Crystallography News

British Crystallographic Association

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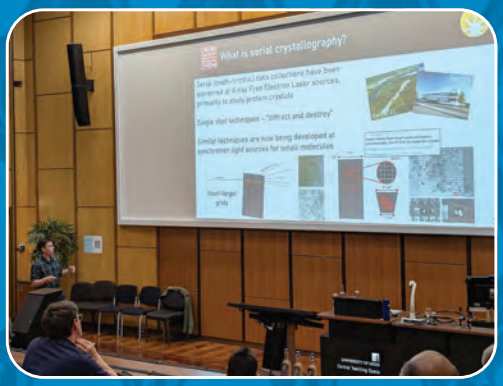

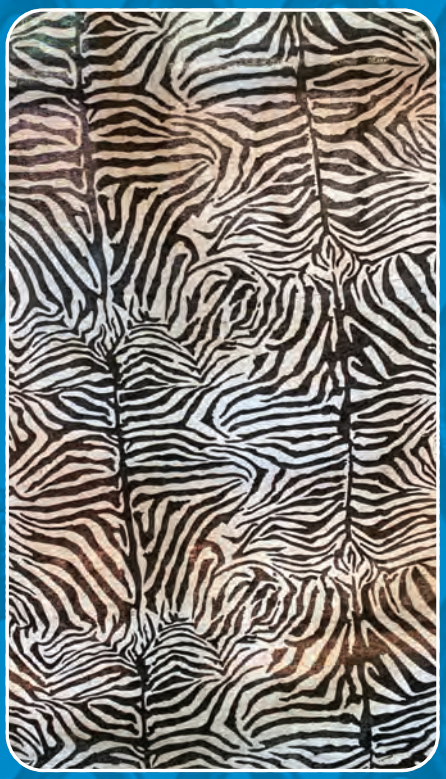

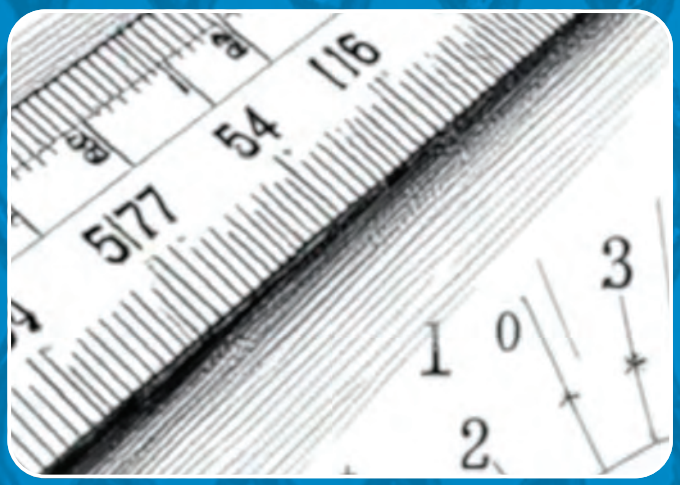

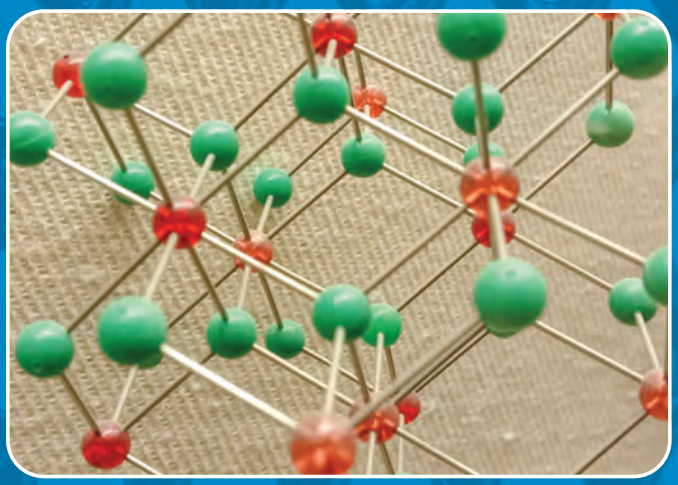

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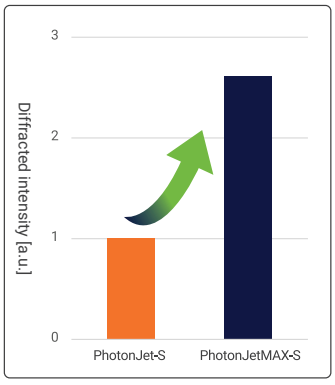

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The Bernal Lecture 2025

Image © Mike Glazer

Bernal Lecture 2025: The Harvest of an eclectic Mind: Alan Mackay and the Rewriting of the Book of Crystallography

Joining Bernal's laboratory some 75 years ago, Alan Mackay delighted in challenging scientific orthodoxy. Inspired by Bernal, he expanded the scope of crystallography to embrace the whole science of structures. Ignoring the crystallographic ban on 5-fold symmetry led to, not only the Mackay icosahedron that other fields have exploited productively, but also to what many consider his crowning achievement – predicting the existence of quasicrystals, the preparation of which earned others a Nobel Prize.

This year's Bernal Lecture will be given on 23 September 2025, 16:00-19:00 at the Birkbeck Main Building, Malet Street by John Finney (see **https://bit.ly/4eidCBq**), who sets Alan's scientific achievements and other products of his fertile mind within the unusual intellectual environment of Bernal's laboratory, one which, unfortunately, could not be reproduced today.

Book the lecture (in-person or live-streamed) here: **http://bit.ly/3FZ2mNP**

You can find the obituary of Alan Mackay at
https://www.iucr.org/news/newsletter/volume-33/number-2/farewell-to-alan-l.-mackay-1926-2025-scientist,-friend

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

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

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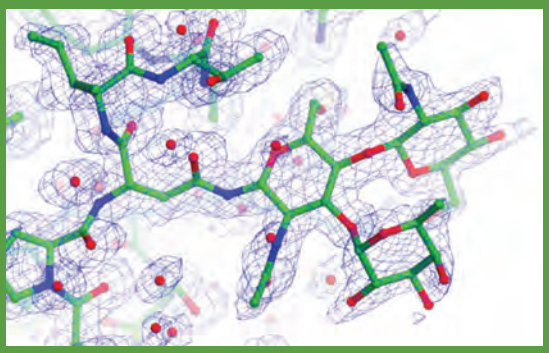
Benefits of Individual BCA Membership:

- 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

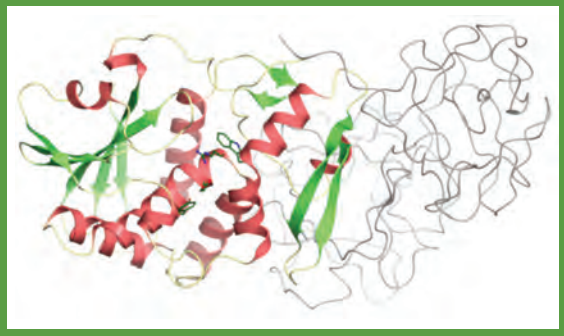
For current rates, and to join, please see **www.crystallography.org.uk/membership/**

Biological Structures Group Winter Meeting 2025

The meeting will be held on **Friday 12th December 2025** at the University of Oxford.



The one-day BSG Winter Meeting provides a fascinating opportunity for members to learn about the latest results and advances in the structural biology field.



More details of the meeting will be posted on the BSG web page.

https://bsg.crystallography.org.uk/

Contents

Late news from BCA President Alexandra Gibbs, St Andrews.

It is with great sadness that I bring your attention to the passing of Pat Doheny, a talented early career researcher who had already made significant contributions to the area of MOF chemistry. I recommend to you his Arnold Beevers Bursary Fund report as well as his obituary later in this issue.

This month's cover:

Scenes from the 2025 Spring Meeting with news of upcoming meetings and courses.

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Text should preferably be sent electronically as MSword documents (any version – .docx, .doc, .rtf or .txt files). Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, .png 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 December 2025 issue are sent to the Editor to arrive before 25 October 2025.

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

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

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From the President

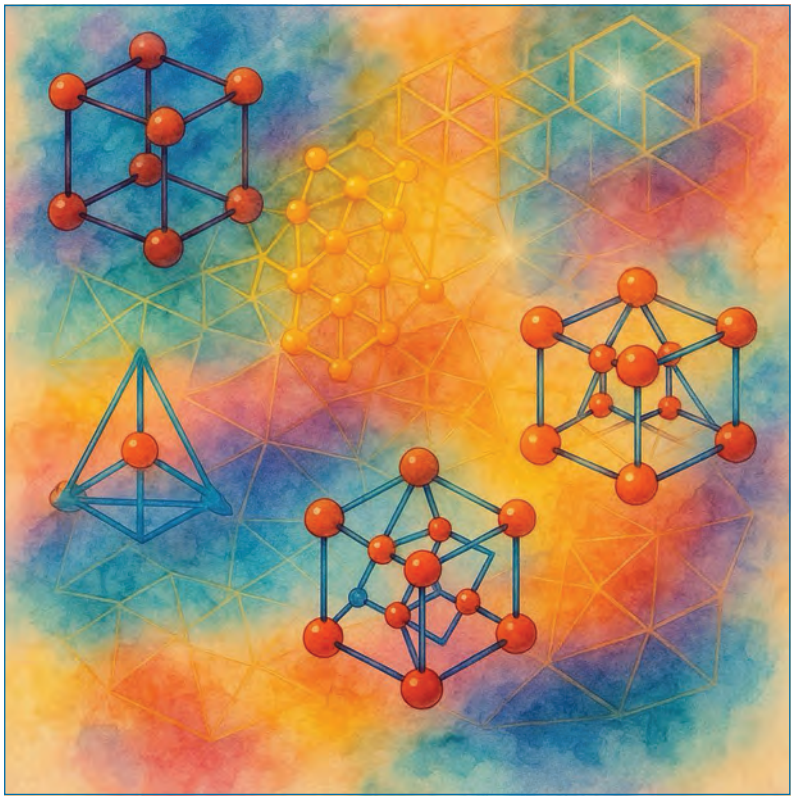
DEAR Members, I hope this column reaches you on one side or another of a restful and sunny summer holiday.

Casting around for a topic for this edition's column I asked ChatGPT (model GPT-4o) the following question (no additional prompts): "What is the most interesting crystal structure?" The answer came:

"Most interesting" depends on whether you're looking at beauty, complexity, or scientific significance – but a few crystal structures consistently stand out across physics, chemistry, and materials science:

1. **Quasicrystals (e.g. Al–Mn alloy, discovered by Shechtman)**
2. **Ice XV and Exotic Ice Phases**
3. **Diamond and Lonsdaleite**
4. **Perovskites (ABX_3)**
5. **Protein Nanocrystals (e.g. Photosystem II)**
6. **Metal–Organic Frameworks (MOFs)**

This is presented exactly as received, minus the explanatory text for each item. The potential for amusement of readers has been sacrificed by my concern for your blood pressure, having already experienced an outbreak of furious pedantry myself!



ChatGPT (model o4-mini-high) output in response to prompt "create an artistic representation of crystallography please." Its explanation of the image has been censored for the benefit of everyone's sanity.

By extreme serendipity I am looking to highlight two upcoming events for you which have direct and important links to the above results. The first, associated with item 3 in the above, is the Kathleen Lonsdale Public Lecture, part of a celebration of the 200th anniversary of the discovery of benzene, to be hosted by the University of Leeds on the 10th September. The second event, relating to item 1, will be recommended to you in a couple of pages' time by Jon – I leave it to him to elaborate!

Richard Cooper discussed the potentials/pitfalls of ChatGPT use in a previous *From the President* (issue 164, March 2023). Although much progress has been made in the last couple of years I still concur with his assessment of its usefulness. It seems it remains the case that it can be an excellent source of food for thought as long as it is not relied on for coherent and accurate details in cases where critical reasoning is required. I have recently begun using it to update me on the latest papers of interest in my field, having created a bot and given it keywords of interest. When asked what's new in the last week it can give me a handful of very interesting papers which I would not necessarily have picked up from simply scanning the RSS feeds of my favourite journals, given the current volume of paper output. It is pretty good at adapting when I tell it a paper is not of interest for a specific reason and is now quite well trained. But although it can tell me what one should look like, it still cannot "draw the unit cell of an fcc lattice" correctly… 6 independent tries… no… prompt "this is incorrect"… it has another go… still wrong… another few iterations…nope. Perhaps I need training!

For those of you who were unable to attend the AGM at the Spring Meeting, I have a couple of topics of discussion which I would like to bring to your attention in more detail. (1) Future Spring Meeting formats and location. This was opened for discussion with no pre-determined directions or boundary conditions. The timing of the Spring Meeting and its length were a key item – do we want to keep the immediate pre-Easter dates? Should we compress the meeting? We received a lot of feedback on Leeds as a venue both positive and negative, with accessibility in general, and the relative locations of talks and breaks specifically, being important concerns. (2) Best practice in collecting and reporting EDI data for the membership and meeting attendees, along with supporting this as a whole was also a core theme. I would like to thank the members present for their willingness to engage in an open and lively discussion. I encourage those who could not attend (and attendees who have further thoughts) to please pass these on to me, other Council members or group officers.

I would like to end with a quote from a junior BCA associate. Following an exercise in symmetrising shapes, the nursery of my 4-year-old son Euan tells me he exclaimed "Look, look, I did some symmetry!" With that cheerful reminder of the simple joys to be had in our day-to-day business, I hope you enjoy this issue of CN and I particularly commend to you Jon's article Going Back to our Roots!

Alex Gibbs
St Andrews

BCA Council 2025

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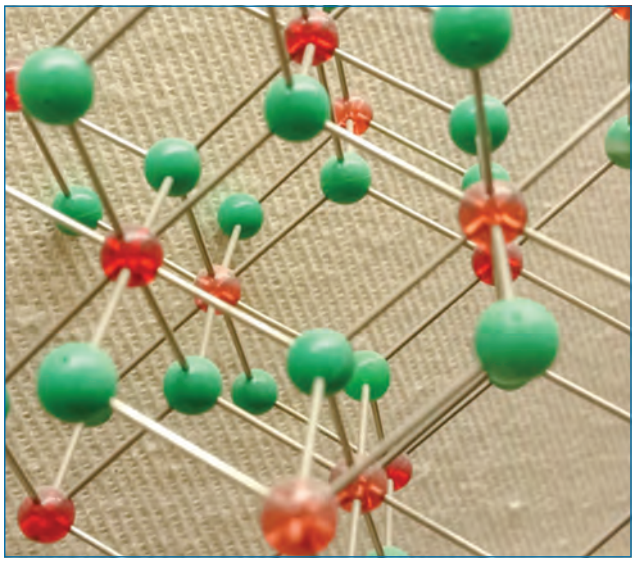
(The dates in parentheses indicate the end of the term of office).

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

From the Editor

IT is a great pleasure to bring you the September 2025 issue of Crystallography News which features a preliminary programme for the 2026 Spring Meeting. We also have reports on the many excellent sessions at the BCA Spring Meeting in Leeds this year, including those organised by Early Stage Crystallographers Group (ESCG), the Industrial Group (IG) and the Chemical Crystallography Group (CCG). Due to the constraints of time and space in the last issue of Crystallography News, we were unable to publish the reports by the Arnold Beevers bursary fund awardees, but these have now been collated and are printed immediately after the Spring Meeting group reports. I am extremely grateful to everyone who sent me accounts of meetings at home and abroad as well as notes on the sessions they attended – in some cases incredibly detailed notes!



We then have two very interesting news sections, one from the CCDC and another from the wwPDB. These are followed by a report on the launch of an excellent text book entitled "Mathematics for Biosciences. From Theory to Worked Examples and Applications" by former BCA President, **Elspeth Garman** (Oxford) and **Nicola Laurieri** (Oxford). This was a very well-attended event in Oxford and it made a great day out back in the Spring. It also triggered some not very advanced and probably errant mathematical thoughts of my own (Going Back to Our Roots) which are included towards the end of this issue for the amusement (or more likely bewilderment) of members! We hope to bring you a proper review of Elspeth's book in the near future.

All of this took me back to the late 1970's and early 80's when the University of London (thankfully) allowed the use of silent calculators in school examinations. Back then I found I could learn the rules or patterns for doing differentiation and integration, etc, but I think without a calculator beside me to do the number crunching in exams, I would not

have passed anything – full stop. Anyway, interestingly AI disagrees with my own lived experience on this point and confidently states "Calculators were generally not allowed for O-level (Ordinary Level) examinations in the late 1970's, despite their increasing availability and affordability." In spite of its brilliance at predicting protein structures, clearly there is some scope for improvement in machine learning algorithms, on this point at least! I did study maths to A-level too and I continue to like it as a subject very much, but I have to confess failing the S-level (sorry, Elspeth) although I passed Chemistry! However, always being a bit piqued by the maths result seems to have given me a life-long interest in the subject (not to mention crystallography) which I might not have otherwise had!

Back to this issue of Crystallography News which we conclude with our regular Puzzle Corner and Meetings of Interest sections. In the latter please have a look at the flyer for the 2025 Bernal Lecture at Birkbeck which will be given by **John Finney** (UCL), the previous Crystallography News editor, later in the month. John's lecture is entitled "The Harvest of an eclectic Mind: Alan Mackay and the Rewriting of the Book of Crystallography." The lecture is devoted to the life and work of Professor Alan Lindsay Mackay FRS (1926 – 2025) who made pivotal contributions to generalised crystallography and the study of quasiperiodic materials. A short obituary for Alan Mackay can be found in the last issue.

We hope to resume the series of ***Crystallographic Forteana*** and **Corporate Member Profiles** in a future issue!

Jon Cooper
UCL

Photographs by the editor taken at the Fitzwilliam Museum in Cambridge.

2026 Spring Meeting Programme

ESCG Early Career Satellite Meeting, University of Leeds

Monday 30th March 2026

EARLY STAGE CRYSTALLOGRAPHERS GROUP (ESCG)

11:00-18:00	*Room:* **Rupert Beckett Lecture Theatre, Michael Sadler Building** The ESCG 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.
11:00-11:30	**ESCG Opening Plenary:** *Chair: TBC* *Speaker:* **Ines Collings** *(Natural History Museum)* *Talk title: TBC*
11:30-12:15	**ESCG Research Sessions** *Session Chair: TBC* Contributed talks from the ESCG community
12:15-12.45	**Flash Poster Presentations** *Session Chairs: TBC* Researchers have an opportunity to present an overview of their poster in 30 seconds with one PowerPoint slide.
13:45-16:00	**ESCG Research Session 2&3** *Session Chair: TBC* Contributed talks from the ESCG community
16:00-16.30	**ESCG Annual General Meeting**
16:45-17:15	**ESCG Research Session 4** *Session Chair: TBC* Contributed talks from the ESCG community
17:15-17:45	**Parkin Lecture:** *Session Chair: TBC* *Speaker: TBC*

MAIN MEETING

	Room: **Rupert Beckett Lecture Theatre, Michael Sadler Building**
18:00-18:45	**Lonsdale Lecture:** *Session Chair: TBC* *Speaker: TBC*
18:45-19:00	**Exhibitor Talks**
19:00	**Poster Session with Dinner and Wine**
21:00	*Evening concludes*

Tuesday 31st March 2026

EARLY STAGE CRYSTALLOGRAPHERS GROUP (ESCG)

08:30-08:15	**IG Plenary** **Rupert Beckett Lecture Theatre, Michael Sadler Building** *Session Chair: TBC* *Speaker:* **John Helliwell** *(University of Manchester)* *Title: TBC*
09:15-10:00	**BSG Plenary** *Room:* **Rupert Beckett Lecture Theatre, Michael Sadler Building** *Session Chair: TBC* *Speaker:* **Basil Gerber** *(The Institute of Cancer Research)* *Title: TBC*
10:30-12:00	**Parallel Sessions** **BSG: Structure-Based Drug Discovery** *Session Chair: TBC*
	CCG/ESCG/IG: Crystal Formation (Crystallisation/Crystal prediction/Crystal Engineering) *Session Chair: TBC*
	PCG: Energy materials *Session Chair: TBC*
12:00-12:30	**AGMs**
	BSG Annual General Meeting
	CCG Annual General Meeting
	PCG Annual General Meeting
13:30-15:00	**Parallel Sessions** **BSG: Complex structures** *Session Chair: TBC*
	Commemorative session for George Sheldrick: his life and impact *Session Chair:* **Judith Howard,** *Durham*
	PCG: Quantum Materials *Session Chair: TBC*
15:30-17:00	**Parallel Sessions** **BSG: Complementary techniques/Disorder** *Session Chair: TBC*
	CCG: Open Session *Session Chair: TBC*
	PCG/CCG: Functional materials *Session Chair: TBC*
17:10-17:55	**PCG Plenary** *Room:* **Rupert Beckett Lecture Theatre, Michael Sadler Building** *Session Chair: TBC* *Speaker:* **Abbie McLaughlin,** *University of Aberdeen* *Title: TBC*
18:00-19:00	**BCA Annual General Meeting**
19:30-00:00	**Conference Dinner, Networking & Ceilidh**

Wednesday 1st April 2026

BCA 2026 MAIN MEETING PROGRAMME

09:00-09:45	**CCG Plenary** *Room:* **Rupert Beckett Lecture Theatre, Michael Sadler Building** *Speaker:* **Neil Champness,** *University of Birmingham* *Session Chair: TBC*
09:45-10:30	**Exhibitor Talks**
10:30-12:00	**Parallel Sessions**
	BSG: Open Session *Session Chair: TBC*
	CCG: Investigating molecular crystals *Session Chair: TBC*
	PCG: Open Session *Session Chair: TBC*
13:00-14:10	**Parallel Sessions**
	BSG: Protein Design Workshop *Session Chair: TBC*
	CCG: Workshop: Micro crystals analysis *Session Chair: TBC*
	IG/PCG: PDF Workshop *Session Chair: TBC*
14:40-15:45	**BCA Prize Lecture** *Speaker: TBC* *Session Chair: TBC*
15:35-16:45	**Early Career Prize Lectures**
	Biological Structures Group Early Career Prize The BSG will award a prize to someone who has had an impact in the field of Structural Biology (with an emphasis on crystallography) and recently obtained a personal fellowship, a lectureship or equivalent position.
	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.
17:05-17:20	**Poster prizes and close** *Room:* **Rupert Beckett Lecture Theatre, Michael Sadler Building** *Session Chair: TBC*
	CLOSE OF CONFERENCE

2025 Spring Meeting Reports

ESCG Satellite Meeting Report

THE Early Stage Crystallographers Group (ESCG) satellite meeting took place this year on the 14th and 15th of April, once again returning to the familiar surroundings of the University of Leeds. This year, Jake Hill (Leeds) and Sam Lewis (Cardiff / DLS) had the pleasure of acting as the programme chairs for what proved to be a highly productive, friendly, and insightful event that covered a broad range of topics.

The Opening Plenary was chaired by **Sam Lewis** (Cardiff / DLS) and was delivered by **Mark Warren** (DLS) who is the senior beamline scientist on the small molecule crystallography beamline I19. The speaker's lecture was entitled "Beyond recrystallisation: accelerating structure solution with serial methods." Mark presented insights into the development of the emerging field of small molecule serial crystallography on the beamline which involves structure determination, permitted by the merging of data collected on hundreds or thousands of microcrystals. Mark expertly detailed the general data collection methodologies involving reduced X-ray flux and small wedge rotations on each individual crystal which affords the necessary reflections from which to index and integrate the dataset. Low temperature data collection is possible and mounting the crystal suspension involves special holders with a fly-swat design which are customisable in terms of size and shape of the grid. We were then informed of a number of case studies for which the technique has been applied, including sub-micron crystals, gas absorbing metal-organic frameworks and photoinduced reactions. The talk was then rounded off with some future outlook with movements towards image recognition and machine learning to further optimise data collections. A highly informative and approachable talk, Mark truly set the tone for the satellite meeting.

Mark Warren (DLS) delivering the opening plenary of the ESCG satellite meeting.

The first session in which the reins were handed to early career researchers was chaired by **Jake Hill** (Leeds) and directly followed the opening plenary. Things were started off by **Daniel Rainer** (Southampton & NCS) who spoke on the subject of "Sodium carboxylate coordination polymers – from environmentally friendly mechanochemistry to 3D ED structure determination." The speaker described the use of the rapidly expanding field of 3D electron diffraction to study sub-micron crystals of sodium carboxylate coordination polymers generated by environmentally green mechanochemical synthesis. Such materials have advantages as battery anodes and shaker ball mill mechanochemistry provides a green and economic means of synthesis. Subsequently, **Matthew Edwards** (Warwick) spoke on "Investigating short-range structural fluctuations in cuprate superconductors." Matthew explored rare-earth cuprate superconductors, their short-range structural fluctuations, and phase transitions by variable temperature X-ray powder diffraction studies. The speaker explained how high-temperature superconductors require doping and covered how phase diagrams investigating various parameters can be used to tune the structure, such as the polarisibility of the A-site metal. The next speaker was **Thomas Smith** (Newcastle) who presented on the subject of "Data management for high-throughput pattern discovery." Thomas provided an insightful look into data management strategies and systems for the large amounts of data being generated in Newcastle by their high-throughput parallel crystallisation experiments. The speaker covered encapsulated nanodroplet crystallisation (EnaCt) technologies and the management of crystallisation outcome data and the issues with meta-data. Plates are scored according to their behaviour under polarised light. Data mining with the Pytomicity python library allows trends to be observed with respect to the experimenter, oil and solvent, etc. Next, "Discovery of a new high-pressure phase of Posaconazole" was the title of the talk by **Banaz Fetah** (Strathclyde) who finished the session by turning attention towards the pharmaceutical target Posaconazole. This compound was explored under high pressure conditions in a diamond anvil cell to analyse previously observed effects in compacted tablets. Multiple forms of the compound (hydrates, solvates, etc) were analysed, demonstrating a crystalline-to-amorphous phase transition during tabletting at 100 MPa pressure. This effect was studied with F19 solid state NMR and by XRD using a diamond anvil cell, which allows pressures of up to 10 GPa to be achieved. These experiments showed a phase transition at 0.33 GPa from $P2_1$ (Z=3) to $P1$ (Z=6) although no clear amorphisation was observed at higher pressures under the conditions of the experiment.

Session 2 of the ESCG satellite meeting was chaired by **Ben Coulson** (DLS) and was kicked off by an engaging talk from **David Coventry** (Edinburgh) who delivered a study carried out on solid caloric materials. David's lecture was entitled "Advancing caloric materials under high pressure and electric fields" and began with an introduction to the field of refrigeration which is estimated to represent something like 20 % of the world's energy consumption. The aim is to develop more efficient solid state refrigerants by exploiting

such effects as solid-to-solid transitions with a high ΔS, hysteresis and pressure sensitivity of barocaloric solids. Tetramethylammonium- and tetramethylphosphonium-$[FeX_4]$ crystals have potential, demonstrating a large ΔS and hysteresis in differential scanning calorimetry (DSC) studies. The system has been studied by powder and single crystal diffraction using high temperature and pressure with various halogens (Br and Cl) as the X substituent in different ratios and with zinc instead of iron. This was followed by a lecture entitled "Radiation damage in molecular crystals – a comparison of X-ray sources and electron diffraction" given by **Stephen Brown** (Warwick). The speaker explained some unexpected X-ray damage that they had observed during beamtime experiments, highlighting the impact that high flux and specific wavelengths can have on inorganic samples. Studies of a titanium-oxo cluster (Ti_6O_6 core) compound which undergoes UV-induced single crystal transformations were described. This process involves photoreduction causing the white cluster to darken and involves a Ti^{3+} d-d transition. A similar colour change was observed on a home X-ray source but with no change in the structure. The session was rounded off with a talk entitled "Novel hydrostatic medium-pressure cell on the I11 high resolution powder diffraction beamline at Diamond Light Source" by **Celine Beck** (Glasgow / DLS). The speaker explained a system she is developing at I11 for carrying out medium pressure powder diffraction studies in a talk which was later awarded the ESCG oral presentation prize! The set up involves a sapphire capillary cell which can achieve pressures of up to 1000 bars in 1 bar steps and temperatures in the range 200 – 420 K, with changes being isobaric or isothermal, as required. The system satisfies a niche requirement of studies falling somewhere between the capabilities of low and high pressure beamlines and there is also freedom of choice in the pressure transmitting medium.

Celine Beck (DLS / Glasgow), winner of the ESCG oral presentation prize, delivering her talk on the liquid pressure cell for use in synchrotron powder diffraction experiments.

The final talk session to round off the first day of the ESCG satellite meeting was chaired by **Rebecca Clulow** (Uppsala) and began with a talk by **Emma Hawking** (CCDC) entitled "Informatics meets energetics: combining crystal structure prediction and knowledge of the crystal landscape." Emma was the winner of the Cruickshank prize for their fantastic participation and involvement throughout the meeting. Emma detailed their work at the CCDC exploring the combined effects of crystal structure prediction (CSP) with the wealth of experimental crystal structure data in the Cambridge Structural Database to better understand the thermodynamic stabilities of small molecule polymorphs. Using the example of mefenamic acid, the speaker described conformational analysis and the evaluation of torsion angles across the CSP landscape. The comparison with Mogul distributions and hydrogen bond network analysis, including H-bond propensity versus actual coordination, were also covered. Emma outlined the assessment of important features using removal of cross-correlation variables and machine learning in the classification of low and high energy states. The rate-limiting step in the analysis is the generation of the CSP landscape. On the theme of polymorphs, **Chengdao Hu** (Edinburgh) then described their research into the discovery of three new polymorphs of the herbicide glyphosate which were revealed under high pressure conditions. Chengdao's presentation was entitled "Three new polymorphs of glyphosate under extreme conditions" and covered the collection of diamond anvil cell data at the DESY source in Hamburg using the P02.2 extreme conditions beamline equipped with a Bruker D8 detector. Previous experiments had detected three crystal forms occurring in the pressure range of 0 to 5.24 GPa and the current study extended this to 8.56 GPa revealing a new crystal phase. Finally, **Rob Carroll** (Leeds) concluded the session with a discussion on the study of amorphous-crystalline MOFs by scanning transmission electron microscopy and electron pair distribution function analysis to unearth structural information. Rob's title was "Electron nano-analysis of amorphous-crystalline MOFs" and during the lecture he covered the commercialisation and device integration of MOFs, mentioning that processibility has been a barrier to their wider use. The lecture encompassed non-crystalline glasses and hybrid glasses which are formed by melt-quenching as well as the use of scanning TEM to study MOF particles. The speaker covered the role electron pair-distribution function (ePDF) analysis in understanding the amorphous nature of MOFs including zeolitic imidazolate frameworks (ZIFs) and a dynamic study of liquid MOFs. The speaker concluded by describing preliminary electron diffraction studies of ZIF-62 which suggested that thinner crystals will be required.

Next on Monday evening, the session of Flash Presentations was chaired **Ellie Dempsey** (Edinburgh) and **Stephen Brown** (Warwick). In this a selection of brave crystallographers took to the floor to show off their research, the only catch being a strict 30 second time limit! **Daniel Rainer** (Southampton), **Chengdao Hu** (Edinburgh), **David**

Participants in the ESCG Flash Presentation session: Ellie Dempsey (Edinburgh, chair), Daniel Rainer (Southampton), Chengdao Hu (Edinburgh), David Coventry (Edinburgh), Lewis Williams (Essex / DLS), Lewis Jackson (Kent), Calum Sangster (Edinburgh) and Stephen Brown (Warwick, chair).

Coventry (Edinburgh), **Lewis Williams** (Essex / DLS), **Lewis Jackson** (Kent) and **Calum Sangster** (Edinburgh) all accepted the challenge and entertained us with some fantastic graphics and speedy crystallography. This made a great warm up to the poster session and sparked much discussion over the drinks and buffet.

This year's Parkin Prize lecture was chaired by **Tom Hitchings** (Kent) and was given by the **Ilaria Gimondi** (CCDC) who also gave the plenary talk for the joint ESCG/CCG Outreach workshop. The Parkin Lecture is always a highlight of the meeting, and this year Ilaria's prize talk entitled "Celebrating collaboration and collective impact in education and outreach" was no different. We were delighted and engaged by the concept of elemental bingo within the crystal structures as we were walked through some successful projects and guided on how we too could get involved with similar activities. Ilaria also leaned on this year's theme of 'Learning from Others', highlighting available crystallographic teaching resources and where to access them – ideal for early-stage crystallographers, as well as engagement grants.

Ilaria Gimondi (CCDC) delivering the Parkin lecture and introducing an interactive game of bingo played during the presentation

The Tuesday morning ESCG session followed on from the Parkin lecture and was chaired by **Stephen Brown** (Warwick). This session began with an excellent talk entitled "Magic ratios or pure coincidence: the rational design of novel pressure transmitting media" given by **Cameron Wilson** (Warwick), the highlight being a very sad racoon having their sample dissolve away and an excellent insight into phase space of multicomponent systems. The speaker covered the basis of diamond anvil cell experiments and what makes a good pressure transmitting medium (PTM) e.g. it should not interact with the sample, and described how most PTMs are liquids or gases. The magic ratio of 4:1 for a methanol:ethanol mixture has a hydrostatic limit of 10.5 GPa, but what is the role of the individual components? The speaker described experiments using isopropyl alcohol rather than ethanol which can raise the hydrostatic limit to 11.5 GPa and theoretical work using dynamic simulations to aid the design of improved PTMs. Following on from this was a talk from **Thomas Fellowes** (Liverpool) on looking at light driven charge transfer reactions using an event-based detector Tristan at DLS I19 which records individual photons instead of frames, allowing for nanosecond time resolution. Thomas's title of the "Identification of a charge-separated transient species by time-resolved X-ray diffraction" relates to studies of this molecular photo-catalytic system consisting of donor-acceptor push-pull molecules that are capable of generating O_2 and N_2. Pseudo steady-state data have been collected using an in house diffractometer with a 3D printed LED holder, allowing charge-density analysis of the dark and light states. The speaker concluded by discussing some of the challenges in the on-going analysis of time-resolved data collected at DLS including the observation that 2D slicing struggled to keep up with the rate of reaction. Next, **Lewis Williams** (Essex / DLS) spoke about quantifying and benchmarking beam damage at the very high intensity XFEL sources, demonstrating that their short pulse durations can prevent dose dependent beam damage in protein crystallography as atomic rearrangement does not significantly occur during each pulse. The speaker's title of "Damage before destruction? X-ray induced changes in single pulse serial femtosecond crystallography" firmly alludes to this point. The speaker described experimental work on ferredoxin, the peroxidase DtpA and thaumatin using the SwissFEL and XFEL sources. The resulting structures were found to be free from the iron-to-water ligand lengthening and disulphide bond reduction effects which are observed with synchrotron data. Next, **Viktorija Mikaite** (UCD) gave a lecture on the subject of "Big ligands, big possibilities: shining a light on NDI-based coordination polymers." The speaker covered studies of naphthalene diimide (NDI) precursors which are relatively easy to synthesise as well as being redox active, photochromic and photoluminescent. They have many applications in inkless printing, batteries, explosives, etc, and can coordinate metal ions such as zinc and bismuth. Structurally, they possess solvent accessible voids and physically, they change colour when exposed to a 385 nm LED. Indeed, over time they return to their original colour and the process can be cycled up to five times. Radical lifetimes vary from 1 to > 3.5 h, depending on the compound framework, and this has been confirmed by EPR.

The Closing Plenary session was chaired by **Ben Coulson** (DLS) and was delivered by **Jeremiah Tidey** (Warwick / NCS) who took spoke on the subject of "3D electron diffraction via the scenic route" and took us on an engaging walking tour through his crystallographic career. This spanned high pressure single crystal XRD of macrocyclic coordination complexes, polymorphism and highly disordered phases as well as charge-density and topological (asphericity) analysis of energetic materials for studying their impact sensitivity. The speaker explained how further work on pXRD of metal oxides shed light on the importance of symmetry and how these studies can be constrained by scXRD. EM and pXRD studies of ferrorelaxors combined dark field imaging of twin domains within the crystal with the use of DFT models to constrain pXRD refinements. This progression led to his current role at the 3DED facility in Warwick as part of the NCS. Jere's talk inspired the members of the ESCG to step outside of their comfort zone and explore the benefits of, in his own words, "the scenic route."

Jeremiah Tidey (Warwick / NCS) delivering the Closing Plenary of the ESCG satellite meeting.

Lonsdale lecture

The BCA awarded the Lonsdale Prize Lecture 2025 on recommendation from the ESCG to **Emma McCabe** (Durham). The prize lecture, which was chaired by **Tom Hitchings** (Kent), was a fantastic opener to the main meeting and was entitled "Breaking inversion symmetry: strategies and consequences." After highlighting the work of the late Kathleen Lonsdale and acknowledging her as a source of inspiration regarding her beliefs and pacifism, Emma began by discussing the fundamental crystallographic concept of non-centrosymmetric point groups. These point groups were elegantly organised into a Venn diagram, which related them to the macroscopic properties expressed by the crystals, sometimes referred to as Neumann's principle, with a focus on polar structures. This was also explored through discussion of chemical concepts such as chirality, which are conventionally associated with molecular species, but can manifest through crystal packing of non-chiral units, in forms such as helices to give enantiomorphic systems. This led concisely on to discussing strategies to design and achieve such properties through the breaking of inversion symmetry to find and design new proper and improper ferroelectrics, semiconducting and photocatalytic materials. Examples of these strategies in action were drawn on with some recent work on the anion ordering in oxychalcogenides as photocatalysts. Notably, the meeting was held in Leeds this year, where Kathleen spent much of her early life and career and where she conclusively settled the planar nature of benzene. In all, Emma delivered an engaging and insightful talk on symmetry, structure and fundamental crystallography, which set an exceptional tone for the rest of the meeting.

CCG / ESCG Joint Session: Would you publish it? Interesting problems in Crystallography

Once again the CCG and ESCG joined forces to deliver a unique session in which we pondered intriguing problems in chemical crystallography, what determines something to be of publishable quality, and later on philosophically what it even means to publish something. This session was chaired by **Toby Blundell** (Durham) and **Sam Lewis** (Cardiff / DLS) and featured a star-studded line up of speakers that made it a session to remember. The National Crystallography Service (NCS) got the proceedings started with an impressive tag-team approach to delivering their talk on what makes a structure acceptable for publication. **Simon Coles** (Southampton) took on the role of headliner for the trio detailing the NCS and the services it provides in-house and interfacing with DLS. Simon's talk title was "Pushing the boundaries of crystal structure analysis – what is acceptable?!" and he used the opportunity to introduce the concept of crystallographic data FAIR-ness, namely that original measurements should be Findable, Accessible, Interoperable and Reusable, as well as fit-for-purpose. The speaker emphasised that challenging samples and experiments as well as new structure determination methods mean that measured data should be available for re-analysis. This should, of course, be part of the driving force for experimentalists to collect the best, most complete data with the best available instrumentation. The speaker also described the crystal sponge method of structure determination, raised the question of whether structures in databases should be graded and mentioned the new journal IUCr Raw Data Letters before passing the baton on to **Peter Horton** (Southampton) and **Daniel Rainer** (Southampton) to describe a number of examples studied by X-ray and electron diffraction, respectively. Then, **Gary Nichol** (Edinburgh) then took to the stage and detailed a number of accounts from his work as the crystallography service manager in Edinburgh. From misconceptions of *R*-factors, battling reviewers on difficult structures, and teaching students on new powerful diffractometers, Gary expertly covered a broad range of topics. Gary also touched on the legacy Ortep Of The Year (OOTY) award which was a reflection of how extremely elongated thermal ellipsoids and other issues allowed the trained eye to spot problematic structures in publications. Using an example where collecting data to 0.5 Å resolution required 2.5 hours compared to the 44 minutes needed for 0.7 Å, the speaker emphasised that one should not sacrifice data quality for throughput and discussed the application of non-spherical form factors, as well as the validity of criteria currently used for assessing structure quality from analysis of the CSD database. This was followed up by a lecture entitled "What are the criteria of isostructurality?" given by **Petra Bombicz** (HUN-REN Research Centre for Natural Sciences). Petra gave a discussion on the criteria for isostructurality, covering the fact that its definition lacks clarification on the requirement of stoichiometry, Z', symmetry elements and space groups. Using a series of crystal structures introducing fine chemical changes, the speaker demonstrated that, in contrast to polymorphism, isostructuralism can be characterised by numerical descriptors. The speaker mentioned the Mercury crystal packing similarity tool in CSD-Materials and discussed new interpretations of the IUCr definitions of isostructurality. Last but by no means least, **Bill Clegg** (Newcastle) contemplated what the modern-day concept of a publication can be defined as. Conventionally, this was considered to be a physically printed manuscript in a peer-reviewed book or journal, however contemporary methods include purely electronic sources, conference presentations, document repositories and structural databases. Bill concluded with a request for people to not only ask ***if*** something could be published, but additionally ***how*** it should be appropriately published.

Stephen Brown, Warwick
Ben Coulson, DLS
Ellie Dempsey, Edinburgh
Thomas Hitchings, Kent
Sam Lewis, Cardiff / DLS
Mark Montgomery, Syngenta

Speakers and chairs of the CCG / ESCG Joint Session: Would you publish it? Interesting problems in Crystallography. Sam Lewis (Cardiff/DLS), Gary Nichol (Edinburgh), Daniel Rainer (Southampton), Simon Coles (Southampton), Peter Horton (Southampton), Bill Clegg (Newcastle), Toby Blundell (Durham) and Petra Bombicz (HUN-REN Research Centre for Natural Sciences).

IG Conference Report

The session entitled "A journey through structural modelling: amorphous, mixtures and more" was chaired by **Tony Bell** (Sheffield Hallam) and **Natalie Johnson** (CCDC). This session featured four excellent speakers whose contributions covered different methods of analysing structures of a variety of different systems.

The keynote lecture was given by **Michael Devlin** (CMAC, Strathclyde) who presented the "Effect of simulation box size and shear on the structure of amorphous hydrochlorothiazide" which detailed the importance of validation of the simulation box size in molecular dynamics simulations. A range of box sizes were investigated to assess the consistency of the simulations and pair distribution functions (PDF) calculated for the structural models were presented as a good method for doing a quick assessment of the structural consistency of the boxes. For simulations of hydrochlorothiazide, it was found that a box size of 100 molecules was the minimum required to have consistent short-range interactions, with 250 molecules required to capture the intermediate-range structure. The chosen number of molecules in the box was also shown to affect the distributions of interactions in the box.

This was followed by 'It's PDF, Jim, but not as we know it…' where **Michael Wharmby** (Bruker AXS) began by describing the requirements for a good PDF and how synchrotron PDF beamlines are optimised to collect high quality data (and the compromises needed to achieve this). Until recently, good PDF data could only be collected at dedicated synchrotron beamlines, for which access to beamtime is required. It was then presented how the same optimisations from synchrotron beamlines have been applied to lab instruments and shown that in many cases, through the proper configuration of an instrument, data can be collected that are more than suitable for publication.

Next **Paul O'Meara** (Malvern Panalytical) delivered a talk entitled "Structure determination of new phases from complex mixtures: a laboratory perspective." It can be challenging to determine the structure of a multiphase sample from powder diffraction, however, this talk demonstrated workflows for structure solutions using the HighScore Suite and data, measured in 5 minutes, from a compact benchtop machine. This was extended to show the successful structure solution of a Li/Na battery material with impurity and unknown phases to be deconvoluted in the data. The accuracy of the structure solutions was confirmed with DFT calculations.

Finally **Fraser White** (Rigaku) described the advancements of electron diffraction instrumentation in "XtaLAB Synergy-ED: Solving the Unsolvable." Several examples of structure solutions from the XtaLAB Synergy-ED were presented, including MOFs, impure powders and absolute structure determination, showing that valuable information can be obtained from sub-micron crystals.

This year's thought-provoking IG plenary was delivered by **Fanny Costa** (Leeds) with a talk entitled "Navigating polyamorphism in amorphous pharmaceuticals: insights and open questions." Dr Costa began by describing the challenge of low water solubility in pharmaceuticals. Poor solubility impacts how well the body absorbs a drug – possibly requiring higher doses which can increase the risk of side effects and toxicity. One strategy to increase the solubility of a drug is the usage of its amorphous form, although this poses different challenges in preparation and storage. From here, Dr Costa described the concept of structure in amorphous materials – while having no long-range order, the materials do have some short-range order over the length scales of many Å. The question was posed: could there more than one amorphous state of the same material? This introduced the potentially controversial topic of polyamorphism – 2 amorphous states separated by a clear phase transition. Dr Costa then discussed recent highlights from scientific literature studies into the phenomena, including studies of paracetamol and hydrochlorothiazide. Finally, questions were posed to the audience: whether the currently available analytical tools are sufficient to demonstrate the presence of polyamorphism, if pseudo-polyamorphism was a more appropriate term and if further investigation into polyamorphism should be considered.

Speakers and chairs on "A journey through structural modelling: amorphous, mixtures and more" Tony Bell (Sheffield Hallam, chair), Fraser White (Rigaku), Paul O'Meara (Malvern Panalytical), Michael Wharmby (Bruker AXS), Michael Devlin (CMAC Strathclyde) and Natalie Johnson (CCDC, chair).

Natalie Johnson (CCDC, chair) and IG Plenary lecturer Fanny Costa (Leeds) consider "Navigating polyamorphism in amorphous pharmaceuticals: insights and open questions."

Natalie Johnson, CCDC
Tony Bell, Sheffield Hallam

CCG sessions

The CCG Plenary lecture entitled "Be a crystallographer to investigate the past, the present and the future" was given by **Lucia Maini** (Bologna) and was chaired by **Hamish Yeung** (Birmingham). The speaker described the hermaneutic approach of text-searching ancient chemical texts from classical antiquity, with the aim of discovering long forgotten mechanochemical methods. For example, the successful extraction of mercury metal from cinnabar (mercury sulphide) by grinding it either in vinegar or copper powder was described in detail, the discovery of these two reactions being attributed to Theophrastus and Pliny, respectively, around 2000 years ago. Sometime after their work, Maria the Jewess, who is claimed to have founded an alchemical academy in Alexandria, discovered that grinding lead with cinnabar had the same effect. The speaker moved on to describe some of the discoveries of syriac and arabic alchemists. Lucia then described studies of enzalutamide, a drug currently used for treatment of metastatic prostate cancer, which was analysed by powder diffraction. Recrystallisation three times in isopropanol yielded a new crystal form R3 with a substitution impurity of the drug being reduced to an acceptable level. Lucia then described studies of barbituric acid which undergoes mechanochemical keto-enol tautomerism on the 24 hour timescale. NMR studies of the hydrogen bonding along with reactions with alkali halides which yield ionic co-crystals were also described. The speaker outlined a range of studies on perylene diimide polymorphs by melting-point and structure analysis, covering their thermo- and mechano-chromic behaviour, the latter having applications in damage detection. These effects were studied by whole powder pattern modelling. The speaker emphasised that the future of research in this field is looking extremely promising.

*Chair of the CCG **Hamish Yeung** (Birmingham) with the CCG Plenary lecturer **Lucia Maini** (Bologna).*

Thus to summarise, Lucia described a fascinating collaboration with historians in understanding the alchemical production of mercury from mineral ores based on ancient texts, using laboratory experiments to reproduce old techniques and modern techniques to investigate the chemistry involved. Lucia presented studies of polymorphism and thermal behaviour relevant to pharmaceutical applications and, finally, the discovery of new smart mechanochromic materials that could be applied to detection of mechanical failure in composites. In all these real-world examples, Lucia showed where her expertise as a crystallographer proved necessary to solve relevant problems, providing inspiration and encouragement to all of us in the crystallography community that our skills and experience remain essential in the modern age.

Next up, following an introductory mini-biography by the session chair **Alex Gibbs** (St Andrews), the CCG Early Career Prize lecture was given by **Wojciech Stawski** (Ulm). With an impressive chemistry background spanning Wroclaw, Cambridge and Oxford, Wojciech spoke on the subject of "π-Conjugated macrocycles in the solid state: structural manifestations of anti-aromaticity and some really cool structures." The prize itself was presented by **Suzanna Ward** (CCDC) in the session. Wojciech described his fascinating and detailed work in synthesising, crystallising and characterising the structures of aromatic and anti-aromatic molecules. He gave the audience a highly engaging tour through his re-investigation of the structure of [18] annulene, determination of global (anti)aromaticity in [24] paracyclophanetetraene and the discovery of polymorphism in six-porphyrin nanorings. Not only was his crystallography impressive, Wojciech's skills in synthetic chemistry and crystallography education were clearly evident – a very worthy winner of the 2025 Prize.

***Suzanna Ward** (CCDC) presenting the CCG Early Career Prize to **Wojciech Stawski** (Ulm) with CCG chair **Hamish Yeung** (Birmingham).*

During his talk, Wojciech described the shielding and de-shielding effects which arise in NMR studies of aromatic compounds. Some published historic work on [18]annulene which had been reduced with potassium metal revealed a very unusual spectrum. The speaker described repeating the experiment and obtaining the correct structure by NMR. Subsequent crystallographic studies of [18]annulene which had been reduced by Li instead of K revealed the full nature of the lithium complex which was similar to corannulene – a molecular bowl structure formed by five fused benzene rings surrounding a cyclopentane ring at the base of the bowl, also known as buckybowl due to it being a fragment of buckminsterfullerene. The speaker reported a large number of very impressive structure analyses of lithium, sodium and potassium sandwich complexes including those of paracyclophanetetraene before moving on to outline the photosynthetic reaction centre and how its numerous constituent porphyrins can be mimicked synthetically by nano-rings. The speaker then reported further even more impressive structures of porphyrin nano-rings and their polymorphs co-crystallised with buckminsterfullerene which adopt herringbone arrangements in the crystal packing. The high porosity of these materials suggests they may have applications in light-harvesting organic frameworks. The speaker has prepared a number of videos on structure solution and refinement which are available on YouTube.

Excellent summaries of the other CCG sessions (including the **Outreach Workshop**, the **Open Session** and the session on **Polymorphism, hydrates and co-crystals**) can be found in the following Arnold Beevers Bursary Awardee reports.

Hamish Yeung, Birmingham
Jon Cooper, UCL

Arnold Beevers bursary awardee reports

The BCA is very grateful to GSK for their very generous sponsorship of the Spring Meeting which has allowed us to award a significant number of bursaries, both this year and last.

Stephen Brown, Warwick

The Tuesday morning ESCG session followed on from the Parkin lecture with an excellent talk about pressure transmitting materials for high pressure studies from **Cameron Wilson** (Warwick), the highlight being a very sad racoon having their sample dissolve away as well as excellent insight into phase space of multicomponent systems. Following on was a talk from **Thomas Fellowes** (Liverpool) on looking at light driven charge transfer reactions using an event-based detector Tristan which records individual photons instead of frames, allowing for nanosecond time resolution. Finally **Lewis Williams** (Essex) spoke about quantifying and benchmarking beam damage at the very high intensity XFEL sources, demonstrating that the short pulse durations at XFELs can prevent dose dependent beam damage in protein crystallography as atomic rearrangement does not significantly occur.

***Stephen Brown** (Warwick, chair) with the Keynote Lecturer of the Outreach Workshop **Ilaria Gimondi** (CCDC) and **Ellie Dempsey** (Edinburgh, chair).*

The outreach workshop was well attended with people from varying stages of their careers and I thoroughly enjoyed hearing people's ideas and experiences with bringing crystallography to the public. The workshop began with an overflowing presentation from **Ilaria Gimondi** (CCDC) about the work she and her team do in outreach as well as sharing the projects the CCDC has helped fund and host. Joining together crystallographers and educators from around the world with resources from top trump cards, activity books and web resources to inspire the scientists of tomorrow. This was followed by discussion groups about future outreach ideas including crystal Guess Who, Lego polymorphs and waves in a pond which *requires* **Peter Horton** (Southampton) to dress in a duck costume.

Matt Cliffe, Nottingham

The final session of Wed 16th April 2025 at the BCA Spring Meeting in Leeds was the plenary talk given by **Robert Palgrave** (UCL) entitled "The Role of AI in materials Discovery." Prof Palgrave gave a lively and entertaining summary of recent efforts from major tech corporations to use generative AI and automation to discover new inorganic compounds and how these efforts have not yet achieved the striking improvements seen in other applications of generative AI in structural problems (e.g. AlphaFold). In particular, he highlighted how crystallographic and chemical understanding will prove crucial for any successful efforts to harness this new technology in materials discovery. The importance of this topic, and the surprising examples of 'discovery' uncovered by Prof Palgrave and coworkers, sparked lively discussion during the session, in the poster session and long after.

Rebecca Clulow, Uppsala

The BCA spring meeting took place at the University of Leeds from the 14th – 17th of April this year. The programme encompassed a wide range of topics and included the PCG session on Phase Transitions which was chaired by **Struan Simpson** (Warwick). The keynote lecture was given by **Rebecca Scatena** (DLS) who covered research on the pressure induced phase transitions in a range of coordination compounds. Her talk highlighted the role of polyatomic ions in pressure induced phase transitions. The first contributed talk was given by **Farheen Sayed** (Cambridge) who presented her work on $LiNbO_3$ coated LNMO cathodes. The talk was followed by a presentation from **Eliza Dempsey** (Edinburgh) on the phase transitions and thermal expansion of the $NbO_{2-x}F_{1+x}$ system. The system has tuneable thermal expansion behaviour

depending on the fluorine/oxygen content. The final talk of the session was given by **Sam Thompson** (Durham) who presented his work using the CSD to find missed ferroelectric materials. The approach identifies polar structures which have closely related non-polar phases.

David Coventry, Edinburgh

I recently attended the BCA's Annual Spring Meeting at the University of Leeds, a simple train ride away from my own university in Edinburgh. The proceedings began on Monday the 14th of April with the Early-Stage Crystallographers' Group meeting. After delivering my own presentation, many other students gave thorough explanations of their own projects. On top of formal presentations, I and the other students made more casual poster presentations with our scientific findings, and displayed them during networking sessions.

The next day, the main group meeting commenced, with main plenary presentations and satellite sessions with specialised themes for their lectures. Across the next three days, I generally attended sessions centred on physical crystallography. One session which interested me greatly was focused on collaborative approaches using X-ray diffraction and additional spectroscopic and diffraction techniques.

The session was chaired by **Evie Ladbrook** (Warwick) and **Karen Johnston** (Durham) and began with **Dave Collins** (Leeds) presenting his research into the surface functional groups of crystal facets, and how they impact the solubility of crystals. Using Raman spectroscopy, certain vibrational modes can be excited at different orientational angles of the crystal, allowing for surface characterisation to be used alongside X-ray crystallography.

Then, **Pedro Nunes** (DLS) presented an upcoming high-energy electron crystallography instrument (or HeXI) which is being developed at Diamond, to open at the end of 2026. As X-ray crystallography gives an indication of a crystal's electron density, electron crystallography can provide the additional data of the crystal's electrostatic potential. The high-energy electrons make the system optimised for intermediate crystal sizes, of 300 nm to 3 μm and minimise the level of secondary and tertiary diffraction, which often plagues electron crystallography.

Afterwards, **Kieran Griffiths** (Lancaster) explained the use of solid-state NMR to identify photoswitching between isomers in pores of metal-organic frameworks, or MOFs. In salicylidene- anilines, interconversion can only occur in its photochromic enol structure, which has a torsion angle between 30-40°, whereas its cis-/trans-keto non-photochromic structures are seen to be planar. NMR was used to evaluate the torsion angle in the salicylidene-aniline molecules when placed in the pores of MOF MIL-53, which showed that the pores afforded greater twisting freedom and therefore were able to convert some non-photochromic species into photochromic ones.

Finally, **Tim Easun** (Birmingham) gave an overview of a variety of collaborative approaches. This spanned from using IR spectroscopy to monitor the photoswitching of nitro-nickel(II) complexes at a range of temperatures, or the UV-induced carbonyl removal of the manganese coordination complex $\{Mn(DMF)_2[C_{12}H_6N_2O_4Re(CO)_3Cl]\}$, to the use of Raman, UV-vis and an LED flash bulb to follow the photochemistry of spiropyrans, as they go back and forth between structures as they absorb photons and then relax.

After a wonderful final dinner, an awards ceremony lauding the best posters and presentations of the meeting, and a celebratory cèilidh on the Wednesday night, the meeting ended on Thursday the 17th April 2025 with knowledge exchanged, connections made and new inspiration acquired for where to take my own research as my PhD project progresses.

***Karen Johnston** (Durham, chair), **Dave Collins** (Leeds), **Pedro Nunes** (DLS), **Evie Ladbrook** (Warwick, chair), **Tim Easun** (Birmingham) and **Kieran Griffiths** (Lancaster) at the joint PCG/ESCG session on Complementary Techniques.*

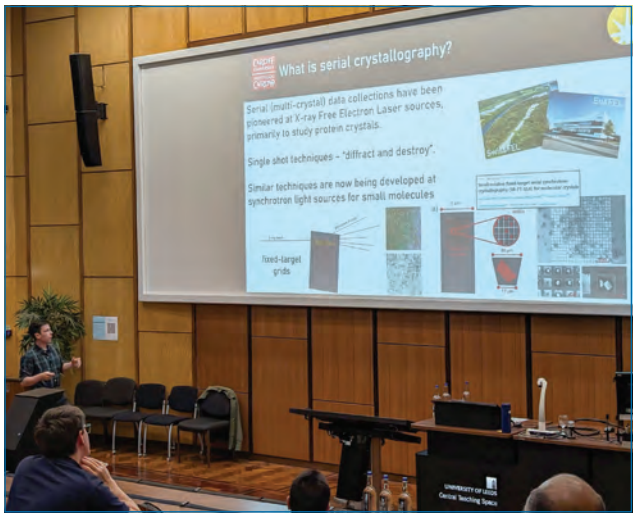
Patrick Doheny, Birmingham

This year's BCA Spring Meeting was again held at the University of Leeds with its theme being 'Learning from Others' which emphasised the necessity and benefits that are to be gained from collaboration in the structural sciences. The conference was marked by an excellent line-up of speakers, both established and early career researchers, that highlighted the diverse and innovative research currently taking place in the field of structural science.

One particular highlight was the CCG Open Session on the final day that featured talks from a number of diverse areas across chemical crystallography. This session, chaired by **Tony Keene** (UCD), featured four speakers beginning with **Gustavo Santiso-Quinones** (ELDICO Scientific AG) who gave a presentation entitled "In the footsteps of Pasteur: identifying conglomerate systems using state-of-the-art electron diffraction" on the use of this technique to determine the absolute structure of natural products, biomolecules and drugs. His talk highlighted the ability of electron diffraction to determine the structures of conglomerate samples, racemic compounds composed of separate crystal entities, from nanometre-sized samples. His talk demonstrated how the use of electron diffraction can lead to much more streamlined structural characterisation of conglomerate samples with higher throughput versus more traditional X-ray diffraction methods.

The second talk was entitled "Serial synchrotron crystallography as a tool for materials discovery" and was given by **Sam Lewis** (Cardiff/DLS) who covered the development of serial synchrotron crystallography (SSX)

methods at the I19 beamline at DLS. The I19 team's development of fixed-target SSX, in which microcrystals are deposited on a grid and rapidly scanned to identify suitable crystals for data collection, was discussed alongside photoirradiation and time-resolved data collection methods used to optimise the structural data obtained for short-lived and poorly diffracting samples. The talk concluded showing the potential for SSX methods to be used in solving small molecule structures characterised by micro crystallites that diffract poorly, are vulnerable to beam damage and may be short-lived, in addition to the continuing development of SSX methods at I19.



***Sam Lewis** (Cardiff/DLS) speaking on serial synchrotron crystallography (SSX) methods in the CCG Open Session.*

Paul Niklas Ruth (Durham) then introduced an open source, web-based crystal structure visualiser called CifVis in a lecture entitled "CifVis – a JavaScript library and widget for crystal structure visualisation." This widget allows the visualisation of CIF files directly in a web browser without the need for external programs and with a wide range of options to customise the visualisation of a structure and its specific properties.

The session then concluded with a presentation entitled "Amino acid-based multicomponent crystals as alternative optical and piezoelectric materials." Given by **Suman Bhattacharya** (Limerick), this lecture looked at multicomponent amino acid-based crystals as potential piezoelectric materials. Suman's talk focused on the use of polycrystalline molds to achieve rapid co-crystallisation of amino acid-based piezoelectric materials. Variation of the organic molecules chosen for co-crystallisation such as γ-glycine and sulfamic acid achieved enhanced piezoelectric performance and demonstrated the potential for these organic-based materials as alternatives to piezoelectrics that contain toxic compounds such as lead, while also achieving greater designability and property control.

***Speakers in the CCG Open Session: Gustavo Santiso-Quinones** (ELDICO Scientific AG), **Sam Lewis** (Cardiff / DLS), **Paul Niklas Ruth** (Durham), **Suman Bhattacharya** (Limerick) and **Tony Keene** (UCD, chair).*

Overall, both the BCA Spring Meeting and Early Stage Crystallographers Group Meeting featured an excellent lineup of speakers particularly from students and early career researchers as well as poster presentations that all showed the exciting research being carried out in crystallographic analysis and structural science.

Banaz Fetah, Strathclyde

I recently travelled from Glasgow to attend the Early-Stage Crystallographers Group (ESCG) satellite meeting, which was hosted at the University of Leeds. I always look forward to these meetings in the lead up to the main meeting. It is a very relaxed and supportive environment to share ideas, discuss research findings and exchange techniques with other PhD students and early-career researchers.

I was honoured to present my talk during the opening session, where I discussed the discovery of a new high-pressure phase of Posaconazole. The experience also helped improve my public speaking skills and made me more comfortable discussing my work with a wider audience. I also presented a poster which gave me the chance to engage with many attendees from the main meeting and resulted in useful conversations and valuable feedback on my work. There were many poster sessions throughout the day which made it easier for networking and gaining confidence in talking about my research area.

During the parallel sessions on the afternoon of day 3, I attended the CCG session entitled "Polymorphism, hydrates, and co-crystals" which was chaired by **Iain Oswald** (Strathclyde). This session had many excellent talks and one of the highlights for me was the lecture by **Emma Hawking** (CCDC) entitled "Informatics meets energetics: combining crystal structure prediction and knowledge of the crystal landscape." Emma's presentation highlighted how polymorphism plays a major role in the pharmaceutical process and how finding the most stable form can be difficult but experimental and computational techniques such as crystal structure prediction (CSP) can help us understand these forms. I also found the talk by **Calum Sangster** (Edinburgh) entitled "3-Dimensional electron diffraction and in situ activation of metal-organic frameworks" particularly interesting. Calum spoke about a topic I am not very familiar with, so it was an amazing opportunity to learn more about this area of research.

Beyond the scientific sessions, the conference dinner was a great social highlight. It was a lovely opportunity to unwind and connect with fellow PhD students. After dinner, there was the announcement of poster prizes, and I was thrilled to be one of the winners of the industrial poster prize. It was a reassuring moment that gave me a bit more confidence in the direction of my research. The night ended with some cèilidh dancing, adding a Scottish twist to the night. Overall, the conference was a good experience and has also helped me reflect on my own career path.

Jake Hill, Bradford

The ESCG satellite meeting was opened by **Mark Warren** (DLS), who gave an excellent opening plenary about their work developing serial methodology for chemical crystallography. Adapting methods more common to macromolecular crystallography, they have developed a method using a small rotation of the chip to overcome the sparse reflection data otherwise produced. This approach allows the exploration of dynamics and, with increasingly bright light sources coming online, is likely to be a key way to deal with increasing radiation damage.

The first session of the ESCG covered a whole range of crystallographic topics. **Daniel Rainer** (Southampton/NCS) started the session with a talk about more environmentally friendly coordination polymers and efforts to characterise them using electron diffraction. This was followed by **Matthew Edwards** (Warwick) with a talk on structural changes in cuprate superconductors. **Thomas Smith** (Newcastle) provided details on their efforts to improve and standardise data management of the increasingly large and complex crystal conditions generated by techniques such as ENaCt. The session ended with an excellent talk by **Banaz Fetah** (Strathclyde) on the discovery of a new phase of the drug Posaconazole at high pressures.

The day continued with two more sessions. **Dave Coventry** (Edinburgh) presented his work on barocalorics which change from an ordered to disordered state with increasing temperature. Using DSC, and a pressure jump cell they mapped the phase change and reported structures for each of the phases. **Stephen Brown** (Warwick) gave a stand-out talk about radiation damage in titanium oxo clusters. Comparing the effects of UV irradiation, a home source, synchrotron and electron diffraction revealed both different disordered and damage states but also allowed an understanding of the change in ligand oxidation. **Celine Beck** (Glasgow / DLS) told us about the development of a new liquid pressure cell on I11 allowing experiments up to 1000 bar with fine control to set the pressure in 1 bar increments.

Emma Hawking (CDCC) gave a talk describing the use of energetic and conformational prediction and analysis to improve crystal structure prediction. **Chengdao Hu** (Edinburgh) presented work on glyphosate polymorphs under extreme conditions. Using high pressure diamond anvil cells at synchrotrons, they showed that slow or fast pressure increases revealed different phases. An initial rapid compression, then gradual increases lead to discovery of a new phase. Finally, **Rob Carroll** (Leeds) gave a talk detailing how they are using electron microscopy to explore heterogeneity as well as Bragg and diffuse scattering to improve the processability of amorphous MOF's for ultimate use in devices.

The day was concluded with a lively poster session and the opportunity to catch up with friends and discuss the day's talks. As always the ESCG meeting showcased the entire breadth of crystallography with excellent talks in a friendly and welcoming way. I am very much looking forward to next year.

Thomas Hitchings, Kent

This year's BCA Spring meeting was full of thought-provoking and engaging contributions across crystallography. Some personal highlights included the 'Would you publish it?' session, where we reflected on the purpose of crystallographic analysis and the importance of data quality and availability, and the fantastic PCG plenary from **Robert Palgrave** (UCL), examining the use of AI for the discovery of crystal structures. I was delighted to see the restoration of the workshop format this year at Leeds 2025! The parallel session I attended was the Outreach workshop, superbly chaired by **Stephen Brown** (Warwick) and **Eliza Dempsey** (Edinburgh), which was unlike many conference sessions I have attended before. The session got underway with a talk from this year's Parkin Prize winner, **Ilaria Gimondi** (CCDC), who focussed on the qualities of successful outreach programmes she had been involved with. This nucleated many ideas within the room, which were then discussed and 'workshopped' in small breakout groups. The session format allowed for constructive

discussion with considerations on audience, environment, and funding sources. This format also facilitated structured networking within breakout groups, which conventional sessions omit, and enabled structured and focused conversations, providing perfect opportunities for early-stage crystallographers to engage with those in more established careers. Overall, a very enjoyable and productive session, and hopefully, it will lead to some excellent crystallographic outreach programmes that I look forward to seeing take shape.

Phillippa Partridge, Edinburgh

The Materials Research Society (MRS) Spring Meeting of 2025 was held in Seattle, WA, USA. This five-day conference, running from the 7th to the 11th of April, attracts nearly 6,000 researchers globally to present their work across 67 diverse symposia. These sessions covered a broad range of topics from materials theory, computation and data science to characterisation, structural and functional materials and their broader impacts on society.

My primary interest lay in a symposium entitled "Solid materials for sustainable cooling: caloric effects and devices." This session was organized by **Helen Walker** (STFC, UK), **Pol Lloveras** (Catalunya, Spain), **Anthony Phillips** (QMUL, UK) and **Karl Sandeman** (Brooklyn, USA). Spanning three out of the five conference days, the symposium focused on various topics related to caloric materials and their applications in solid-state cooling devices. The caloric effect, which involves inducing reversible changes in isothermal entropy and adiabatic temperature through the application of an external field, presents an environmentally friendly alternative to traditional vapour-compression cooling technologies. Throughout the symposium, researchers presented advances in materials, devices, and theoretical modelling in magnetocalorics, elastocalorics, barocalorics and multicalorics with contribution from both academia and industry.

One particularly engaging session, entitled "Barocaloric materials" chaired by **Heike Herper** (Uppsala) and **Anthony Phillips** (QMUL), showcased a diverse array of presentations focused on enhancing barocaloric efficiency through material tuning. The session opened with a talk by **Patrick Shamberger** (Texas A&M, USA), entitled "Isolation of geometric contributions to plastic crystal transformations through selective deuteration of neopentyl glycol." Their research focussed on a series of selectively-deuterated neopentyl glycol (NPG) compounds which have identical chemical interactions but span a spectrum of molecular sphericity. These offered valuable insights into the role of molecule geometry on the resulting rotational degrees of freedom in the plastic crystalline phase. Following this, **Xavier Moya** (Cambridge) delivered a presentation on "Barocaloric plastic crystals for sustainable cooling." They highlighted both innovative methods and materials, notably showcasing direct measurements that revealed adiabatic temperature changes of up to 30 K. **Daniel Laorenza** (Harvard, USA) then presented on the subject of "Organic molecules in a box – barocaloric cooling from confined order-disorder transitions" demonstrating how pressure sensitivity and thermal transport properties may be modulated based on the metal node and central cation compositions in three-dimensional perovskite-like materials.

Continuing the theme of molecular design, **Faith Chen** (Wellesley, USA) discussed "Barocaloric design principles in asymmetric dialkylammonium salts." Their work explored chain-melting materials and illustrated how manipulating chain lengths in these asymmetric dialkylammonium salts enables controllable tuning of barocaloric properties. **Joshua Levinsky** (Edinburgh) followed with a talk entitled "The role of hydrogen bond competition in the colossal barocaloric response of choline-based plastic crystals." This talk linked structural disorder identified through single-crystal X-ray diffraction with hydrogen bond competition observed via ab initio molecular dynamics simulations. Finally, **Chase Somodi** (Texas A&M, USA) closed the session with a

The 2025 Materials Research Society (MRS) Spring Meeting in Seattle, USA.

lecture on “Unraveling thermal hysteresis in plastic crystals – a pathway to efficient solid-state refrigerants.” Their presentation detailed calorimetric and optical microscopy analyses aimed at isolating the primary contributors to energy dissipation during solid-solid transformations.

As evident from the breadth of research presented, barocaloric behaviour can be observed across a wide range of materials. The ability to tailor structure-property relationships remains an evolving and promising area of ongoing investigation within this field.

On a final note, I would like to extend my sincere thanks to the symposium organisers, the speakers across all three days and the Arnold Beevers Bursary Fund (ABBF) for providing the financial support that made my attendance possible.

Daniel Rainer, Southampton

The second CCG session of the conference featured talks on the topic of “Polymorphism, hydrates, and co-crystals” and was chaired by **Iain Oswald** (Strathclyde). The keynote speaker **Amy Hall** (Durham) opened the session by presenting her work investigating the importance of hydrogen-bonding in predicting stability of co-crystals. In her talk entitled “Are hydrogen bonds really queen in molecular cocrystals?” Amy first described the parameters for the CSD search to find suitable dimeric systems for which energy calculations could be performed to elucidate interactions present and their relative strength. The study focused on 1:1 dimers in order to create a manageable but still representative dataset. Amy’s findings show that despite H-bonds (HB) being clearly a strong indicator for a stable co-crystal, stacking and T-type interactions (ST) must equally be considered. When taking both strength and occurrence of HB and ST interactions into account they may be referred to as King (ST) and Queen (HB) of co-crystal predictors. A comprehensive description of the concepts and findings can be found in Amy’s Nature paper from last year [1].

The next talk was given by **Emma Hawking** (CCDC), who was able to step in at the last minute as a substitute speaker and present her work entitled “Informatics on Energetics”, which she had previously given at the ESCG satellite meeting on Monday. Emma developed a robust pipeline with the aim of overcoming the bottleneck of computationally intensive CSP calculations. Using mefenamic acid as example molecule, she demonstrated that a CSP landscape and information from the CSD can be used to highlight differences between high energy and low energy structures. By removing cross-correlations, the relative importance of different features could be determined, giving a good indicator for the stability of different polymorphic forms. In the case of mefenamic acid, this analysis shows that the stable form 1 features weaker H-H repulsion compared to the meta-stable form 3.

The following presentation was given by **Olivia Breen** (Dublin), showcasing her work on polymorphs in her talk entitled “Diverse polymorphism in metal ammonia oxalate hydrate coordination polymers.” Using a range of transition metals (Mn, Fe, Co, Ni, Cu, Zn), 3 main types of compounds are distinguishable, based on the metal-ammonia-oxalate-hydrate (MXYZ) stoichiometry. Intriguingly, compounds with different composition may still crystallise in related crystal structures, such as Fe210 and Zn012, which both feature metal-oxalates connected via bridging ammonia or water bridges, for the iron and the zinc compound, respectively.

The final talk was given by **Calum Sangster** (Edinburgh), in which he demonstrated “3-Dimensional electron diffraction and in situ activation of metal organic frameworks.” He was able to utilise the often-detrimental high vacuum in TEMs / electron diffractometers to his advantage by in-situ dehydration of a copper-based MOF and determining its crystal structure before and after the treatment. Additionally, crystals from which data had been collected prior to the dehydration showed evidence of beam damage in the form of a disorder present in the crystal structure, in contrast to pristine crystals, which solved into an ordered structure.

[1] Cruz-Cabeza, A. J., Spackman, P. R. & Hall, A. V. (2024). The interplay between hydrogen bonds and stacking/T-type interactions in molecular cocrystals. *Nature Commun. Chem.* **7**, 284. https://doi.org/10.1038/s42004-024-01380-3

Chair and speakers in the CCG session on “Polymorphism, hydrates, and co-crystals” namely Iain Oswald (Strathclyde), Calum Sangster (Edinburgh), Amy Hall (Durham), Emma Hawking (CCDC) and Olivia Breen (Dublin).

Thomas Smith, Newcastle

The joint CCG/BSG session on “In-situ crystallography” opened with a keynote lecture from **Amy Thompson** (DLS) who gave a fantastic overview of the work being done to automate data collection and processing from multi-crystal experiments. The VXMi beamline is designed to handle crystals grown in multi-well crystallisation plates, with a Formulatrix Rock Imager storing plates at a controlled temperature and providing automated optical micrographs. Crystals grown in these plates are often both very difficult to remove, and grow in large, overlapping clumps. A small beam (down to 10 x 10um!) allows the beamline to only collect from the most ideal regions of such samples. Crystallisation plates are completely analogous to diamond anvil cells in the restrictions they place on access to reciprocal space, therefore in macromolecular crystallography it has been commonplace to collect many incomplete datasets and merge them together to form one final set. It was fantastic to see how well-integrated their data processing system is from the automatic detection and ranking of up to 100 objects from each droplet, through to the intensity-based clustering algorithm used to detect different samples and only merge datasets from the same sample together. Finally, Amy touched on validation experiments performed with human, pig and cow insulins, and how the system was able to accurately identify and cluster the structures together.

*Chair and speakers in the CCG/BSG session on "In-situ crystallography" namely **Phoebe Allan** (Birmingham), **Alexandra Longcake** (Newcastle), **Ross Angel** (Padova), **Manuel Fernandes** (Johannesburg) and **Amy Thompson** (DLS).*

Next was an interesting example of the use of in situ crystallography as an analytical technique. **Manuel Fernandes** (Witwatersrand) presented their work in which solid-state Diels-Alder reactions were monitored using single-crystal X-ray diffraction. This talk showed two example reactions, and in both the progress of the reaction was shown to change the symmetry of the system in such a way that it could be tracked using refinement statistics of solutions in different space groups. To me this was an incredible use of crystallography fundamentals to track the completion percentage of a reaction in real-time, akin to the relative heights of NMR peaks or HPLC traces.

Ross Angel (CNR) was next-up, talking about his newly released software package: CrystalPalace. As the author of the EosFit and a high-pressure crystallographer by trade, the speaker explained how CrystalPalace was born of a frustration with incompatibilities with different software packages used during the analysis of parametric extreme conditions experiments. It ingests a concatenated CIF containing all the experiments to analyse, and an algorithm finds all equivalent atoms across structures, regardless of the site naming scheme or occupancy. This represents a huge usability improvement when comparing data from different sources. Data are presented in formats suitable for direct inclusion in reports, minimising the chance of a "copy-paste" mistake sneaking in. Finally, each value is presented alongside an estimated standard uncertainty which, despite not having access to the entire variance-covariance matrix, agrees with those produced by Shelx.

The final talk of the session was given by **Alexandra Longcake** (Newcastle) who told us about her work producing an in situ diffraction workflow for the ENaCt technique. Central to this was the use of a Rigaku XtalCheck system alongside the XtaLAB Synergy-S diffractometer. This involved a drastic reduction in thickness of the glass usually used for ENaCt experiments to increase transmission of X-rays – from 1.0 mm all the way down to 100 µm! A series of different plate holders and adapters were prototyped using 3D printing to try and mitigate most of the difficulties in manually handling glass so thin. She demonstrated the process of selecting, centering and running a crystal, showing that merging a single-digit number of datasets was enough to obtain a structure solution for 2 out of her 3 trial samples.

Spring meeting prize winners

IUCr Prize

BSG02 **Lewis Williams** (Essex) “Damage before destruction? X-ray induced changes in single pulse serial femtosecond crystallography.”

CCG03 **Giovanna Martins** (Newcastle) “High-throughput nanoscale in situ derivatisation reactions for the crystallisation of “uncrystallisable” carbonyl-containing organic molecules.”

PCG06 **Farheen Sayed** (Cambridge) “Structural characterisation of new Li-rich d^0 metal containing phases via combined diffraction, EXAFS and NMR spectroscopy.”

AIPP/ACA Structural Dynamics Prize

CCG04 **Stephen Brown** (Warwick) “Radiation damage in molecular crystals a comparison of X-ray sources and electron diffraction.”

ESCG Prize

Best Poster CCG05 **Catherine Dunsford** (Kent) “Synthesis and characterisation of room temperature Fe (II) spin-crossover materials with N_4O_2 Coordination Spheres.”

Best Oral GI02 **Celine Beck** (Glasgow / DLS) “Novel hydrostatic medium-pressure cell on the I11 high resolution powder diffraction beamline at Diamond Light Source.”

Cruickshank IG01 **Emma Hawking** (CCDC) “Informatics meets energetics: combining crystal structure prediction and knowledge of the crystal landscape.”

Group poster prizes

GI03 **Owen Hewitt** (NCS) “Apprenticeships: how to produce a new generation of scientists.”

ESCG – PCG05, **Evie Ladbrook** (Warwick) “Enhancing polar distortions by pressure in a metal.”

BSG02 **Lewis Williams** (Essex) “Damage before destruction? X-ray induced changes in single pulse serial femtosecond crystallography.”

PCG04 **Banaz Fetah** (Strathclyde) “Discovery of a new high-pressure phase of Posaconazole.”

CCG07 **Lewis Jackson** (Kent) “Novel series of lutidine-based spin-crossover co-crystals.”

A collage of Spring Meeting prize winners in Leeds 2025. Photos: Chloe Naylor (HG3).

CCDC

A new series of free virtual workshops scheduled for October and November

Join us for a series of interactive virtual workshops to explore how to visualize, analyse and simulate the behaviour of porous materials and crystal structures. Learn how structural features relate to particle properties and how to apply virtual screening techniques using powerful CCDC tools.

Each session includes live demonstrations using the CCDC software such as Hermes, GOLD, the CSD-Particle suite, Mercury and the CSD Python API. You will also have plenty of time for hands-on practice, with our tutors available to guide you and answer your questions.

Save your place:

7th October, 13:30 (BST)

Advanced Structural Visualization and Analysis of Porous Materials Using Mercury

21st October, 9:30 (BST)

How to Use Particle Informatics Tools to Connect Crystal Structure to Particle Behaviour

4th November, 15:30 (GMT)

How to Use the Docking Software GOLD to Perform Virtual Screening Simulations

If you have any questions, get in touch at hello@ccdc.cam.ac.uk!

CCDC Engagement Grants 2025/2026

We are excited to announce that applications for the CCDC Engagement Grants are now open! Are you passionate about structural science? Do you have an idea for a video, social media series, poster or activity to get others excited about the topic? Whether you are planning a workshop, school visit or creative science communication project, you can apply for funding to make it happen.

This is a great opportunity to share your enthusiasm for chemistry and crystallography with a wider community. Applications must be received by 12th October 2025. To learn more and apply, visit the CCDC website.

Research Highlights from Our PhD Students

The latest PhD Students Science Day meeting on the 27th of June brought together a dynamic group of early-career researchers, each tackling fascinating challenges in the world of crystallography, nucleation, molecular modelling and drug design.

Nathan Hennessy, a PhD student from the University of Leeds, has researched how thermodynamic factors shape nucleation and crystallisation – critical processes in pharmaceutical manufacturing. Using histidine as a model compound, Nathan has investigated whether activation barriers during nucleation correlate with key product properties like polymorphism and particle size. By measuring nucleation rates and applying a reversible aggregation model, he has calculated thermodynamic parameters such as entropy and enthalpy of crystallisation. Nathan has also examined how different co-solvents, including alcohols and glycols, affect solubility and crystallisation. His results show that solvent structure plays an important role – glycerol, for example, promotes higher solubility due to stronger hydrogen bonding. Interestingly, the crystallisation behaviour did not directly follow these solubility trends, and the Gibbs free energy remained consistent across solvents. Nathan's research could open new pathways for fine-tuning crystallisation processes in drug development.

Emilia Prandini, a PhD student from Politecnico di Torino collaborating with the CCDC and Imperial College London, combines Crystal Structure Prediction (CSP) with particle informatics to forecast polymorphism and morphology – two critical aspects of crystal behaviour. Her focus is xanthone, a natural antioxidant with promising medicinal potential. Emilia used CSP to generate a crystal structure landscape and identified the global minima, which match closely with experimental data. Applying particle informatics, she predicted the likely morphologies of these structures, finding strong alignment between CSP lattice energies and morphological predictions. Her research lays the groundwork for better control of crystalline properties in pharmaceutical and materials science. Next, Emilia aims to extend this approach to explore surface properties and packing.

Harry Nash, who recently completed his PhD at the University of Sheffield, collaborated with Lee Brammer and Grant Hill to predict σ-hole interaction energies. His work focuses on halogen bonding and other σ-hole interactions – a growing area in crystal engineering. Using a large dataset from the Cambridge Structural Database (CSD) and machine learning models, Harry built a predictive tool for interaction energies validated against high-level DFT calculations. By investigating geometric factors like contact distances and angles, Harry uncovered key trends in σ-hole interactions between different donors and acceptors. His consistent, large-scale dataset now serves as a valuable resource for computational chemists and experimentalists

aiming to understand non-covalent interactions in crystals. Harry has been honoured as a co-recipient of the Turner Prize, recognizing the best PhD thesis in Chemistry at the University of Sheffield.

Aaron Horner tackled a tricky challenge in structural chemistry: assessing the quality of molecular models, particularly crystal sponges. He highlighted the pitfalls of relying solely on traditional descriptors like the *R*-factor, which can be misleading due to disorder, overlap or solvent ambiguities. To address this, Aaron introduced a distortion score that quantifies geometric distortions by measuring changes in bond lengths and angles as restraints are adjusted. He also presented a bond likelihood score tool, which assesses the plausibility of bonds based on probability density functions from crystallographic data. These tools give structural chemists practical, real-time feedback to refine complex models – especially valuable for early-career researchers.

William Midgley focuses on PROTACs (proteolysis-targeting chimeras) – innovative molecules that harness the body's natural degradation machinery to eliminate disease-causing proteins. Unlike traditional drugs, PROTACs can target "undruggable" proteins without clear active sites, but they come with challenges like large size and limited bioavailability. William's research uses computational pipelines and molecular dynamics to design and rank PROTACs for challenging targets, including the Epstein-Barr virus protein EBNA. His next steps aim to enhance computational models, optimize PROTAC linkers and apply advanced techniques like cryo-EM to understand protein structures better.

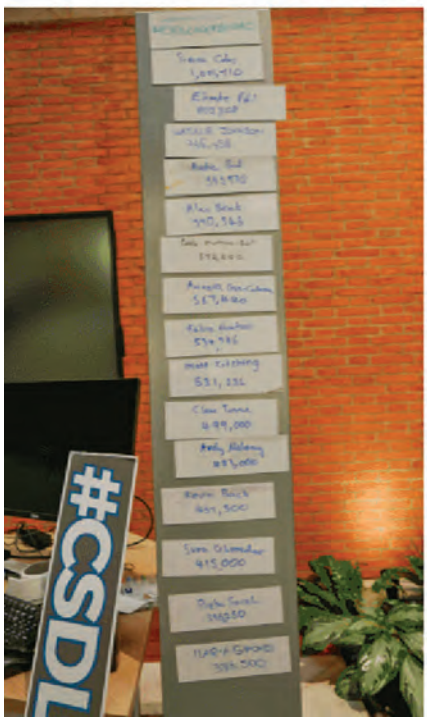
Our lightning talk session spotlighted the impressive progress of the 1st and 2nd year PhD students – Alex D. Lee, Henry James Broster, Omar El-Habbak, and Henry Holleb – who shared snapshots of their developing research. We also gave a warm welcome to Paulo Nunes de Souza, who joined us from the University of São Paulo, Brazil, this March to start his PhD journey.

We wrapped up the day with a lively panel discussion featuring former CCDC-sponsored students who shared invaluable advice on navigating career paths, followed by a well-earned CSD60 celebration – complete with cake and good company.

Thank you to everyone who shared their work and joined us for a day of inspiring science and community. We look forward to seeing where your research takes you next!

Find out more about our sponsored PhD programme at the CCDC website.

Ana Machado, CCDC




Outline


Can Machine Learning Models
Ligand Docking Learn Physics?

Transitioning to PDBx/mmCIF and extended PDB IDs

wwPDB strongly encourages all users to adopt the extended PDB ID format and transition to PDBx/mmCIF file format as soon as possible. This includes making changes to software; referring to structures by the full 12-character ID in all communications; and encouraging your communities to do the same.

Transitioning to extended PDB IDs

As the PDB archive continues to expand, the four-character PDB accession codes (PDB IDs) are expected to be fully assigned before 2028. To support the growth of the archive, the wwPDB has extended the length of PDB IDs to 12 alphanumeric characters including "pdb_" prefix (e.g., "1abc" will become "pdb_00001abc", case insensitive) to improve text mining capabilities in the published literature. Users or journals will be able to parse/recognize PDB IDs using the prefix "pdb_". The prefix and zeros must be included in the extended PDB ID.

Once four-character PDB IDs are fully assigned, new entries will only receive extended PDB IDs; data will not be provided in the legacy PDB file format files.

Access further details, including a transition plan, example files, and supporting FAQs at wwPDB: Extended PDB ID With 12 Characters.

Users can adopt usage of extended PDB IDs for all PDB entries immediately using the _database_2.pdbx_database_accession data item in the PDBx/mmCIF formatted structure files.

For example:

```
loop_
_database_2.database_id
_database_2.database_code
_database_2.pdbx_database_accession
_database_2.pdbx_DOI
PDB 2HYV pdb_00002hyv 10.2210/pdb2hyv/pdb
WWPDB D_1000038924 ? ?
```

New PDB DOI Format

All existing PDB entries with four-character PDB IDs issued have DOI formatted as 10.2210/pdb[4-character_PDB_ID]/pdb that resolve to the corresponding wwPDB DOI landing page. For example, PDB entry 8y9m (pdb_00008y9m) has the DOI https://doi.org/10.2210/pdb8y9m/pdb. Importantly, this DOI will remain unchanged in the future.

When all 4-character PDB IDs have been exhausted, all new PDB entries will be issued extended PDB IDs issued and a NEW DOI formatted as 10.2210/[Extended_PDB_ID]/pdb that will resolve to the corresponding wwPDB DOI landing page. For example, PDB entry "pdb_10001xyz" will have the DOI https://doi.org/10.2210/pdb_10001xyz/pdb.

Transitioning to PDBx/mmCIF Format

To help users adopt extended PDB ID and PDBx/mmCIF file format, wwPDB offers an mmCIF User Guide and software resources such as mmCIF parsers and CIF Editor.

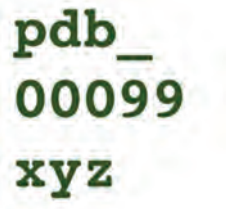
In addition, wwPDB will provide a Beta PDB Archive organized by extended PDB ID (including file naming, directories, and datablock naming) in early 2026. The current PDB archive organizes data files grouped by data type, e.g., coordinates, experimental data, assemblies, validation reports, etc.

A major change in the Beta PDB archive will be the re-organization of file directory at entry level, following the same file organization as the PDB Versioned Archive. In other words, all the data files associated with an entry will be grouped together under its PDB ID (extended PDB ID) with two letter hash. Please watch wwPDB.org and community bulletin boards for announcements on the file organization for the Beta PDB archive later this year.

We recommend users fully adopt all of these these changes before the end of 2026. Early adoption will contribute to the long-term sustainability and interoperability of 3D biostructure data across the scientific community.

In particular, journals should begin adopting the Extended PDB ID format (in Text, Tables, and Data Availability Statements), updating links included in journal articles for PDB IDs to the wwPDB DOI landing page via CrossRef, and verifying software tools linked from a journal article (e.g., FirstGlance or Jsmol for 3D visualization) support extended PDB IDs and PDBx/mmCIF.

Should you have any questions or require further assistance, please do not hesitate to contact us at info@wwpdb.org. We greatly appreciate your support and cooperation as we work together to enhance the future of structural data accessibility.



Extension to EMDB Accession Codes

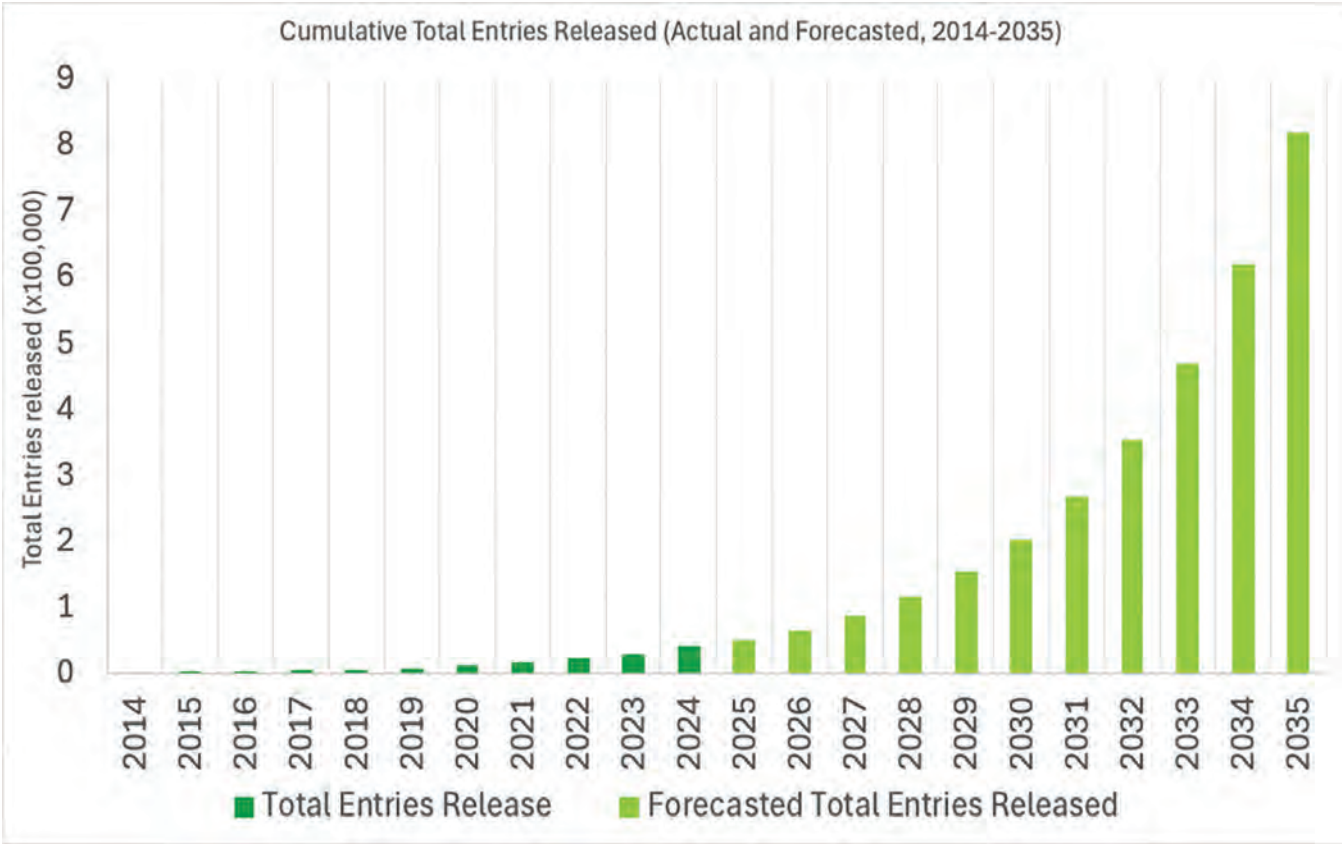
The EMDB archive is experiencing near-exponential growth. To support this rapid expansion, the wwPDB has been working to prepare our systems for the future and ensure seamless deposition, validation, and dissemination of data in the years ahead.

As part of this effort, we are announcing an important change:

EMDB IDs will be extended to support up to six digits, allowing for identifiers such as EMD-123456. Currently, the archive uses four and five-digit IDs (e.g., EMD-0123, EMD-45678), with support for identifiers up to the EMDB ID: EMD-99999. The change to six-digits will increase our capacity ten-fold and ensure ID availability into the next decade, up to EMD-999999.

We do not anticipate surpassing 99,999 released entries until around 2028, however, we expect to begin assigning six-digit EMDB IDs sometime in 2026. As such, as early as 2026, depositors should anticipate being assigned six-digit IDs within the wwPDB OneDep deposition system, and the user and developer community can expect six-digit EMDB IDs in the EMDB archive.

We appreciate your support as the archive grows and thank you for your contribution to the worldwide effort to archive structural biology data. We remain committed to ensuring a stable, sustainable and scalable infrastructure that supports the continued successes and productivity of the scientific community using structural biology and cryoEM in their research. For questions or feedback, contact the EMDB team at emdbhelp@ebi.ac.uk.



Paper Published: 3DEM Structure-Map Validation Recommendations

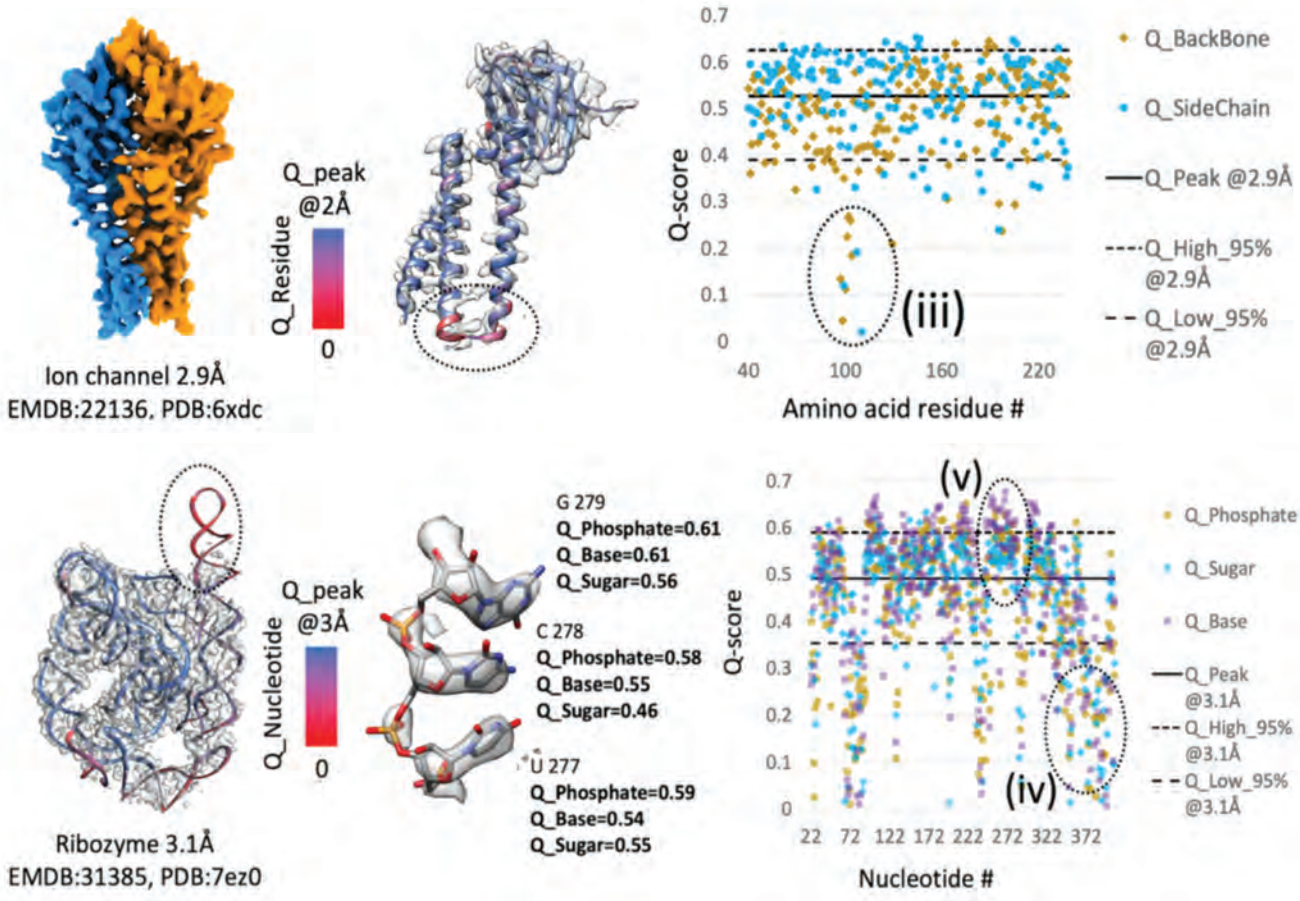
A new publication describes two percentile-based metrics: Q_relative_all and Q_relative_resolution. The publication presents a statistical analysis of Q-score and these new percentile based validation metrics.

Q_relative_all is a single value percentile, representing the overall quality of the model-map fitness. It is derived by comparing a model-map average Q-score to all model-map average Q-scores calculated for 3DEM structures in the PDB/EMDB. Higher Q_relative_all percentile values, infer higher quality in the model-map fitness.

Q_relative_resolution is a single value percentile, derived by comparing the average Q-score of a model-map with the Q-scores of other model-map entries of similar resolution. This metric was developed from the principle that average Q-score is correlated with map resolution. Q_relative_resolution percentile values close to 50% therefore represent a score that is commonly observed for entries in the PDB/EMDB of similar resolution, inferring model-map fitness is typical for an entry of a particular resolution. Notably low or high Q_relative_resolution percentiles may be helpful to guide further review of model-maps.

The EMDB has made these metrics available since Spring 2024 via emdatabank.org and since the publication of the paper, the wwPDB is in the process of incorporating these metrics into wwPDB validation reports by providing the

Q-score percentile slider for the assessment of model-map fitness of 3DEM entries. This validation enhancement will help depositors, reviewers and the community to improve the quality of data submissions and assist users to assess 3DEM data quality in the PDB and EMDB, wwPDB core archives.



EMDB ID	Resolution (A)	Q-score	Q-relative-all	Q-relative-resolution
EMD-22136	2.9	0.51	71%	51%
EMD-31385	3.1	0.43	47%	26%

Examples of Q-score application in proteins and in nucleic acids adapted from: doi: 10.1107/S2059798325005923

Q-score as a reliability measure for protein, nucleic acid and small-molecule atomic coordinate models derived from 3DEM maps

Grigore Pintilie, Chenghua Shao, Zhe Wang, Brian P Hudson, Justin W Flatt, Michael F Schmid, Kyle L Morris, Stephen K Burley, Wah Chiu (2025) Acta Cryst D81: 410-422 doi: 10.1107/S2059798325005923

The above three articles are reproduced from the News and Announcements section of the World Wide Protein Data Bank website (wwpdb.org) with their permission.

OBITUARY
Patrick W. Doheny 1993-2025

IT is with great sadness that I write that Dr Patrick Doheny, commonly known as Pat amongst friends and colleagues, has passed away. The materials chemistry and crystallography communities, along with friends, colleagues and collaborators, mourn the untimely loss of an excellent, kind and generous scientist and teacher. Our deepest sympathies lie with his parents, Peter and Jo, and his brother, Brendan.

Patrick was born and grew up on the Central Coast of New South Wales and lived in the suburb of Berkeley Vale, approximately one hour north of Sydney. He commenced primary school in February 1999 and completed his primary education in 2005 at St John Fisher Catholic School at Tumbi Umbi. During his time at primary school Patrick was awarded numerous Certificates of Achievement and Certificates of Merit. He attended St Peter's Catholic College Tuggerah Lakes at Tuggerah between 2006 and 2011. There, he received numerous Certificates of Achievement, Merit awards and Commendations for his academic performance and extra-curricular activities, which included fundraising for charity, the Duke of Edinburgh's Award, Karate, and participating as an Honorary Junior Director for Wyong Town Financial Services Limited. In his final year he received the Principal's Award for Academic Achievement for notable performance in Physics, Economics, Studies of Religion, English and Chemistry.

Patrick completed a Bachelor of Science degree with majors in Physics and Chemistry at the University of Sydney, Australia, between 2012-2014, followed by attaining Honours Class I in 2015. His Honours thesis, "Computational Techniques as a Means of Elucidating the Electronic and Magnetic Properties of Metal-Organic Framework Materials" was supervised by Prof. Deanna D'Alessandro and Prof. Cameron Kepert. He stayed with the same supervisors at Sydney to carry out doctoral research, completing his PhD in 2019 with a thesis entitled, "Elucidation of the Properties of Electroactive Metal-Organic Framework Materials via a Combined Experimental and Computational Approach". During his PhD, in 2018 he was awarded a Dr Joan R Clark research scholarship, through which he travelled to the UK to perform experiments at the EPSRC National Research Facility for EPR Spectroscopy at the University of Manchester. This was a formative time for Patrick, and his work there with Floriana Tuna and David Collinson led to papers in *Chemical Science and Faraday Discussions*, adding to others in *JACS* and *Materials Advances* resulting from his PhD research.

Patrick (second from right) at the Yeung group 2023 Christmas dinner in Birmingham.

Patrick (third from right) with members of the d'Alessandro group during a visit to Sydney in 2024.

Towards the end of his PhD, he was selected as a finalist for the Don Stranks Award at the 19th Royal Australian Chemical Institute Inorganic Chemistry Conference (IC19) in Wollongong, 2019.

In 2020 Patrick moved to the UK to undertake postdoctoral research with Dr Paul Saines at the University of Kent, investigating magnetically frustrated frameworks for magnetocaloric applications and extending his experience into the realms of thermal expansion and neutron scattering. He also collaborated with several other academics, including Helena Shepherd and Maria Alfredsson, and participated in several experiments with Maria at the XMaS beamline at the ESRF. His work while in Kent was published in *Inorganic Chemistry, Chemistry a European Journal, APL Materials, Journal of Materials Chemistry A, Chemistry of Materials* and *Journal of Magnetism and Magnetic Materials*. Patrick then moved to the University of Birmingham in 2023 to work with Dr Hamish Yeung on the elucidation and role of intermediates in the formation of metal-organic frameworks, developing his experience of in-situ diffraction and total scattering through several experiments at Diamond Light Source. While in the UK, he was a regular contributor to conferences of the British Crystallographic Association (Spring and Winter meetings) and the Royal Society of Chemistry (Porous Materials and Solid-State Chemistry interest groups) amongst others. The award of the CCDC Chemical Crystallography Prize for Younger Scientists in 2024, and the award of an ARC DECRA Fellowship, which Patrick was due to begin back at the University of Sydney in Autumn 2025, were due recognition of his excellent scientific contributions and a highly promising career.

Throughout his career, Patrick took on several roles that helped, trained and educated other students and researchers. At various times, he was officer for single crystal X-ray diffraction, officer for electron paramagnetic resonance, laboratory demonstrator and lecturer on molecular symmetry and group theory. He helped many PhD students and researchers and made highly valued contributions to lots of different projects within his group and beyond. His wide scientific interests and his willingness to help others – be it in the office, in the lab or during an experiment at a central facility – were hallmarks of his character. Patrick was a highly valued member of the materials chemistry and crystallography communities, and he was a valued friend to many. His untimely passing has affected all those he worked with, and his chats and contributions will be sorely missed.

Hamish Yeung,
Birmingham

Going back to our roots

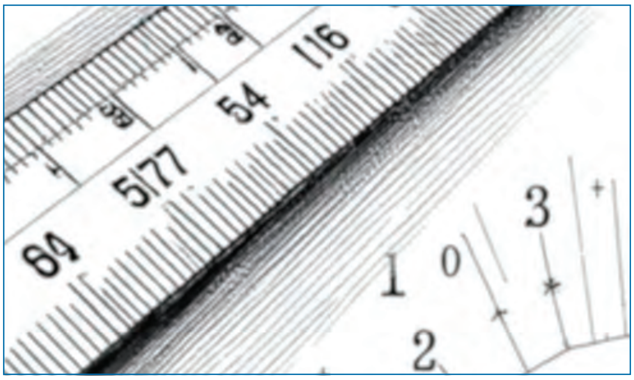


Image from the Surreal Graphics Generator at deepai.org.

AT the end of May, it was a pleasure to attend the launch of the book "Mathematics for Biosciences" by Elspeth Garman (Oxford) and Nicola Laurieri (Oxford) (World Scientific, DOI: https://doi.org/10.1142/q0473). Attendees received a welcome from Francis Bar (Oxford) the head of the Biochemistry Department which was followed by a presentation from Alison Woollard (Head of Teaching) who emphasised the role of integral complex biological systems and the foundations of computational biology. Elspeth then presented a mini-autobiography starting with teaching work in Africa followed by undergraduate studies in physics at Durham and postgraduate research in Oxford. Elspeth remained in nuclear physics until a career change in 1987 saw her become the X-ray facilities manager in Biochemistry and in 1995 she instigated a maths course for 1st year students in the department. Nicola then described his career path from undergraduate studies in Lyon to postgraduate research in Oxford followed by postdoctoral work in Bari and then on to higher education research and teaching in Italy.

Elspeth then introduced two of her former students and tutors on the course who have progressed to very great things. We also heard from project collaborator **John Fink** (Kalamazoo) who described the formulation and understanding that goes into mathematics as giving us a world of ideas, in contrast to our world of humble ordinary experience. On more practical issues, John emphasised the manifold benefits of learning to use a graphing calculator or software package to bridge the gaps between symbolic expressions, actual numbers and the visual display of results. We hope to bring you a review of the book in a future issue.

The introductory chapter of Elspeth's book reminded me of a number of quandaries I had encountered not so long ago when trying (very hard) to read the book "Understanding Analysis" by Stephen Abbott (Springer, DOI: https://doi.org/10.1007/978-1-4939-2712-8). The preface of Abbott's book very rightly states "This lively introductory text exposes the student to the rewards of a rigorous study of functions of a real variable." However, at this point, members should be made aware that, sadly, the editor did not manage to get very far with Abbott. This was mainly because I stumbled while trying to understand rational and irrational numbers, which is very fundamental stuff for mathematicians who would probably say something like "Well, if you don't get that, just go and do some biology instead."

Thus, I thought it might be useful, if only for myself, to summarise what I understand about the subject I got so stuck on, only a few years ago. The idea is that mathematicians put numbers into different categories, the most humanly understandable ones being the *natural numbers* which are positive *integers*. These are the whole round numbers one gets from counting on your fingers and toes, etc, and are easy to understand. Of course, we know that integers can also be negative; so we say that the natural numbers are a subset of all integers.

Mathematicians also have a class of numbers which they call *rational numbers* and these consist of two integers in the form of a fraction. A general rational number might be:

$$\frac{a}{b}$$

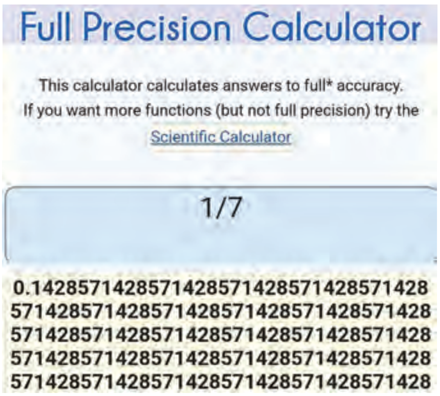
where *a* and *b* are integers. One of the things about rational numbers which I had forgotten or did not know is that when you express a rational number as a decimal, the result either terminates fairly quickly (e.g. ½ = 0.5 and ¾ = 0.75) or becomes highly repetitive; you could even say symmetric. Of course, I knew that the fractions:

$$\frac{1}{3} \text{ and } \frac{1}{6}$$

are equal to 0.33333... and 0.16666… respectively, with the last digit repeated *ad infinitum*. With the one sixth fraction, the first digit after the decimal place (1) does not repeat, but the subsequent digit (6) clearly does. However, I regret I did not realise that this repetition of a pattern is a general feature of *all* rational numbers. At this point I recommend readers to find the Full Precision Calculator (https://www.mathsisfun.com/calculator-precision.html) on the internet and enter the fraction:

$$\frac{1}{7}$$

This gives us the following:



where we can see from the columns of numbers that the sequence of six digits after the decimal place (142857) is repeated indefinitely. Using a handheld pocket calculator with limited screen-size, one probably would not notice the repetition with most fractions, but I gather it is always there! So let us try some more adventurous fractions like this:

37÷57

0.649122807017543859649122807017543859
649122807017543859649122807017543859
649122807017543859649122807017543859
649122807017543859649122807017543859
649122807017543859649122807017543859

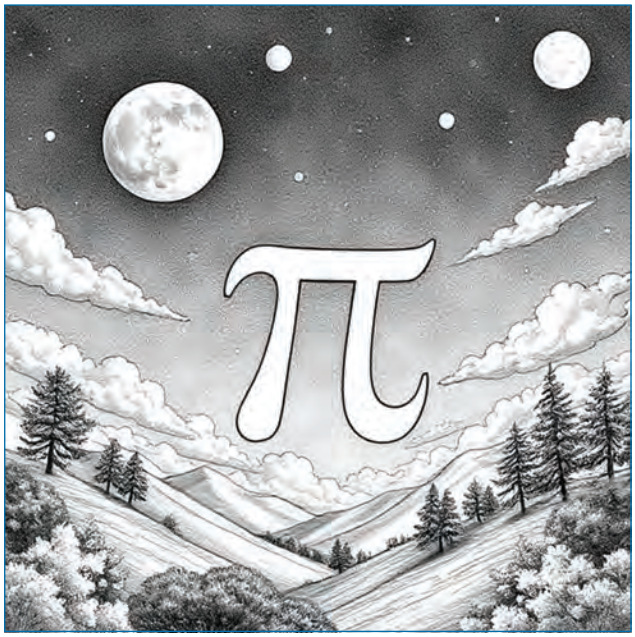
and again from the columns of numbers we see a sequence of 18 digits (649122807017543859) repeated infinitely after the decimal place. In defence of my failing to understand Abbott at the first read, I will say that having done most of my calculations to considerably fewer decimal places than that, perhaps one could be forgiven for not noticing it?

We have all heard of the fraction $^{22}/_{7}$ as a common approximation to π, so let us see what it works out as:

22/7

3.142857142857142857142857142857142857
142857142857142857142857142857142857
142857142857142857142857142857142857
142857142857142857142857142857142857
142857142857142857142857142857142857

So the 3.142 is about right but the huge amount of repetition after the decimal place seems a bit odd for π. Indeed it is, of course, the same repeat sequence that one gets with $^{1}/_{7}$. However, I always thought that π was a transcendental sort of number that was not constrained by the sort of symmetry that we see in molecular crystals! Still $^{22}/_{7}$ is a good approximation for π as long as you do not go more than about 3 places beyond the decimal point.

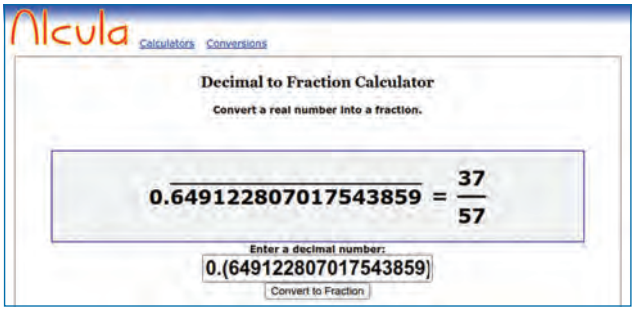


Pi is a transcendental sort of number! Image: deepai.org

It is interesting that with a bit more dabbling you can find relatively simple fractions of integers which have insanely long repeat sequences e.g. $(11/17)^2$ repeats every 273 digits!

It is worth trying that out. However, the mathematicians know best so let us accept the general rule that the rational numbers either terminate or become repetitive, which is basically saying the same thing (e.g. 0.5 is the same as 0.50000...).

Truly, there are calculator web sites (such as Alcula) where you can enter any repeated sequence of digits and they will generate the corresponding fraction for you (see figure below for the 18 digit example above). Note that a repeating sequence of digits is commonly indicated using an overline or bar, much like crystallographers use for the rotoinversion symbol in point groups and space groups.



The repeating nature of rational numbers means that they therefore represent only a tiny subset of all possible numbers. The remaining numbers, which are not repetitive and therefore cannot be represented by rational numbers, are called *irrational*. I have to be careful here because irrational numbers can still have repetition within them but the repetitive regions are likely to be short compared to the length of the whole number.

The reason I found Abbott very difficult is because he starts on the question of whether numbers like $\sqrt{2}$ can be represented by rational numbers. I have to confess that I didn't know that they couldn't. The idea is to prove that $\frac{a}{b} = \sqrt{2}$ where a and b are integers can never be a correct expression. Since we can square both sides, the problem is tantamount to saying that the ratio of two squared integers can never equal 2. Surely we can find two integers which when squared will be in a 2:1 ratio!? To me that seems reasonable so let's try it with a script which generates a lot of integers, square them, get their ratios and see what sort of numbers we get.

```
ratios={}  -- Our list of (a/b)^2 ratios
for a=1,1000 do
    for b=1,a do
        found=false
        if a^2%b^2==0 then  -- Check if the ratio is an integer
            ratio=a^2/b^2    -- If so, get the value of the ratio
            for i,j in ipairs(ratios) do
                if j==ratio then found=true break end
            end  -- Add any new ratios to the list
            if not found then table.insert(ratios,ratio) end
        end
    end
end
table.sort(ratios)  -- Sort the ratios and print first 20
for i=1,20 do print(math.tointeger(ratios[i])) end
```

The above lua script, which can be found here: https://pastecode.io/s/52omdaih generates about half a million different fractions (a/b) and prints out the lowest integral ratios of a^2/b^2 that one gets with $a \geq b$. This gives us a series of numbers, the first 10 of which are 1, 4, 9, 16, 25, 36, 49, 64, 81, 100. Indeed it does seem that 2, 3, 5, 6 and thus any natural number which is not a perfect square seems not

to be here. This suggests that the ratio of two squares can never be one of these missing numbers (2, 3, 5, 6, 7, 8, 10, 11, 12, etc) and that the square roots of any of these missing numbers (not just 2) can never be rational. It looks like I have missed something pretty fundamental for a long period of time! I am hoping it was drummed into my head a long time ago and that I simply managed to forgot it. On reflection, it does fit with the observation that rational numbers have the weird repeating effect which does not occur with square roots and other constants such as π, *e*, etc.

The hard bit is where Abbott tries to prove that the ratio of two squared integers cannot be 2 by contradiction! The proof starts with the equation $\frac{a^2}{b^2}=2$ in which it is assumed that all common factors in *a* and *b* have been divided out. This equation can be rearranged to give $a^2=2b^2$ and this implies that a^2 is divisible by two and must therefore be even. Since a^2 is even, *a* must be even, too. Hence we can write $a=2n$ where *n* is an integer. Substituting this into the rearranged equation gives us $(2n)^2=2b^2$ or $2n^2=b^2$ and this implies that b^2 is even and therefore *b* must be even as well. Herein lies a logical impasse because we said that we had factored out all of the common terms in *a* and *b* which means that both of them simply cannot be even and the equation is disproved. That is not too bad – in fact, I get that.

The problem is with the first exercise in Abbott, which is as follows: "Prove that √3 is irrational. Does a similar argument work to show that √6 is irrational?" The equation that is relevant to the first question is $a^2=3\,b^2$ and I gather that 3 times an even number gives another even number and 3 times an odd number gives another odd number, so a^2 could be odd or even, right? I then drove myself batty trying to answer the question by using the odd or even argument which had worked so well for √2 and I did not manage to sort it out, let alone answer the question on √6.

A much clearer way to solve the problem is provided by the book: "The Mathematics Lover's Companion – Masterpieces for Everyone" by Edward R. Scheinerman (Yale University Press, 2017) which I chanced upon in a local charity shop! This approach relies on what is called (somewhat embarrassingly) the Fundamental Theorem of Arithmetic. Wikipedia (the free encyclopedia) states that this is also called The Unique Factorization Theorem or The Prime Factorization Theorem, both of which sound better! This theorem states that every positive integer can be factored into prime numbers and that its factorisation is unique, *up to* the order of the factors. I assume the last bit means that the factorisation is unique *ignoring* the order of the factors since what matters is how many prime factors of 2, 3, 5, etc, are required to generate the number of interest, rather than the order that we multiply them in. Any integer that is not a prime number can be expressed as multiples of prime numbers e.g. 12 = 2 x 2 x 3. The key thing is that the composition of the number in terms of how many times we use each prime number is unique e.g. 12 is made from two 2's and one 3, 24 is made from three 2's and one 3 much like a chemical formula, although we are using numbers instead of atoms.

Scheinerman's book gives a nice explanation although I have adapted it a lot in my own (simpler) terms. Consider the fraction $^{99}/_{70}$ which has a value of 1.4142857142857 (note the repetition) and is therefore a good approximation for √2 or 1.4142135623731. Hence we can state the approximation:

$$\frac{99}{70} \approx \sqrt{2}$$

Breaking the numerator and denominator down into prime numbers gives:

$$\frac{3x3x11}{2x5x7} \approx \sqrt{2}$$

Squaring both sides gives:

$$\frac{3x3x3x3x11x11}{2x2x5x5x7x7} \approx 2$$

In this case there are no common factors in the numerator and denominator, but if there were, we could cancel them out at this stage. Note that all the prime numbers are now in pairs, so they would cancel in pairs and we would be left with only pairs of primes in the result. The smallest integral values the overall result could have would be 1 x 1, 2 x 2, 3 x 3, ... (or 1, 4, 9, …). Hence values of exactly 2, 3, 5, 6, 7, 8, 10, 11, etc, could not arise. I think I get that now.

With our final expression for the square of $(^{99}/_{70})$, because the numerator and denominator now consist only of prime numbers which refuse to divide roundly into each other, however many primes we have and however big or small they are, there is no way that the numerator can be divided by the denominator to give a factor of exactly 2. After any factorisation that is needed, the remaining prime numbers in our fraction can never be multiplied and divided to give a single prime number like 2 or 3. This follows from the fact that prime numbers are just that – prime numbers. Since the prime numbers in a squared fraction (like this one) are all present in exact pairs, neither could we get a number like 6 which is a product of two different prime numbers (2 and 3). Thus √2 can never be represented by a rational number and neither can √3 or √6 or indeed any number that isn't already a perfect square! I get the hint of a cyclic argument somewhere in all of this, but I think it makes sense. Just let me know!

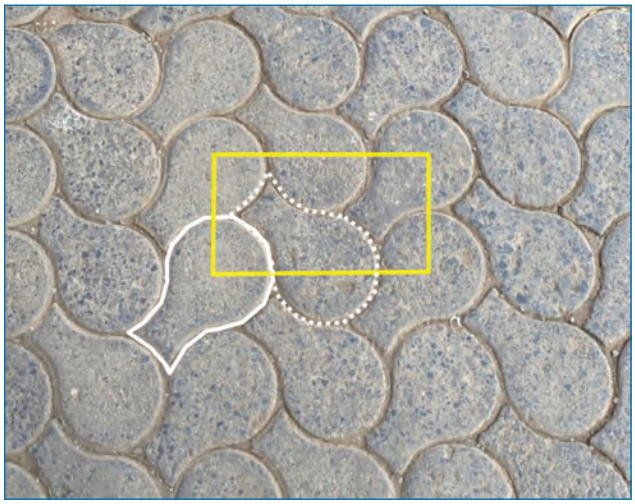
Jon Cooper,
UCL

Puzzle Corner

HERE are my best efforts at a set of answers for last month's quiz. Please let the editor know if you spot any errors.

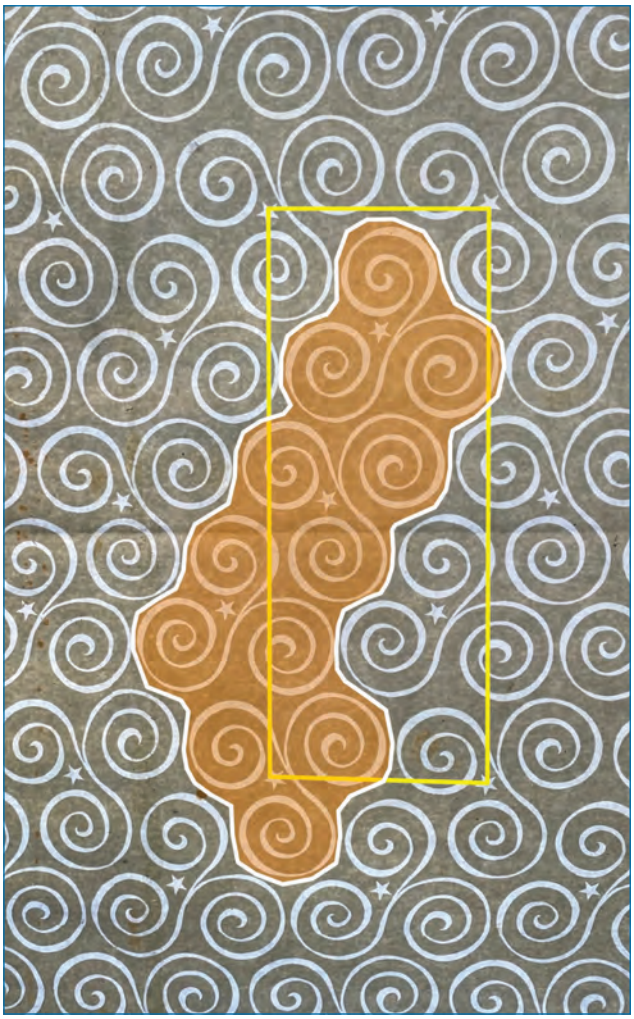
(a) Removing a bit of perspective from this striking pattern with the website lunapic.com has allowed the motif (my arbitrary choice of which is shown with a white boundary) and a unit cell (yellow) to be identified. I think the plane group is *p*1, which the International Tables for Crystallography Vol. 1 (1969) identifies as oblique. It generates a centred rectangular pattern (not shown).

(b) Again, using lunapic.com to remove some of the distortion due to perspective from this interesting cobblestone pattern made with flask-shaped motifs, I arrived at the following.

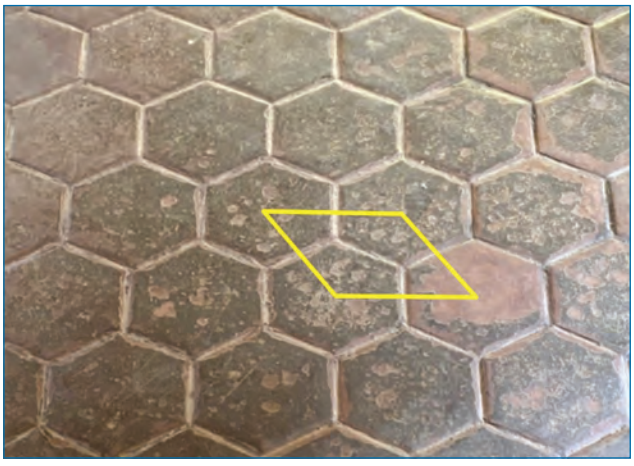


For this one I can see a rectangular cell with a horizontal glide plane which makes it *pg*. If we take the flask motif on the lower left hand origin of the cell, reflect it through a horizontal mirror line and translate it half a unit cell to the right, we get the motif shown with a dashed outline.

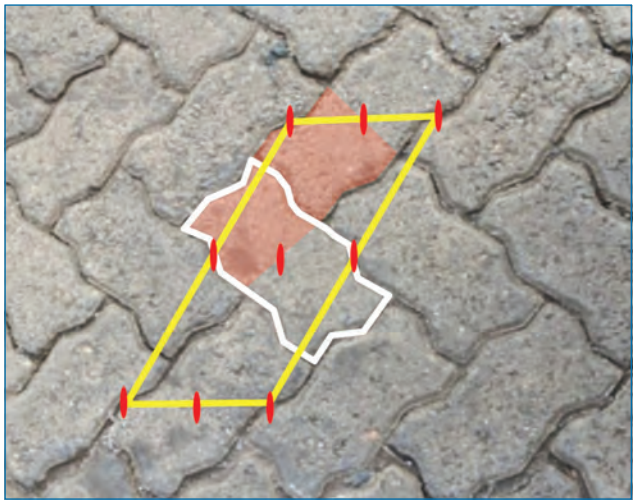
(c) This is quite a hard one with all of the face-like swirls and pseudo reflection and three-fold symmetry. I think it is rectangular p1 with 4 of the trefoil motifs per asymmetric unit. I cannot see how to generate the exact pattern with fewer motifs in the asymmetric unit and alternative cells, etc, but I am open to all suggestions.



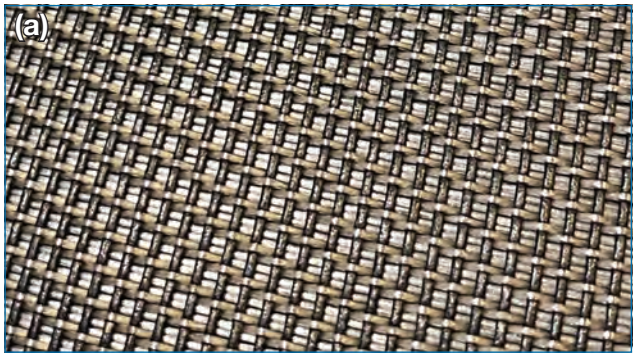
(d) This one needs very little explanation as it is a great example of *p6m*. *i.e.* hexagonal with mirror lines or planes at 30° to one another.

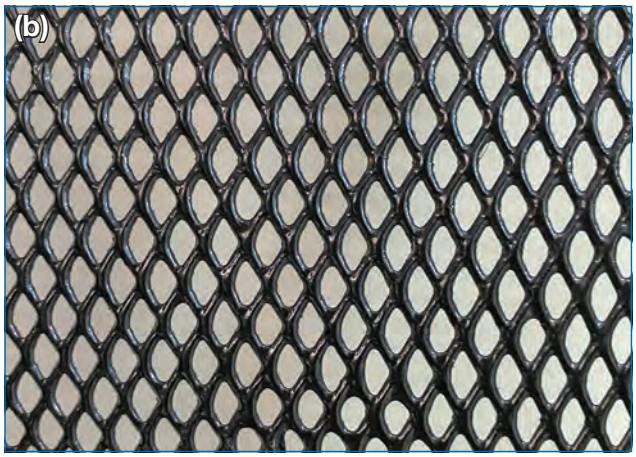


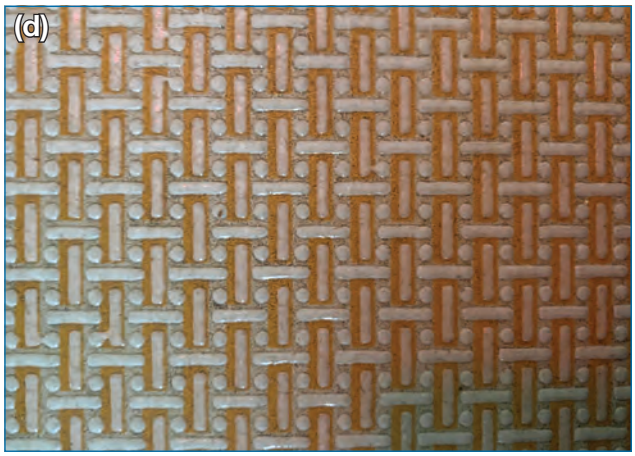
(e) For this one, I think the plane group is *p*2. The motif (a brick) is shown with a white outline and has a two-fold within it. So I think the asymmetric unit (shown with a brick-like hue) is two half-bricks placed at about 90° to each other. The two-folds are shown as red diad symbols and are in exactly the right place according to the International Tables.



For this issue we have five new patterns from **John Lisgarten** (London) which members are invited to comment on, ideally in terms of their symmetry, up to the point of identifying a plane group, if possible. One of them might even involve layer groups, which is an unfamiliar subject for the editor, but one which sounds very interesting! Answers on a postcard to jon.cooper@ucl.ac.uk.







Jon Cooper,
UCL

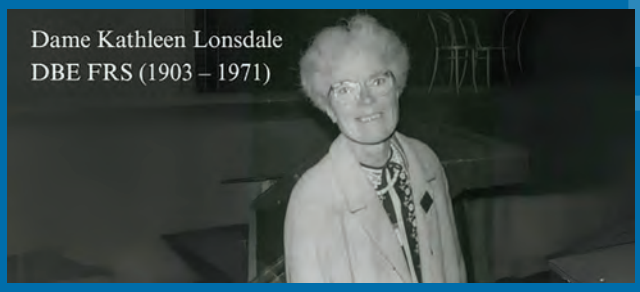
Meetings of Interest

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**.

Kathleen Lonsdale Public Lecture



You are warmly invited to attend the Kathleen Lonsdale Public Lecture, to be held on Wednesday 10th September 2025 at the University of Leeds (School of Chemistry and Sir William Henry Bragg Building), as part of a national programme of events marking the 200th anniversary of the isolation of benzene by Michael Faraday in 1825.

The bicentenary is being celebrated through a series of events coordinated by the Royal Institution and the Royal Society of Chemistry, recognising this milestone in the development of modern chemistry. We are pleased to contribute to these celebrations by hosting a dedicated lecture in honour of Kathleen Lonsdale, whose seminal crystallographic work at Leeds provided the first conclusive evidence that the benzene ring was a planar hexagon – a crucial discovery which has had major implications for chemical bonding theory.

As well as two of our Leeds colleagues presenting their work, the event will feature two prestigious talks from external speakers: one exploring the life and legacy of Kathleen Lonsdale, and the other focusing on the crystallographic and scientific significance of her work.

Programme

14:00 Arrival and registration

14:30 Welcome: Professor Colin Fishwick, Head, School of Chemistry, University of Leeds

14:45 Professor Dame Jocelyn Bell Burnell – Introduction to Kathleen Lonsdale

15:15 Dr Briony Yorke, School of Chemistry, University of Leeds

15:35 Dr Fanny Costa, Faculty of Engineering & Physical Sciences, University of Leeds

15:55 Professor Arwen Pearson, Institute for Nanostructure and Solid State Physics, University of Hamburg

16:45 Closing remarks: Professor Sir Richard Catlow, Department of Chemistry, University College London

17:00 Drinks reception and poster session (TBC)

18:00 Event close

Booking is required to attend the event: click here to book. Deadline: 1st September.

If you have any questions, please contact the EPS CPD Conference and Events team via **cpd@engineering.leeds.ac.uk**

Twenty-Seventh Congress and General Assembly of the International Union of Crystallography

Calgary, Canada, 11th-18th August 2026

IUCr2026 is set to be held in the magnificent city of Calgary, located in the heart of Alberta, Canada, from 11th to 18th August 2026. Calgary, a city renowned for its breathtaking natural beauty and warm hospitality, has been chosen as the host for this remarkable occasion. Nestled amidst stunning landscapes and boasting a rich cultural heritage, this vibrant metropolis promises to provide an unforgettable experience for all attendees.

More details and registration are available at https://www.iucr2026.org/

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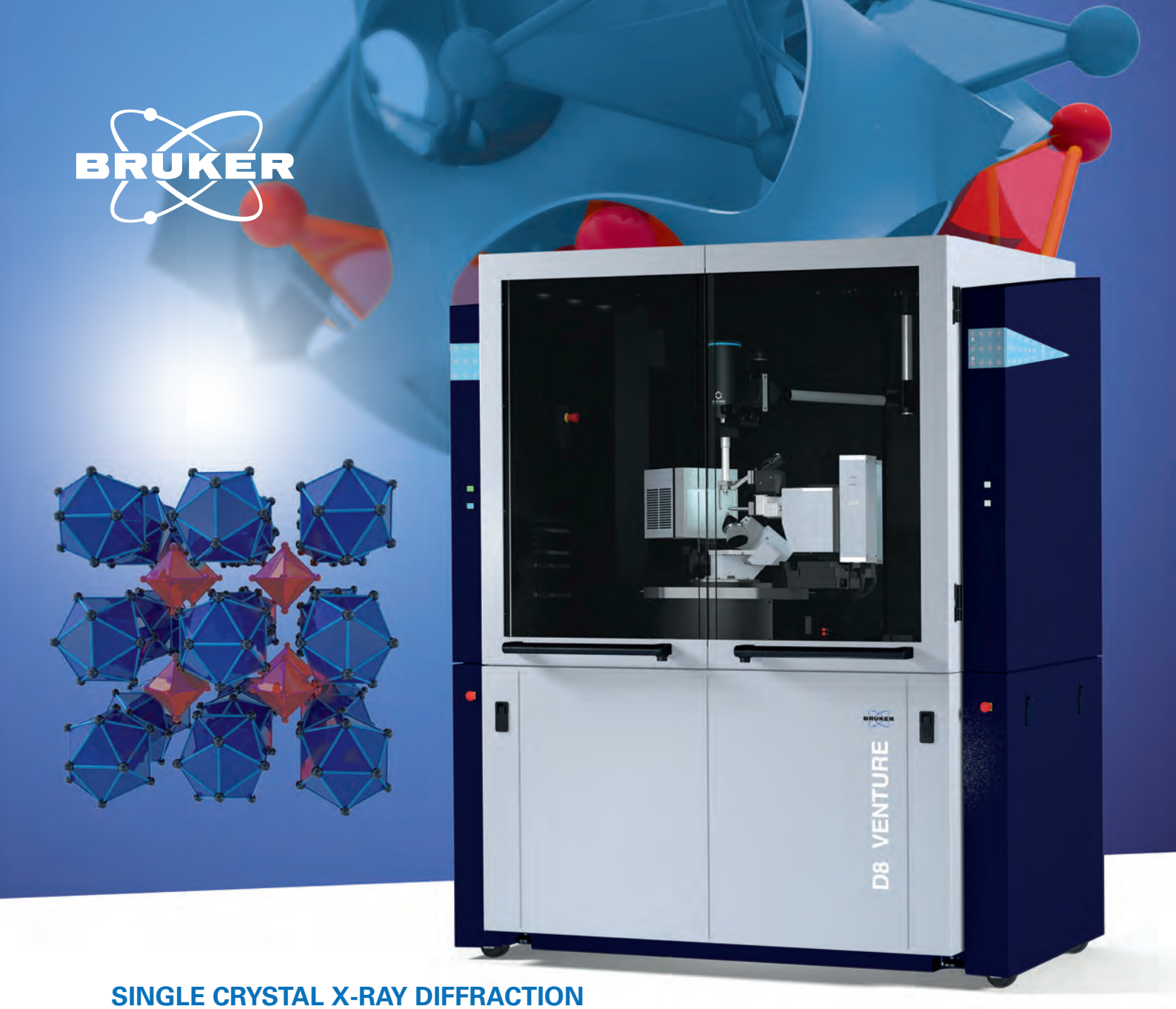

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