

**14) AOB**

Elspeth Garman thanked the BCA Council for their work.

The meeting closed at 18:50.

# Report on the 2023 Industrial Group Autumn Meeting

Pharmaron Hoddesdon

**THE 2023 BCA-IG Autumn Meeting was held on 28th November 2023 at Pharmaron UK's Hoddesdon site. This was the first time Pharmaron Hoddesdon had hosted the BCA-IG meeting and the first in-person BCA-IG meeting since 2019! The meeting consisted of a variety of academic and industrial talks and multiple networking sessions.**

We arrived to a nice set of refreshments (and coffee!) with some time for networking and getting to know each other. The meeting was introduced by the chair: **Joseph Benson** (Pharmaron). The morning session started with a talk presented by **Anthony Bell** (Sheffield Hallam) whose work was entitled "Dynamic high temperature crystallisation and processing properties of industrial soda-lime-silica glasses." Tony presented a thorough and meticulous temperature-controlled analysis of multiple glass materials heated between devitrification and melting temperatures. Aside from the *in situ* observation of cristobalite, wollastonite, quartz, and tridymite phases, his team observed an unknown primitive cubic phase, and several unassigned Bragg reflections. These interesting findings could be the seed for a potentially interesting PhD project. The session continued with a talk from **Ian Scowen** (Lincoln) entitled "Structure hierarchy in multi-component organic crystals." Ian presented a series of projects from his research group, ranging from studies of proton transfers in salts and co-crystals, to molecular photochromic donor/acceptor systems with reversible colour changes. The latter was an example of a serendipitous discovery after a batch of a crystal was stored inside a drawer and another batch of the same crystal was left close to a window that received lots of sunlight. After some time, one was colourless and the other was a beautiful purple! A deep dive into this intriguing phenomenon showed this process to be reversible, and triggered by UV light in one direction, and heat in the other. Concluding the morning session was a talk from **Michael Hall** (Newcastle/Indicatrix) entitled "High-throughput oil-encapsulated nanodroplet crystallisation for organic-soluble small molecules." Michael presented an investigation into the use of Encapsulated Nanodroplet Crystallisation (ENaCt) to aid the search for new polymorphs and co-crystals, and crystallisation of salts and structural elucidation of natural products in a high-throughput fashion. Using ENaCt, his team was able to successfully identify the 13th and 14th polymorph of 5-methyl-2-[(2-nitrophenyl) amino]-3-thiophenecarbonitrile (a.k.a. ROY) which holds the current record for the largest number of fully characterized organic crystal (true) polymorphs. ENaCt also facilitated the structural elucidation of a natural product, identifying 24 new structures of it!


*Introduction from the IG Autumn Meeting chair* ***Joseph Benson*** *(Pharmaron).*

*Morning session speakers:* ***Ian Scowen*** *(Lincoln),* ***Michael Hall*** *(Newcastle/Indicatrix) and* ***Tony Bell*** *(Sheffield Hallam).*

The generous lunch break provided an ideal occasion for networking with fellow crystallographers, spanning across academia and industry. Moreover, it allowed us to address any lingering questions from the talks within the first session. It was also accompanied by a lab tour of the main materials science facilities at Pharmaron Hoddesdon. After lunch, the talks turned from an academic to an industrial setting, starting with technology updates from multiple companies.

*Lunchtime networking at the IG Autumn Meeting.*

The afternoon session was chaired by **Anthony Carter** (Pharmaron). The first of the technology updates was presented by **Christopher Smalley** (Bruker) who introduced the Bruker D6 PHASER and how it has changed XRD history. The main advances that stuck out from this update were the 600W and the 1200W tools that provide high-quality XRD data and do not require a chiller! They also include motorised slits and a motorised anti-scatter screen and have the capability to hold a 12-position sample stage which is very useful for high-throughput applications. This continued with an update by **David Walker** (Warwick) who introduced the new National Electron Diffraction Facility (NEDF). This consists of three partners including Rigaku Synergy ED instruments that specialize in electron diffraction. The goal of the facility is to create a step change in crystallographic structure determination by introducing an accessible alternative to single-crystal XRD while operating at large scale. The NEDF can be accessed by a mail-in service, similar to the NCS, or in-person with a visit to a site where you would be trained to use the instrumentation and run your own samples. The third update was by **Omar Matar** and **Mark Benson** both from Rigaku. Omar gave an insightful technology update introducing a new product line, the MiniFlex. The MiniFlex XpC with ASC-24 has high-throughput capabilities with a 24-position sample stage and a robotic arm, with the option for multiple non-ambient attachments. Complementary to the update about the NEDF, Mark gave an in-depth introduction to the XtaLAB Synergy-ED dedicated electron diffractometer. Probably the most unique capability of a dedicated electron diffractometer is the ability to solve the structure of nm-sized samples. Finally, the last of the technology updates was presented by **James Craig** (Anton Paar) who introduced their new XRD instruments, including the XRDynamic 500, which was designed with non-ambient XRD in mind. In this system, one controller conveniently controls the instrument housing for cooling water, compressed air, vacuum and gas supplies to provide a comprehensive non-ambient range of conditions.

Next, **Jacob Danks** (Pharmaron) gave a fantastic talk surrounding the development of an industrial high throughput co-crystal screening workflow. As co-crystals can be a viable alternative to salts, this was highly insightful. Jacob used three high-throughput techniques to generate co-crystals: slurry, evaporative crystallisation and LabRAM, which is resonance acoustic mixing. The data were evaluated by hits found, ease of experiment, amount of sample used and other high-throughput criteria. It was found that the LabRAM and evaporative crystallisation were complementary techniques to be performed after a typical solubility screen. This was validated by experiments with sulfasalazine which has low permeability and solubility. The final talk was presented by **Margarita Mersiyanova** (Pfizer) whose work, completed during her PhD at Johnson Matthey/University of Reading, was entitled "PXRD in the structural characterisation of opioids". The project aimed to fill gaps in research caused by the restrictive use of opium, despite its historic use as a painkiller throughout thousands of years. PXRD provided the main tool for identification, with DASH being utilized for structure solution, overlayed with the refined structure defined in TOPAS. DFT-D was used for crystal structure validation. With some structures taking a day for identification (and others even months!), Margarita was able to successfully solve all 10 opioid structures.

*Afternoon session speakers: **Margarita Mersiyanova** (Pfizer), **Jacob Danks** (Pharmaron), **Omar Matar** (Rigaku), **James Craig** (Anton Paar), **Christopher Smalley** (Bruker) and **David Walker** (Warwick).*

The meeting concluded with the BCA-IG AGM. Overall it was a well organised day full of very interesting and highly engaging talks on industrial crystallography.

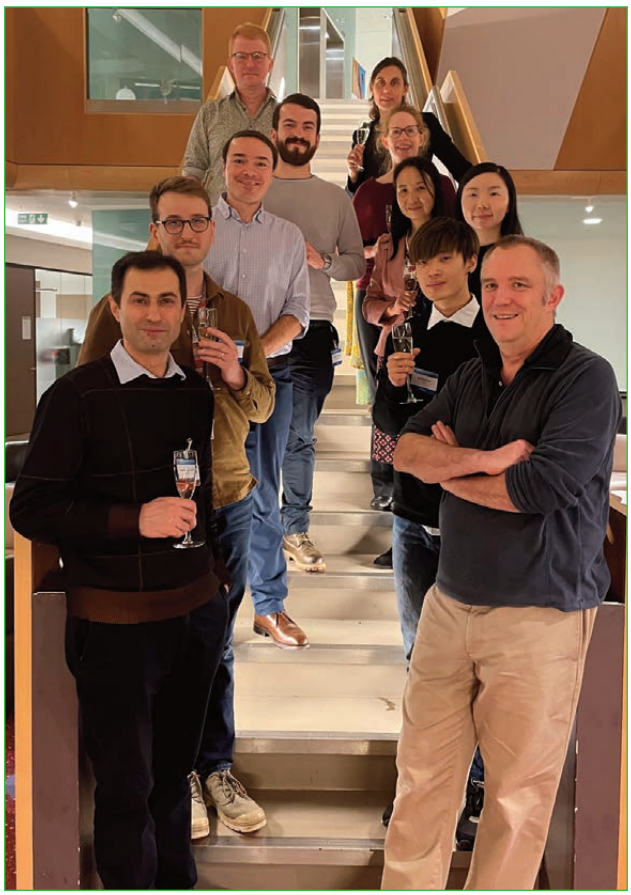
**Andy Molina, Indigo Dean, Alannah Byron**
Pharmaron UK

# Biological Structures Group Winter Meeting

## Oxford 2023

**THE 2023 BSG Winter Meeting on "Breaking Barriers in Structural Biology of Cells and Systems" was held at the University of Oxford on 11th December and was organised by Simon Newstead and Joanne Parker. The conference was generously sponsored by Douglas Instruments, iLab Solutions, Kavli, Molecular Dimensions, Quantifoil, Shimadzu and ThermoFisher Scientific.**

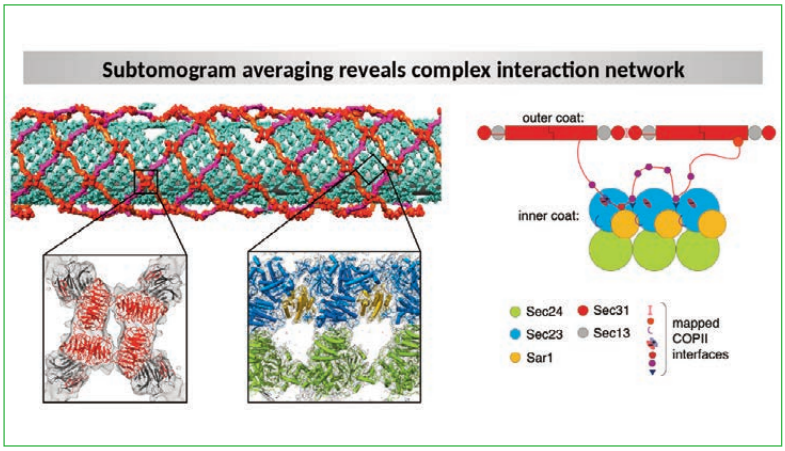
The meeting began with a welcome for attendees by **Simon Newstead** (Oxford) who also chaired the first session which began with a lecture by **Joanne Parker** (Oxford) entitled "Drug recognition and transport via solute carriers." The speaker described how solute carriers (SLC's) are membrane proteins which allow cells to acquire nutrients from their surroundings and also to expel harmful toxins. Humans have 458 genes for SLC's, proteins which use ion gradients, rather than ATP hydrolysis, as their source of energy and are therefore classed as secondary active transporters. They are also attractive drug targets as one can target the SLC's in specific tissues. Structurally they consist of two membrane-spanning 6-helix bundles which are arranged to form a large aqueous cavity in the centre of the membrane. They belong to the major facilitator superfamily (MFS) – the second largest group of membrane proteins. Joanne then described cryo-EM work on the folate transporter PCFT and the organic anion transporter OAT1 which were complexed with an inhibitory nanobody to trap compounds of interest bound to the transporter. Chicken PCFT is a 50 kDa protein with 85 % identity to the human transporter and can be expressed well in yeast. Human PCFT is the target for the antifolate drug pemetrexed which has been approved for cancer treatment. OAT1 is involved in the clearance and excretion of unwanted anionic compounds in the blood stream and is the target for the gout drugs probenecid and tenofovir. These compounds competitively inhibit the reabsorption of uric acid by the proximal tubules of the kidney, thus reducing blood uric acid levels. Chloride ions enhance transport and were shown by cryo-EM of the rat protein to bind in the central cavity close to α-ketoglutarate.



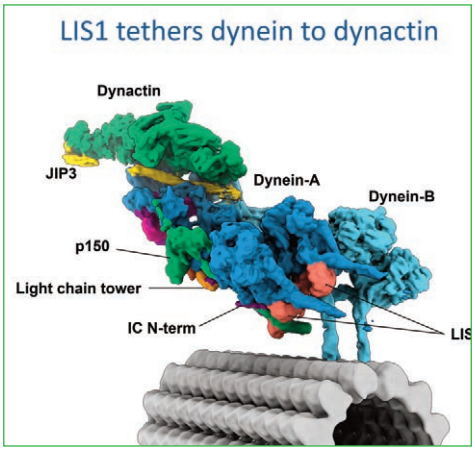
*Speakers and chairs at the 2024 BSG Winter Meeting in Oxford. From front to back on the left:* ***Elton Zeqiraj*** *(Leeds),* ***Alex Cook*** *(Oxford),* ***Simon Newstead*** *(Oxford),* ***Tomas Pascoa*** *(Oxford) and* ***Matt Higgins*** *(Oxford), and on the right:* ***Andrew Carter*** *(MRC Cambridge),* ***Kin Chao*** *(UKRI, STFC),* ***Beijia Wang*** *(Kings),* ***Xiaodong Zhang*** *(Imperial),* ***Joanne Parker*** *(Oxford) and* ***Giulia Zanetti*** *(Birkbeck/UCL).*

The binding of probenecid and tenofovir was also studied by cryo-EM and mutagenesis. The next lecture was given by **Kin Chao** (UKRI, STFC) on the use of molecular dynamics in the analysis of cryo-EM reconstructions. The speaker described using MD to generate synthetic cryo-EM images of the GroEL chaperone which were compared with experimental datasets. Kin then went on to describe simulations of GPCRs in the membrane to identify their cholesterol binding sites and to study the modulating effects of glycosphingolipid GM3 which binds to the extracellular domain. The next speaker in this session was **Alex Cook** (Oxford) who gave a lecture entitled "How African trypanosomes evade the innate immune system." The speaker emphasised how the rapid movement of this extracellular parasite allows it to minimise contact with cells in the bloodstream, as part of its strategy for cellular immune evasion. It also has variable surface glycoproteins (VSGs) such that if one clone of the parasite generates an immune response, there are plenty more which do not. The speaker then described studies of one of the trypanosome's invariant surface glycoproteins (ISGs), ISG65, which is linked to the membrane by its C-terminal tail and helps the parasite to evade the innate immune system. ISG65 was shown to bind to the complement protein C3 and a crystal structure of the complex with C3d was determined as well as a cryo-EM structure of the complex with C3b. ISG65 was shown to be a large 5-helix bundle protein but it is not clear how it inhibits the complement system since the structure and activity of C3b and C3d are unaltered in the complexes and the reactive thioester, which attaches these proteins to invading pathogens, is not affected. Work is ongoing to improve our understanding of the system. The last lecture of this session was given by **Xiaodong Zhang** (Imperial) and was entitled "Macromolecular machines that open double-stranded DNA for gene transcription." The speaker emphasised how double-stranded DNA opening is involved in replication, transcription and DNA repair. RNA polymerase is a flexible, multi-domain protein which binds DNA in a jaw-like manner and initiates transcription by separating the two strands and delivering the template strand to the active site. The speaker explained how the σ factor permits the enzyme to bind to specific promoter regions, $\sigma^{70}$ being the main housekeeping one. In contrast, $\sigma^{54}$ is involved in stress-responses and is inhibitory since it binds in the cleft of the enzyme, preventing the DNA from opening. The speaker then described a huge amount of cryo-EM work on RNA polymerase activators which are hexameric ATPases that facilitate opening of the DNA molecule and cause the N-terminus of $\sigma^{54}$ to slot between the two strands. Conformational changes in the activator protein during ATP hydrolysis appear to pull the N-terminus of $\sigma^{54}$ through the DNA. Xiaodong ended her lecture by suggesting that time-resolved EM studies may shed further light on these processes.

After lunch and posters, the second session was chaired by **Matt Higgins** (Oxford) and began with a lecture by **Andrew Carter** (MRC Cambridge) entitled "Cargo transport by dynein/dynactin." The speaker described how dynein plays an important role in axonal transport of endosomes for signalling, autophagosomes, mitochondria and viruses. Dynein has 12 subunits and functions with a cofactor known as dynactin which itself binds activating coiled-coil adaptor proteins. These adaptors are associated with specific cargo and trigger dynein to 'walk' along microtubules. The speaker emphasised how cryo-EM studies of these complexes require the highly repetitive microtubules to be deleted from the images in order to average the dynein/dynactin complex. Andrew reported numerous adaptor protein structures and described common sequence features of these molecules. Certain mutations in the adaptor protein LIS1 are associated with the smooth brain disease lissencephaly. The speaker described a fascinating complex in which numerous proteins had been captured, demonstrating that LIS1 binds to both the dynein motor domain and p150, the largest subunit of dynactin. The next speaker, **Tomas Pascoa** (Oxford) gave a lecture entitled: "Structural basis of the mechanism and inhibition of human ceramide synthase." Tomas emphasised how ceramides (lipid molecules joined by an amide bond) promote free fatty acid incorporation into triglycerides and high levels of certain ceramides are associated with diabetes, obesity and cardiovascular disease. Inhibitors of ceramide synthesis therefore have therapeutic potential. The speaker described how two enzymes are involved in *de novo* ceramide synthesis, the second being ceramide synthase, which is inhibited by the mycotoxin fumonisin $B_1$. The human enzyme CerS6 has been subjected to cryo-EM studies by the use of nanobodies and this work has revealed a large central acyl-linked palmitoyl chain covalently linked to a histidine residue. The fact that this can be displaced by the second substrate suggests that it is a reaction intermediate. A cryo-EM structure of the complex with fumonisin B1, which forms a covalent adduct with the palmitoyl group, suggests a ping-pong or double-displacement mechanism for the enzyme. The next lecture in this session was given by **Giulia Zanetti** (Birkbeck/UCL) and was entitled: "Membrane trafficking mechanisms in the early secretory pathway." The speaker described the COP II coat proteins which mediate vesicular transport from the endoplasmic reticulum (ER) to the golgi by budding out in the form of polyhedral cages. The speaker described subtomogram




*Subtomogram averaging of in vitro-reconstituted COPII coated tubules by* ***Giulia Zanetti*** *(Birkbeck/UCL) reveals their structure and assembly.*




***Andrew Carter*** *(MRC Cambridge) spoke on cryo-EM studies of axonal cargo transport by dynein and dynactin and the role of the protein LIS1 in the smooth brain disease lissencephaly.*

averaging of reconstituted COP II vesicles and tubules from yeast, revealing the structures and functions of Sec 23, 24, 31 and 13 as well as Sar 1. The speaker described how microsomes allow the cages to be studied further, revealing how the outer coat proteins have very flexible interactions while the inner coat proteins, which are thought to be the main driving force behind the curvature of the system, form a patchy lattice.

Following the afternoon break, the final session of the meeting, chaired again by **Matt Higgins** (Oxford), began with a commercial presentation by **Tom Drake** (Thermo Fisher) concerning transient expression systems using CHO, sf9 and HEK293 cells, as well as strategies for selenomethionine labelling of mammalian proteins. The next lecture was given by **Beijia Wang** (Kings) whose talk was entitled "The nature of the molecular interactions at high resolution of the *Streptococcus pneumoniae* topo-IV DNA complex with the novel fluoroquinolone delafloxacin." This bacterium is the leading cause of community-acquired pneumonia and is becoming increasingly resistant to antibiotics. The topo-IV enzyme is involved in separating the two interlinked chromosomes after replication and is a target for fluoroquinolone drugs, such as delafloxacin. The latter is particularly good at treating antibiotic resistant strains of this organism and at the molecular level it, like other fluoroquinolones, stabilises the G-segment bound complex at the cleaved stage. The speaker described a 2.5 Å structure of topo-IV with an 18 bp fragment of DNA, in which the drug had intercalated, bound to the enzyme with additional contacts being made by a magnesium ion and bridging water molecules. Last but not least, the final talk of the conference was given by **Elton Zeqiraj** (Leeds) and was entitled "Discovery of molecular glues that regulate activity and conformation of dynamic protein complexes." The speaker introduced the area of ubiquitin signalling with an emphasis on JAMM domain deubiquitinases (DUBs) which are heterodimeric complexes requiring zinc for catalysis. These enzymes are of much interest as cancer drug targets since inhibition of DUBs is known to affect cell-cycling and promote apoptosis. The speaker emphasised how knockout of the DUB BRISC-SHMT2 complex increases degradation of the interferon receptor. Cryo-EM and mass-spectrometry have shown that small molecule inhibitors make the BRISC protein dimerise in an autoinhibited state and have anti-inflammatory effects in autoimmune disease.

The meeting was followed by a wine reception and the presentation of poster prizes by **Simon Newstead** (Oxford). These were awarded to **Stanley Fronik** (Oxford) and **Brendan Farrell** (Oxford). In addition an exhibitor prize for a 'Guess the number of cryo-EM grids' competition was awarded to **Girish Ram** (Oxford) by **Claire Naylor** (Quantifoil). This concluded a very interesting and memorable meeting for which the organisers **Simon Newstead** and **Joanne Parker** (Oxford) must be congratulated.

*The post-conference prize-giving and wine reception.*

**Jon Cooper**
UCL

# International Symposium on Industrial Crystallization, ISIC

## Glasgow 5th – 8th September 2023

**THE international conference on industrial crystallization was an excellent opportunity to meet researchers and students working in the field and a fruitful learning experience in the last year of my PhD in Scotland. As I live in Edinburgh, it took less than an hour by train to arrive at the conference venue, the University of Strathclyde Technology and Innovation Centre in Glasgow, which is a spacious and modern building, incorporating CMAC, the platinum sponsor of the conference.**

The program was intensive and versatile, and it incorporated a set of tutorial sessions highlighting the fundamentals and the main aspects of industrial crystallization. The tutorials took place one day before the conference. Upon my arrival, I was warmly welcomed by **Prof. Joop Ter Horst**, one of the organizers and leading scientists in the industrial crystallization field.

The conference kicked off at 9.00 am on the 6th of September, with a plenary session by **Kevin Girard** (Pfizer) explaining the FAST (Flexible API Supply Technology) approach, which aims to build and deploy continuous crystallization processes at Pfizer. Two more lectures by distinguished speakers followed before the parallel sessions took place for the rest of the conference. After the first parallel session, I had the opportunity to present my poster and discuss my findings with the crystallization research community. The poster attracted a good number of participants, and I exchanged contact information with a few for future collaborations.

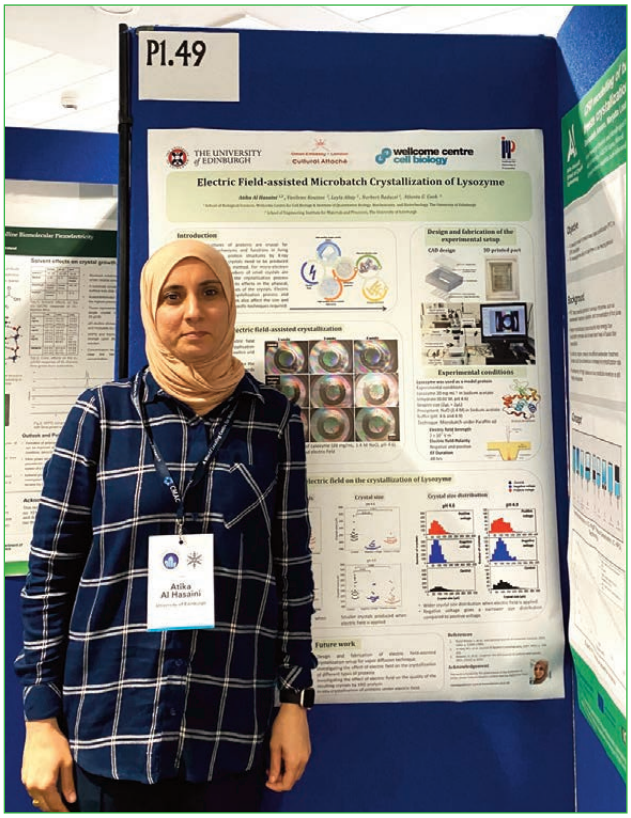
In the parallel sessions, I attended mostly the crystallization fundamentals sessions, which were a versatile blend of industrial crystallization approaches and fields. A number of talks were of high interest to me, such as the laser-induced crystallization approach, the microfluidic continuous crystallization approach and growth rate measurement as well as the mechanochemistry approach.

*Attendees at ISIC 2023: **Atika Al Hasaini** (Edinburgh), **Joop Ter Horst** (Strathclyde), **Jan Sefcik** (Strathclyde) and **Mercedeh Sadat Hosseinalipour** (ETH Zurich).*

Socializing during the event was spontaneous and relaxed, as there was plenty of time during coffee and lunch breaks as well as the social events. I am glad that I had the chance to discuss my research with one of the leading researchers in the field, **Stéphane Veesler** (Marseille), who gave me constructive feedback and suggestions to improve my research methods. I can say that I have made good connections during these times, and I acted as a tour guide for once, taking some of them to see the UNESCO World Heritage Site, Edinburgh.

At the end of the conference, closing remarks were delivered by the organizers, in addition to presenting awards for the best posters and announcing the next conference, which will be held in Hungary in 2026.

**Atika Al Hasaini**
Edinburgh




*Atika Al Hasaini (Edinburgh) presenting in the poster session at ISIC 2023.*

# Highlights from the Proceedings of the ECA Council Meetings 2023

*Logo of the European Crystallographic Association. (Dritan Siliqi, CC BY-SA 4).*

**THE 2023 meeting of the Council of the European Crystallographic Association (ECA) took place over two afternoons on the 20th and 22nd of September. 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 BCA have one representative/vote, with the first council meeting attended by Suzanna Ward, the second by Richard Cooper. 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. However, due to this year's IUCr Congress taking place in Melbourne, it was decided to hold the Council meeting online to ensure as high an attendance as possible.**

A considerable part of the business at ECA Council Meetings naturally concerns the planning of future European Crystallographic Meetings, and Councillors receive progress updates on the planning of upcoming meetings as well as the opportunity to vote for the location of future ECMs. Preparations are well underway for ECM34, which is scheduled to take place in Padova, Italy, from the 26th – 30th August 2024 (more information is available on the conference website: https://www.ecm34.org/). It should be noted that EPDIC18, the European Powder Diffraction Conference, will be held immediately after ECM34 at the same venue (https://www.epdic18.org/).

Due to the ongoing conflict in Ukraine, where ECM35 was due to be held in 2025, a proposal was made by the Polish Crystallographic Association in collaboration with ECM35 organisers and other Ukrainian colleagues to move the location of the conference to Poznań, which was approved by the Council. A bid from Czech colleagues to hold ECM36 in Prague (at the same location as the 25th IUCr Congress) was also presented and approved.

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 the Council meeting in September proposals were heard and approved for the incorporation of two new prizes related to ECA: the George M. Sheldrick Prize (awarded to a non-tenured researcher for outstanding scientific contributions in the field of structural sciences) and the Lodovico Riva de Sanseverino Prize (awarded in recognition of notable contributions to the dissemination of crystallography in the field of education at all levels). 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 8th European Crystallographic School (ECS8), which took place in-person in Berlin, Germany, in June 2023. European Crystallographic Schools combine lectures and hands-on tutorials to provide attendees a fundamental understanding of the principles underpinning crystallography. Each school is unique, however, and offers a variety of topics to cater to a broad range of interests. ECS9 will take place during 2024 in Nancy, France, and a successful bid takes ECS10 to Ohrid, North Macedonia, in 2025. For further information on the ECS, please visit https://ecanews.org/european-crystallography-school/.

**Suzanna Ward**
CCDC

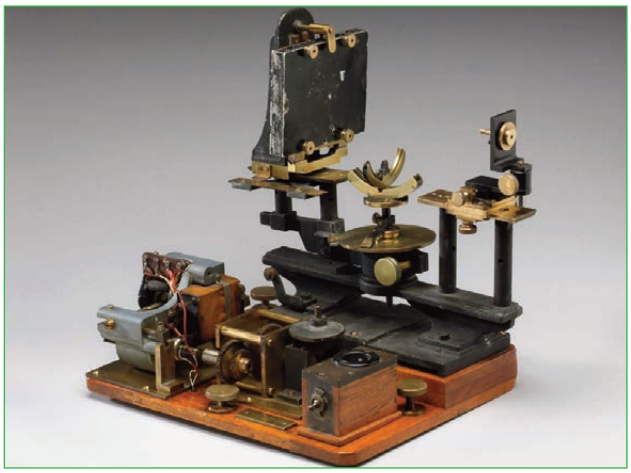
*A view of ECM33 held in Versailles in 2022. Photo: Suzanna Ward (CCDC).*

# British X-ray Crystallographers

**WE are very grateful to Peter Morris of the Royal Society of Chemistry (RSC) Historical Section for organising a meeting on the subject of celebrated X-ray crystallographers who lived and worked in the UK, as well as their scientific parentage of those working in the field today. The meeting was held at Burlington House in London on 18th October 2023, with the option of attending in person or online.**

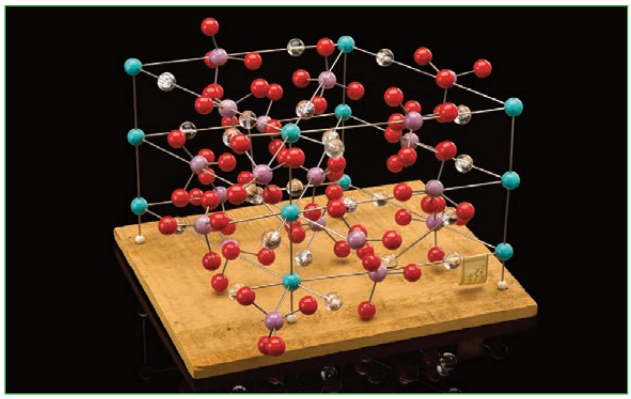
*Speakers at the RSC meeting on British X-ray Crystallographers: **John Finney** (UCL), **Tom Blundell** (Cambridge), **Elspeth Garman** (Oxford), **Georgina Ferry** (Oxford), **Ian Wood** (UCL), **Stephen Neidle** (UCL), **Mike Glazer** (Oxford), **Judith Howard** (Durham) and **Jenny Wilson** (UCL). Photo: **Peter Morris** (RSC).*

In opening remarks, the first session chair, **Mike Glazer** (Oxford) reminded attendees that very early humans are known to have collected crystals as objects of fascination and insightfully suggested that they were pivotal in the development of human scientific thought. The first session began with a lecture by **John Finney** (UCL) about *John Desmond Bernal* who was born in 1901 in Nenagh in Ireland and graduated from Cambridge in 1923. His informal vacation project on deriving all 230 space groups using quaternions landed him a PhD scholarship in the laboratory of Sir William Bragg. As author of this article, I have to add that in the 40 years of studying crystallography I have only encountered one other person who can do this. Anyway, back to the speaker who then described how Bernal had a huge lifelong impact across the full spectrum of science, politics and the arts. Bernal's early work involved studies of the structure of graphite and later at the Royal Institution he worked on bronzes and developed an innovative but humble X-ray rotation camera using an alarm clock as well as inventing what became well-known as the Bernal Chart for analysing rotation photographs. In the late 1920's he gained a lectureship in structural chemistry at Cambridge, working on sterols, steroids and proteins. It was during this time that he recruited Dorothy Hodgkin as a post-graduate who published the first X-ray analysis of crystals of pepsin. Working with Isodor Fankuchen, Bernal developed an interest in viruses and water structure, publishing a seminal paper in 1933 which remains consistent with current state-of-the-art experiments. Bernal also appointed Max Perutz to the Cambridge laboratory before moving to Birkbeck in 1937 where he recruited many who would become great names in the field, including Aaron Klug, Andrew Booth and Rosalind Franklin. The onset of war in 1939 meant that he was appointed as scientific advisor to Mountbatten, studying the effects of bombing, as well as designing a giant floating iceberg and mapping the Normandy landing sites, which he visited twice under cover. Bernal continued his research at Birkbeck after the war, working on cements as well as biological, chemical and generalised crystallography until his untimely death in 1971. The next lecture was given by **Jenny Wilson** (UCL) and covered the life and work of *Kathleen Lonsdale* who was born in Newbridge, Kildare in 1903 and went on to study physics at Bedford College, graduating in 1922. After studying for an MSc at UCL, her external examiner was W. H. Bragg who was so impressed that he offered her a position at the Royal Institution. There she worked on ionisation spectrometry and mathematical crystallography before moving to Leeds and working with William Astbury. Here she obtained grant funding and determined the structure of hexamethyl benzene before moving back to the RI in 1932 where she worked on diffuse reflections and thermal vibrations. In 1935 she authored a handwritten volume of the International Tables for Crystallography and was elected to FRS in 1945 after having served a short prison term for pacifism during WW2. In 1946 she became a reader at UCL and in 1949 she became the first woman professor there, working on diamonds and bladder stones, as well as undertaking much work on prison reform. She was pivotally involved in setting up the IUCr in 1946, being elected president in 1966, a few years before her untimely passing in 1971. The next lecture, given by the session chair, **Mike Glazer** (Oxford), concerned the life and work of another irish-born crystallographer, *Helen Megaw* (1907-2002), whose formative years were spent in Dublin and Belfast before studying at Cambridge, both as an undergraduate and later as a post-graduate with J. D. Bernal. During her PhD work, which involved studies of thermal expansion and diffraction of ice crystals, she was a contemporary of Dorothy Hodgkin. After a scholarship in Vienna, she worked in Oxford and spent several years as a school teacher, before moving to Philips Research in Mitcham. She then moved to Birkbeck in 1945 with J. D. Bernal again and finally to Cambridge in 1946 until her retirement in 1972. She is remembered for her ground-breaking work on



*J. D. Bernal's X-ray oscillation-rotation diffraction camera from 1928. (This image is from the Science Museum Collection, object number 1963-44 and is available under a CC BY-NC-SA 4.0 license https://creativecommons.org/licenses/by-nc-sa/4.0/).*

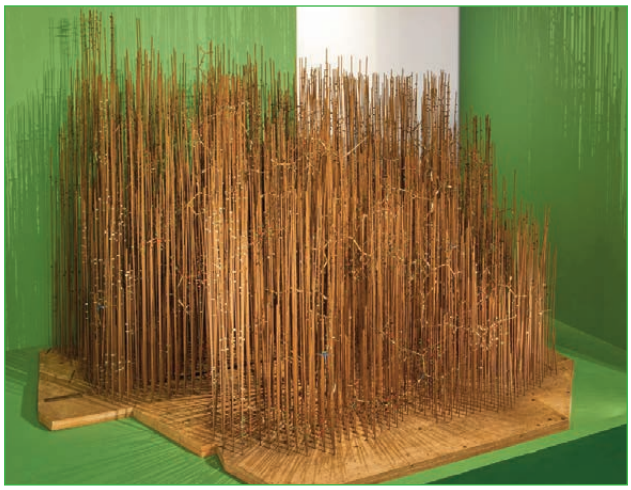
perovskites and feldspars as well as for contributing many crystallographic designs to the Festival of Britain in 1951.



*A molecular model of the biological mineral hydroxyapatite made by Kathleen Lonsdale. (This image is from the Science Museum Collection, object number 1993-421/4/10 and is available under a CC BY-NC-SA 4.0 license* ***https://creativecommons.org/licenses/by-nc-sa/4.0/***

*Helen Megaw of Cambridge was the driving force behind the Pattern Group of the 1951 Festival of Britain. The group created designs for wallpapers, carpets, ceramics and fabrics, for example this haemoglobin-inspired silk tie, based on the work of Max Perutz. (This image is from the Science Museum Collection, object number 1976-644/2 and is available under a CC BY-NC-SA 4.0 license* ***https://creativecommons.org/licenses/by-nc-sa/4.0/***

After the lunch break, the second session was chaired by **Judith Howard** (Durham) and began with a lecture on *John Kendrew* which was given by **Elspeth Garman** (Oxford). Kendrew was born in Oxford in 1917 and graduated in chemistry at Cambridge in 1939 before entering the RAF in 1940 where he undertook operational research, rising to the rank of wing commander. In Ceylon he met J D Bernal who persuaded him to work on protein structure. After the war, he returned to Cambridge to work on globin structures with Perutz and Bragg, for which he received a PhD in 1949. By 1950 he was very interested in the role that electronic calculators could play in crystallography and, together with Perutz, his work on heavy atom derivatives allowed the structure of whale myoglobin to be determined by 1959 – a world first, for which he received the Nobel Prize in 1962. He became one of the founders of EMBO and J. Mol. Biol. in 1963 and by 1974 had persuaded governments to establish the EMBL in Heidelberg, becoming its first director. These achievements were honoured with a knighthood in the same year. The next lecture was given by **Georgina Ferry** (Oxford) and covered the remarkable achievements of *Max Perutz* who was born in 1914 in Vienna where he studied chemistry, graduating in 1936. His PhD in Cambridge with Bernal and Lawrence Bragg on the crystal structure of ice as well as, what was then, very ambitious work on the structures of proteins was completed in 1940. In the late 30's he obtained a Rockefeller grant to study the structure of haemoglobin but progress was interrupted by WW2 when he was interred abroad for several months. In 1941 his expertise on ice led to him being appointed to a team attempting to make a giant floating ice platform for refuelling aircraft in the Atlantic. Back at Cambridge after the war, the award of MRC funding for his globin work led to the pivotal structure determination of haemoglobin in 1959 and his Nobel Prize in 1962. The final lecture before the afternoon tea break was given by **Tom Blundell** (Cambridge) and was on *David Phillips* (1924-1999) who began his crystallographic career in Cardiff. After an interruption to his studies of several years for radar work during the war, he completed a PhD in 1951 with A. J. C. Wilson – an expert on crystallographic statistics and father of the Wilson Plot. After postdoctoral work in Canada he joined the RI where he achieved considerable scientific fame in 1965 for his determination of the first enzyme crystal structure, lysozyme. He was elected FRS in 1967 having moved to the Department of Zoology in Oxford in 1966 to establish the Laboratory of Molecular Biophysics which he led until 1990. David had a great many senior scientific advisory roles to the government and research councils, being knighted in 1979 and gaining a life peerage in 1994. The speaker speculated that David's interest in politics originated from his maternal grandfather who was a Labour MP and acknowledged that it was David who invited him to co-author the field-leading text book Protein Crystallography (Academic Press) published in 1976 with Louise Johnson.

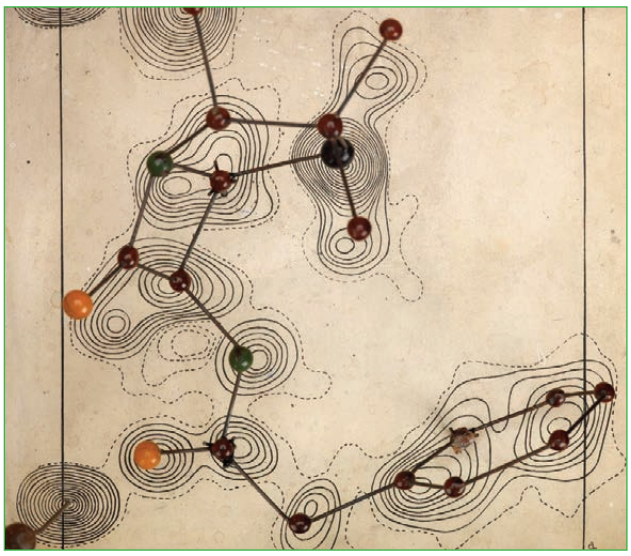


*The Forest of Rods model of myoglobin at 2.0 Å resolution built by John Kendrew and Max Perutz in Cambridge. (This image is from the Science Museum Collection, object number 1977-219 Pt3 and is available under a CC BY-NC-SA 4.0 license* ***https://creativecommons.org/licenses/by-nc-sa/4.0/***

The final session began with a lecture on *Rosalind Franklin* by **Stephen Neidle** (UCL) who described how Franklin studied in Cambridge prior to undertaking a PhD with the British Coal Utilisation Research Association. She then moved to Paris for post-doctoral studies on diffraction of amorphous substances in 1947. From there she succeeded in obtaining a Turner and Newell Fellowship for studies on protein structure at Kings with John Randall, moving there in 1951. The speaker explained how a laboratory reshuffle in which Rosalind was switched from working on proteins to DNA and was given the student (Ray Gosling) of another staff member already working on DNA (Maurice Wilkins) may have contributed to the well-know tension which subsequently arose between Wilkins, who believed he was getting a new research assistant (Rosalind) and Franklin who believed she was an independent researcher. Nevertheless, everyone involved at Kings along with the Cambridge team (notably James Watson and Francis Crick)

received unparalleled scientific acclaim when their structural model for DNA was published in a series of Nature papers in 1953. By this time, Rosalind, whose experimental work at Kings had been pivotal in the DNA story, had moved to Birkbeck to join the team of J. D. Bernal working on viruses. The speaker mentioned her untimely passing from ovarian cancer in 1958. The next lecture was given by **Judith Howard** (Durham) and focussed on the life and work of *Dorothy Hodgkin* who was born into a family of archaeologists, spending her formative years living with her grandparents in the UK, while her parents spent most of their time in the middle east. After graduating in Chemistry at Oxford, she completed a PhD with J. D. Bernal in Cambridge working on sterols before returning to Oxford in 1934. Here she published the structure of penicillin in 1949 and the structure of vitamin $B_{12}$ in 1954, winning the 1964 Nobel Prize, before determining the structure of insulin in 1969, as well as launching a great many of her students and researchers into stellar career trajectories. Last but not least, the final lecture of the meeting was on the esteemed mineralogist *Judith Milledge* (1927-2021) and was given by **Ian Wood** (UCL). Judith studied physics at Rhodes University in South Africa and then worked for De Beers at their Diamond Research Laboratory until 1951 when she moved to London to study for a PhD with Kathleen Lonsdale. This led to a postdoctoral position at MIT before she returned to UCL for the remainder of her distinguished career, in which she focussed on diamonds, publishing 10 Nature papers, and on geological teaching in the Earth Sciences department. She had a special interest in crystallographic computing and in the use of Bayesian methods in structure refinement.

This concluded an excellent meeting for which the organiser **Peter Morris** and the RSC support staff must be congratulated for their considerable time and effort.



*A model of the structure of penicillin by the Nobel Prize winner Dorothy Hodgkin c. 1945. (This image is from the Science Museum Collection, object number 1996-686 and is available under a CC BY-NC-SA 4.0 license https://creativecommons.org/licenses/by-nc-sa/4.0/).*

Recordings of the lectures can be found online at the following URL: https://www.youtube.com/playlist?list=PLLnAFJxOjzZu7N0f5-nVtHcLNxU2tKmpC.

**Jon Cooper**
UCL

# BCA Spring Meeting 2023, CCG Session Report

## Powder Diffraction for Chemical Crystallography

This session was held on Thursday 6th April in the morning and was chaired by **Iain Oswald** (Strathclyde) who took us into the world of structural solution from powder and its use in Chemical Crystallography. The first lecture was by **Kenneth Harris** (Cardiff) and was entitled "Enhancing structure determination from powder diffraction through multi-technique synergy." The speaker provided a tour of various systems where powder diffraction was used in conjunction with DFT and NMR to be able to help determine changes to the structures. He presented cool tricks to ensure you get the best possible data such as the use of amorphous starch to reduce preferred orientation in powders. A lecture by **Christopher Smalley** (Cardiff) on the subject of "Multi-technique approaches for structure determination of organic materials from powder X-ray diffraction data" followed. Chris expanded on work specifically related to alloxazine and its tautomerisation and how DFT and SSNMR were able to elucidate the structural changes. Next, **Charlie McMonagle** (ESRF) gave a lecture entitled "A new sapphire capillary cell: a moderate pressure setup for powder diffraction at SNBL BM01, ESRF." The lecturer described the development of pressure cells at the ESRF and the quality of data that can be obtained from the set-up. He described the development of heaters for capillary work to enable studies of the evolution of structure with temperature to 1200 °C at 100 °C/min. These developments can be used in conjunction with pressure and gas flow cells to expand the region of experimental space that can be accessed. Last but not least, **Carissa Ponan** (UCL) gave a lecture entitled "The future of pharmaceutical solid-state chemistry: hyphenated *in-situ* diffraction techniques." Carissa discussed the in-situ characterisation during ball-milling processes and explained how the modification of the set-up could yield different forms of their secret compound!

**Iain Oswald**
Strathclyde

# News from CCDC

## 2023.3.1 CSD Software Update (January 2024)

This latest software update fixes several bugs following the 2023.3 release last November.

All available software or data updates can be applied by using the CCDC maintenance tool in the installation and selecting the Check for Updates option. If you are using a previous software (version 2022.3 or earlier), or if this is your first time installing CSD software, you will need to install the software from **Downloads**, and this download will contain the latest data update.

If you have problems installing the update, see **our FAQ for more details and other options**. Please contact our **support team** if you have any questions about updating.

## Blog highlights

**Small Molecule FDA Novel Drugs Approvals Increase by 50% in 2023.**

The Food and Drug Administration (FDA) approved 55 new drugs in 2023, an increase of nearly 50% from the 37 approvals in 2022, the second highest number in the past 30 years. A total of 34 out of the 55 approved new drugs are small molecules, representing 62% of the total. The growing number of small molecules from the previous years, corresponding to the 56% in 2021 (28 out of 50) and 57% in 2022 (21 out of 37), shows how this class of drugs continues to be crucial in advancing health care. **Read more on the CCDC website**.

## Online Platforms for Crystal Structures Exploration

The Cambridge Structural Database (CSD) is the largest database of organic and metal-organic experimental crystal structures, containing today over 1.25 million structures. It includes data published in associated scientific articles, patents, institutional repositories, thesis publications, and structures published directly through the database (CSD Communications).

The CSD represents a community effort, with datasets determined by researchers worldwide. Every single CSD entry is enriched and annotated by experts at the CCDC to aid the discoverability of data and knowledge from the resource.

Alongside the multitude of structures, the CSD also contains a wealth of structural information such as over 94 million atomic coordinates, 28 million bond lengths, 40 million valence angles, 14 million torsion angles and 2 million rings, representing a rich and extensive source of data. **Read more on our website**.

**Check out all our blogs on our website**.

## CCDC Online Events

Our next series of CCDC Virtual Workshops is scheduled for April and May. These free, interactive 90 min training sessions are suitable for beginners and more advanced users wanting to increase their skills using the CSD Portfolio. We also regularly host webinars and have an exciting calendar of topics and external speakers planned for 2024.

To find out more about our online events and to register go to the Events tab at the CCDC website.

## In-Person Events

**Cambridge Festival 2024**
16th March, Cambridge

The Cambridge Festival 2024 is a celebration of ideas, innovation, and exploration. This dynamic event will feature a diverse array of talks, workshops, and interactive experiences designed to engage and inspire participants from all ages. Visit the CCDC team at the Crystal Adventures activity and have fun exploring the wonders of crystallography.

## ACS SPRING 2024 – Many Flavors of Chemistry

17–21 March, New Orleans and Hybrid.

The ACS Spring Meeting brings together chemistry experts to exchange ideas and enhance scientific knowledge. The event offers a great chance to share your love for chemistry and connect within a global scientific community.

Join the session Celebrating The Life and Legacy of Dr Olga Kennard in memory of the founder of the CSD and CCDC, on 17th March at 8 am – 12 pm.

## BCA Spring Meeting 2024

25–28 March, Leeds.

The CCDC is exhibiting, speaking, and sponsoring the CCDC Chemical Crystallography Prize for Younger Scientists at the BCA Spring Meeting, at the University of Leeds. Stop by our stand to meet our team and take part on the CSD Leaderboard, a friendly competition for crystallographers.

## HTCC6 – Hot Topics in Contemporary Crystallography 6

7–12 April, Dubrovnik.

Join us for the sixth edition of HTCC6 – an advanced macromolecular crystallography workshop in Dubrovnik. Since 2014, HTCC workshops have been at the forefront of structural research, uniting leading experts as lecturers and enthusiastic scientists from academia and industry. Join us to explore cutting-edge methods in structural science and their practical applications in research.

For more information on how to register, visit our events page at the CCDC website.

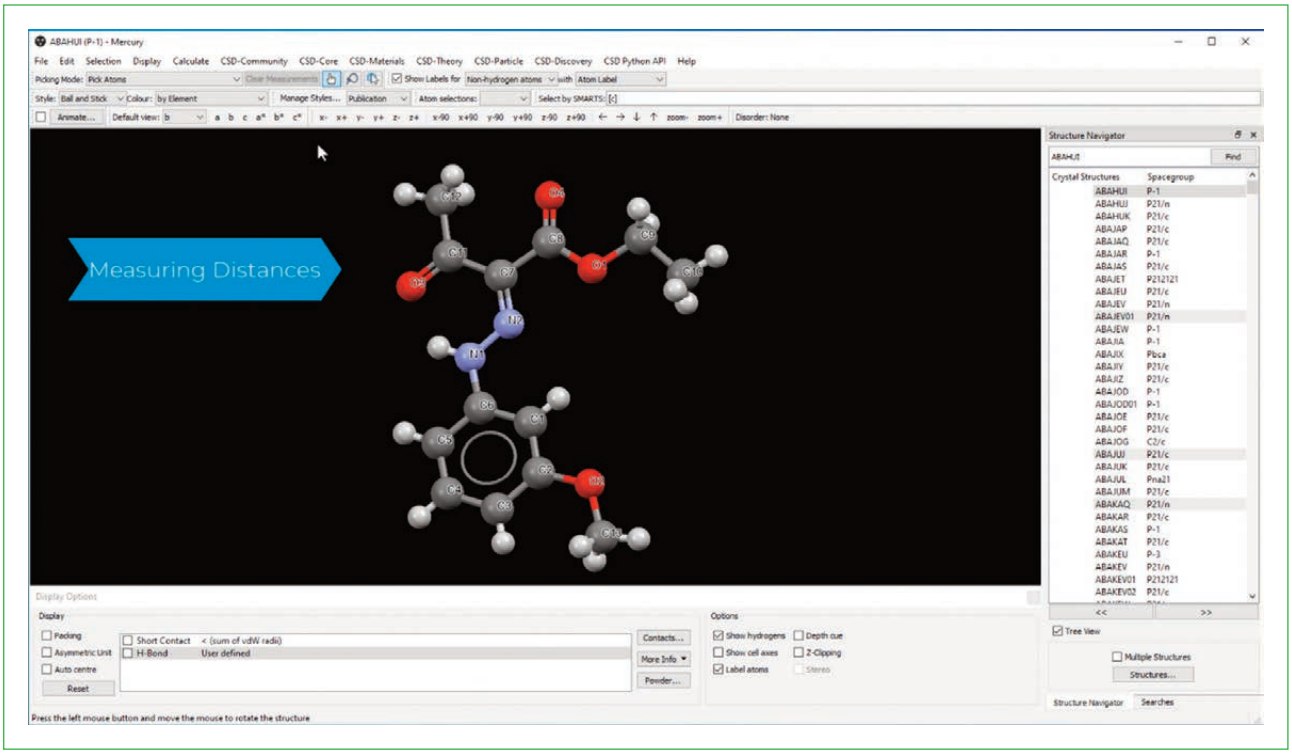
## New Mercury Tutorial: How to measure intramolecular and intermolecular distances, angles and torsions in Mercury

A new Mercury tutorial is now available on our YouTube channel. In this 5 min video you will learn how to measure intermolecular and intramolecular distances, bond angles and torsion angles in molecules and crystal structures using the CCDC's visualisation software Mercury. This functionality could be used in the study of molecular geometry and interactions in the solid form, such as hydrogen bonds. Measuring distances, angles and torsions functionality is available in the free version of the visualization software Mercury.
To **watch the video**, a snapshot of which is shown below, visit the Support and Resources tab of the CCDC website.

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

**Follow us on Social Media.**
Want to learn more about CCDC events, blogs, case studies, and software updates? Follow us on LinkedIn, Facebook, and Twitter.

**Ana Machado**
CCDC




# Historical Reflections on X-ray Crystallography

**AFTER a long career working alongside Durward Cruickshank, I have observed the X-ray Crystallography scene since the 1960s, ending up as his Royal Society biographer jointly with John Helliwell. Here are some aspects of the historical X-ray scene which may be of interest.**

In *Acta Cryst* (1998) A54, 687-696, Durward wrote about the international bodies overseeing the development of X-ray Crystallography (XRC) during and after WW2. This involved Bernal and others who were working on the embryo IUCr. Durward mentions how, in the USA (1941) the ASXRED (American Society for X-ray and Electron Diffraction) was founded and in the UK (1943) the X-ray Analysis Group (XRAG) of the Institute of Physics (IOP) was set up. In 1944, Ewald gave a lecture in Oxford, which it seems started the ball rolling for the formation of an international body for XRC, the IUCr.

My interest at this time is that I would like to know more about XRAG. The Bodleian Archives notes that XRAG dates between 1943 and 1969, with Dorothy Crowfoot Hodgkin elected on the committee in 1944. After my PhD in 1962, I attended IOP XRC meetings at UCL at which Kathleen Lonsdale presided. I have wondered, ever since whether these UCL meetings were the swan-song of XRAG. Perhaps someone knows more about XRAG and whether it ended when Kathleen Lonsdale

retired in 1968/69. Durward arranged for me to move to Oslo, Norway, before I found out! Forming a new overarching XRC organization replacing XRAG took about 10 years.

Around 1980, a working party including D M Blow, D W J Cruickshank, A C Skapski, S C Wallwork and A J C Wilson, organised the setting up in 1982 of the British Crystallographic Association (BCA). I was privileged to be one of the Founder Members. Other Founder Members included Judith Howard, Dorothy Crowfoot Hodgkin, Judith Milledge and David Phillips. In 1984, a retirement symposium was held for Cruickshank, the proceedings of which were published in *J Mol. Struct.* **130** (1985). One of those attending was Dorothy Crowfoot Hodgkin and an additional attachment to these historical reflections, is a photograph of Durward, myself, Dorothy and Prof. Hankins of UMIST. I have a small Cruickshank Archive, including the original photographs of attenders at his retirement symposium. There is a major Cruickshank Archive at the Manchester University Library.

*Durward Cruickshank (Manchester), Brian Beagley (Manchester), Dorothy Hodgkin (Oxford) and Harold Hankins (UMIST).*

**Brian Beagley**
Manchester

Brian raises some interesting questions about where we, as a society, come from, which I think can be answered in part by the information collected by one of the previous *Crystallography News* editors, Kate Crennell (ISIS), who summarised the history of the various X-ray-related groups in the UK as follows.

The "X-Ray Analysis Group" of the Institute of Physics was formed in 1943 and started sending a newsletter to members in May 1957. At that time the officials were:

Chairman: Professor D. G. Cox
Vice Chairman: Sir Lawrence Bragg
Honorary Secretary: Dr R. L. Gordon
Ordinary members: Dr Helen D. Megaw, Dr P. T. Davies

In 1969 the name was changed to the "Crystallography Group" and in 1981 they joined with the Crystallography Group of the Royal Society of Chemistry to form a new association.

The British Crystallographic Association (BCA) was founded in 1982 to advance the education of the public in the science of crystallography, particularly within the British Isles. It is now a Registered Charity No. 284718.

### XRAG newsletter of the IoP

No 1 May 1957 to No 34 May 1969
No named editor in these issues, name changed in 1969.

### Crystallography Group newsletter of IoP

No 35 Jan 1970 to No 64 Dec 1980
Bob Diamond No 35 Jan 1970 to No. 36 Jul 1970
P. J. Baldock, J. A. Bland No. 37 Jan 1971 to No. 42 Jul 1973
David Dyson No. 43 Jan 1974 to No. 48 Jul 1976
Doug Grant No. 49 Jan 1977 to No. 60 Jan 1980
Moreton Moore No. 61 Apr 1980 to No. 64 Dec 1980

### Crystallography News

No.1 Mar 1981 to present time.

As the current editor, I relayed the above information, which can be found on the old BCA web site, to Brian who very kindly pointed out some reports from the 1940's on meetings of the X-ray Analysis Group which were published in *Nature*. Following this up, I found these articles to be a rich vein of information (too much to include here) and I hope to have more to say on this in future issues. Brian also says: "As a Founder Member of the BCA, it is an honour and pleasure to still be involved at the age of 87."

**Jon Cooper**
UCL

# Down Memory Lane

**IN the last issue, I invited members to suggest ways of keeping one's career on a crystallographic track. Professor John Helliwell (Manchester) replied saying: "It would make an interesting session at a BCA Spring Meeting." Thank you very much, John. Now that is a thought! John goes on to say "In France I recall that their famous crystallographer Herbert Curien became the French Minister for Science."**

In that article we looked at two crystallographers who changed field, one of them being the electron diffractionist Dr Richard Beeching who went on to become a household name, albeit perhaps not a very popular one. One thing I failed to mention in that article was that Dr Beeching took the management helm at British Rail at a time of great modernisation of the railways, with the ancient steam rolling stock being phased out and replaced by diesel and electric. Realising this, one can almost sense the excitement that someone keen on ascending the career ladder must have felt in his position. Likewise with A. D. Booth at Birkbeck, his own interests in natural language translation by computer (something we are so familiar with today) inevitably took precedence over the requirements of his crystallographic colleagues and allowed him to achieve considerable recognition as a pioneer in the computer science field, while his disgruntled colleagues were probably left struggling with Beever-Lipson strips to compute their Fourier transforms, for another decade or two.

Maybe it is the challenge of ascending to higher career realms which motivates people to stray from the crystallographic field. One could almost call it a situation in which the player is vertically challenged, not in terms of their own physical height, but by the height to which they can climb the career ladder. Another electron diffractionist who was quite literally vertically challenged and who also became a household name was Prof George Ingle Finch (1888-1970) at Imperial, one of whose interests was mountaineering. Indeed, the names of Mallory and Finch are synonymous with pioneering efforts of the British Mount Everest Expedition in the early 1920's. Finch, the Australian-born, die-hard physical chemist was an unlikely match for the Cambridge history scholar, George Mallory, with his ambivalent personal life and penchant for hill-walking with nothing on. Nonetheless, Finch made a major contribution to the team's efforts by provision of bottled oxygen which was pivotal to the success of this and subsequent expeditions, although with the numerous sherpa fatalities, one does wonder a bit about the ethics of all this. Anyway, with supplemental oxygen, the climbing team reached an astonishing vertical height of 8.3 km in 1922 breaking the previous record. However, Finch had a reputation for being short tempered and fell out with the Everest committee shortly after this attempt and took part in no further trips. This may well have saved his life as the 1924 expedition proved fatal for Mallory whose remains on Everest were not found until 1999. Sadly the remains of Mallory's climbing partner for that ascent (Andrew Irvine) have never been found.

Finch trained in physical sciences in Zurich from 1906 to 1911 and, after research and management positions in Switzerland, he took up a research fellowship at Imperial. Following military service in WW1, he became a lecturer in electrochemistry at Imperial in 1921, gaining a chair in applied physical chemistry in 1936, before being elected FRS in 1938. After retiring from Imperial in 1952 he moved to India for 5 years to head the National Chemical Laboratory in Poona. The 1920's and 30's represented the heyday of his electron diffraction work, which was mainly focused on surfaces and thin films with many applications in the burgeoning aero-engine and automobile industries. He invented the Finch camera in which the electron beam was produced by a gas discharge tube. Curiously, he insisted this should always be a wine bottle. Commercial versions of the instrument were produced up to the 1960s.

His non-biological son became the Oscar-winning film actor Peter Finch of great critical acclaim. I am not much of a movie buff so his only role that I come anywhere near to remembering is that of the Israeli premier Yitzhak Rabin in the 1977 blockbuster Raid on Entebbe, which coincidentally was released only 5 days before the actor's death. All 2 hours and 20 minutes of the film, which is based on truly dreadful real-world events, when the editor was 12 and thankfully being brought up in a sheltered South London suburb, can be seen by members on YouTube.

**Jon Cooper**
UCL

**References:**

Bigelow, W. C. (2012). Early Days of Electron Diffraction. *Microscopy Today* 20, 38 – 44. http://doi.org/10.1017/S1551929512000016.

Blackman, M. (1972). George Ingle Finch, 1888-1970. *Biogr. Mems Fell. R. Soc.*18223 – 239. http://doi.org/10.1098/rsbm.1972.0007.

Wikipedia, the free encyclopedia.

*The electron diffractionist* **George Ingle Finch** *(1888-1970) in mountaineering mode (source: Wikipedia, copyrighted free use, Alpine Journal, 1922).*

*STOP PRESS –*

# Bursary Awardee Reports on the 2023 CCP4-BCA Summer School

*Running for the first time since the COVID-19 pandemic, the school, which was previously held at the University of St. Andrews for many years, has trained hundreds of crystallographers while also providing them with unforgettable collective memories. The York team is to be congratulated for capturing the essence and tradition of the school and blending it with the best the City of York has to offer.*

**IN August 2023 I was lucky enough to be supported by a BCA bursary to attend the CCP4-BCA Macromolecular Crystallography Summer School hosted by the York Structural Biology Laboratory at the University of York.**

I'm currently a third year CRUK-funded PhD student at the University of Southampton working on an interdisciplinary project which combines cancer immunology, structural biology and computational chemistry with the aim of developing more powerful immune-stimulating antibodies as anti-cancer therapeutics.

The Summer School was a fantastic opportunity for me to get to grips with the fundamentals of crystallography. It started on a Saturday with an opportunity for all the students to present their research in 3 minutes with 1 slide. From Sunday, we had six busy days of lectures covering every aspect of crystallography theory and structure solution from crystallisation to data collection, data processing, molecular replacement, refinement, validation and PDB deposition. To build on the lectures, we had a series of computer workshops to teach us how to use various pieces of software including the CCP4i2 suite, DIALS/DUI, Coot, REFMAC and CCP4 Cloud. We also had a couple of lectures on other structural biology methods, including Cryo-EM, Micro-ED and NMR. On Tuesday we had the afternoon off to explore the city (and recap some of the things we had learnt!) and on Wednesday there was an evening session focussing on 'Structural Biology in Industry'. And of course we had the social highlights of the week: the cèilidh, a trip into York and the final night river cruise!

The Summer School was a brilliant experience, allowing me to meet budding structural biologists from all around the world and learn from leading scientists and software developers in the world of macromolecular crystallography. I've already been able to apply lots of the things I learnt during the week to my PhD project, so I'm very grateful to the organisers of the Summer School, the speakers, and the BCA for awarding me the bursary to allow me to attend.

**Izzy Elliott**
Southampton

**AFTER an eventful journey due to train strikes and cancellations, we finally arrived to the University of York for the first CCP4-BCA Summer School since the pandemic, and also the first in-person event of my Ph.D. The student talks on Saturday afternoon gave all the attendees the chance to briefly present their research and later get to know each other over a visit to York City Centre.**

The schedule of the following six days was set up so that we were never more than a couple of hours away from a meal or coffee break, which helped everyone to fully focus on the talks and learn as much as possible. Sunday's lectures introduced the CCP4i2 software and the theory behind symmetry and diffraction, followed by an explanation on the basis of cryo-EM and how it has evolved over the years.

In addition to some very interesting lectures, Monday brought around the first set of workshops on scaling/merging data and data processing with DIALS/DUI. The highlight of that day, however, was the evening activity: the cèilidh, a fun but exhausting dance with lively folk music by The New Fox Band.

Tuesday marked the middle of the Summer School and as such we were granted an early finish to explore York. The morning talk on CCP4 Cloud introduced me to a great alternative for use on personal computers that don't have much memory. The other lectures covered structural biology techniques for samples that are not suitable for X-ray diffraction. A few of us used that free evening to visit the Jorvik Viking Centre and the famous shops of the Shambles.

The Coot lecture and workshop on Wednesday proved invaluable. The guide provided for the Coot workshop has continued to be useful over the past few months and has helped me solve problems I was previously having with my data. The afternoon lectures finished with a talk from an industry partner, supporting careers outside of academia.

Thursday started with an overview of synchrotrons and the facilities available at Diamond Light Source, followed by a lecture and workshop on molecular replacement, and a focus on restraint generation. The day ended with a fascinating talk on serial crystallography, followed by a formal dinner aboard a cruise along the river Ouse.

The final day's lectures covered the last steps to complete the structure determination process: refinement and structure validation for deposition on the PDB. That evening, I made my way back to Cardiff, having thoroughly enjoyed every aspect of the week.

Overall, the Summer School provided an amazing opportunity to improve my knowledge on macromolecular crystallography, meet great people interested in similar areas of research and explore the lovely city of York.

**Sara Royo**
Cardiff

# Meetings of interest

**WHERE** possible, information on the following meetings has been abstracted from the conference websites, where further details may be obtained.

Assistance from the IUCr website is also gratefully acknowledged.

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

## BCA Spring Meeting 2024

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

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

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

## The Astbury Conversation

Date and time: **Monday 8th – Tuesday 9th April 2024**.
Venue: **University of Leeds**.

The Astbury Conversation is the University of Leeds' biennial flagship event for structural molecular biology and is back for 2024. The event brings people from across the globe together to discover, explore and inspire ideas whilst showcasing the latest innovations making waves in molecular biology. This year's theme is 'Illuminating Life', which will shine a light on the hidden world of macromolecules.

For more information and registration, please visit: **https://astbury.leeds.ac.uk/astbury-conversation/**.

## Hot Topics in Contemporary Crystallography 6 – Advanced Macromolecular Crystallography Workshop

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

Since 2014, HTCC workshops have tackled the major achievements in both experimental methods and theoretical approaches, that have brought structural research to the forefront of natural sciences. The course brings together leading experts in selected domains as lecturers and motivated scientists in crystallography or related fields as "students" who may come from both academia and industry. The workshop is ultimately for those interested in acquiring new knowledge on cutting-edge methods in structural science and exploring ways to apply them in their ongoing research. The workshop is organised by the Croatian Association of Crystallographers (CAC).

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

## The Zürich School of Crystallography – Bring Your Own Crystals

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

The Zurich School of Crystallography teaches small-molecule single-crystal X-ray structure determination and consists of lectures, computer exercises and practical work. The School is ideal for anyone for whom a knowledge of small-molecule crystal structure analysis would be particularly helpful in their current research. The goal is that the participants gain hands-on experience plus a theoretical background in the art and science of routine crystal and molecular structure determination of small molecules by single-crystal X-ray crystallography, as well as in the interpretation and presentation of results. Participants will collect data and determine the structure of one of their own compounds that they are currently interested in, as well as working with data sets that demonstrate routine and a range of more challenging situations.

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

## ECM34

The European Crystallographic Association (ECA) and the Italian Association of Crystallography (AIC) are hosting the 34th European Crystallographic Meeting in Padova (Italy) **26th – 30th August 2024**. The organisers of this event are **Gilberto Artioli** (Chair), **Giuseppe Zanotti** (Co-chair) and further details can be found here: **https://www.ecm34.org**.

SINGLE CRYSTAL X-RAY DIFFRACTION

# APEX5 - The world's most powerful crystallographic software package

## Accurate data from the smallest crystals

- Future-proof and performance-oriented.
- New sample management workflow for crystallography service providers.
- Revolutionary automated structure determination.
- Outstanding graphical user interface.
- Unmatched handling of challenging samples.

For more information, visit **bruker.com/apex5**

OXFORD CRYOSYSTEMS

OXFORD CRYOSYSTEMS

# CRYOSTREAM 1000

## 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.

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

# KEY FEATURES

- **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.
- **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).
- **Auto Shield Flow:** Automatically optimised shield gas flow rates.
- **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.
- **Eco Mode:** Continual monitoring of the dry-air module eliminates any unnecessary run time, saving energy and reducing maintenance.
- **Improved Pump-out Port Design:** Relocated to the rigid leg and re-designed for ease of use, this eliminates the requirement to remove the coldhead from the cabinet during vacuum regeneration.
- **2 Year Standard Warranty:** All Cryostream 1000 systems ship with a two year warranty.