Crystallography News

British Crystallographic Association

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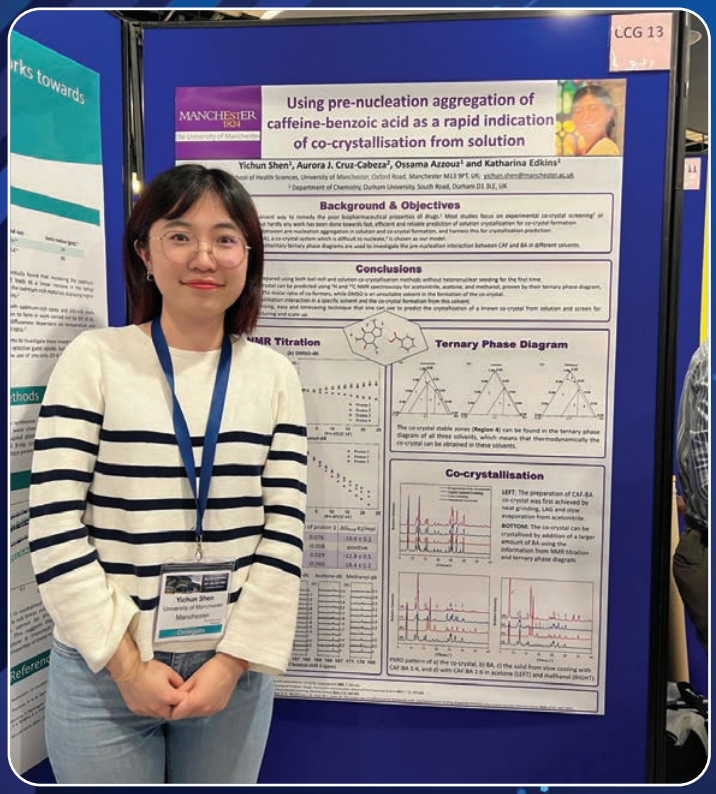

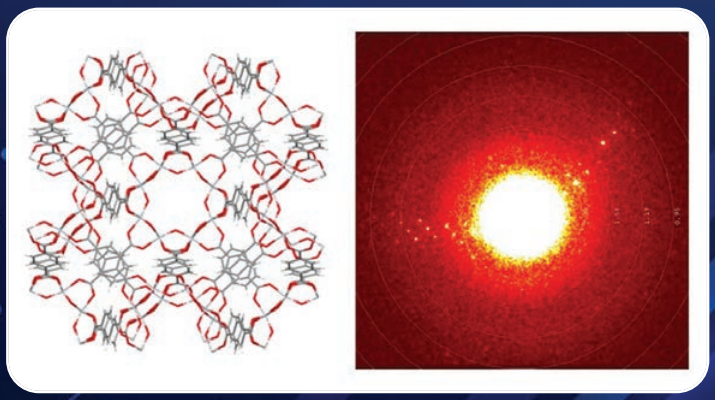

BCA Spring Meeting in Sheffield

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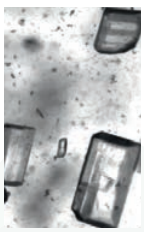
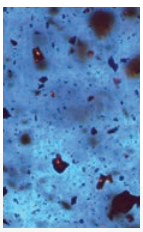
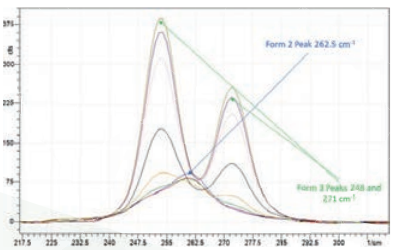
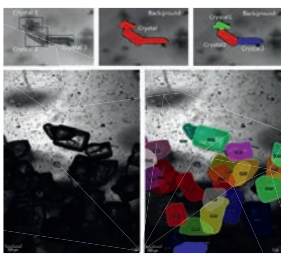


Nucleation within droplet



Colored particle view imaging





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British Crystallographic Association

Conference Bursaries 2023

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

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

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

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

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

Contents

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by North Wolds, York. Text should preferably be sent electronically as MSword documents (any version - .docx, .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.
Please ensure that items for inclusion in the September 2023 issue are sent to the Editor to arrive before 25 July 2023.

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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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This month's cover:

Spring meeting attendee Yichun Shen (Manchester), Dr Olga Kennard OBE FRS 1924-2023, Robert Bannister and Simon Coles (Southampton) with an XtaLAB Synergy-ED, and nano-crystal electron diffraction.

From the President

I was sad to learn of the passing of Dr Olga Kennard at the beginning of March this year. She founded the Cambridge Structural Database in 1965 and was also a Founder member and Honorary member of the British Crystallographic Association. Her legacy to the crystallographic community is the establishment of the CSD and many readers frequently rely on the database in their research.

Since its founding, the CSD has appeared to grow almost exponentially, reflecting the increasing rates of data collection and publication of structures in the field. The bar plot showing this growth is a familiar sight in publications and lectures deriving insights from the database. But what are the implications of this for the future?

In his article "The Great Horse-Manure Crisis of 1894" Stephen Davies[1] notes that we commonly read reports to the effect that "If trend X continues, the result will be disaster". He includes an example from history: "The larger and richer that cities became, the more horses they needed to function. The more horses, the more manure. Writing in the *Times* of London in 1894, one writer estimated that in 50 years every street in London would be buried under nine feet of manure. Moreover, all these horses had to be stabled, which used up ever-larger areas of increasingly valuable land. And as the number of horses grew, ever-more land had to be devoted to producing hay to feed them (rather than producing food for people), and this had to be brought into cities and distributed – by horse-drawn vehicles. It seemed that urban civilization was doomed."

It turned out that cities weren't doomed (at least not as immediately) and were "saved" by the introduction of the motor car. In a world with finite resources (people, crystals and instruments), exponential growth can be supported for a while by technological advances, but growth slows as we approach the capacity of the system.

If the CSD had continued to grow at the same exponential rate as it was growing in 1980, then it would already be seven times larger today, and by the end of this century would be growing at a rate of 17 million structures per day. And that isn't a future that I would wish for our descendants. Extrapolation can often lead to fantastical or impossible results and as fitting data is a large part of crystallography, we know the dangers of using the wrong function. A better measure to fit is the first derivative of the growth, the number of new crystal structures being determined and included in the database each year. New structures are the most resource intensive part of the process and the increase since the turn of the century has been almost linear, increasing from approximately 20,000 structures per year in 2000 to around 60,000 per year now – increasing by about 2,000 extra new structures per year.

Even this increase in rate would eventually exhaust the capacity of the world's labs, but its non-exponential form means that we're not doomed to be buried by CIF files piling up in the streets of London for a while yet, and we can continue to benefit from the marvellous foresight of Olga Kennard and enjoy using and learning from the world's crystal structures.

The 19th BCA/CCG Intensive Teaching School in X-Ray Structure Analysis was held in Durham for the week preceding this year's Spring Meeting. This school runs every two years and teaches students and researchers fundamentals required for single crystal structure analysis including maths, symmetry, instrumentation, structure solution and refinement. A unique feature of the school is the inclusion of group tutorial sessions led by experienced crystallographers, which reinforce the lecture material as it is covered. It was good to be back in person for this edition of the school, and as usual the attendees threw themselves into the work and enjoyed the opportunity to meet fellow scientists. Some of the more invincible attendees made it to the **BCA Spring Meeting** in Sheffield the following week, which was also a great success. Thank you to Programme Chair **Helen Playford**, VP **Suzanna Ward**, the Programme Committee, and Session Chairs for lining up an excellent programme of speakers. Thanks also to Hg3 for managing the meeting and the support of our sponsors and exhibitors for supporting the meeting.

On 5th April the AGM voted to introduce a new Fellow membership category: this membership level recognises those with an established career in crystallography and offers a simple way to support the organisation through the membership subscriptions. The next AGM will also see a proposal for a small change to the statutes: the Young Crystallographers Group have changed their name to the **Early Stage Crystallographer Group** (ESCG) – and we can now update the statutes to match.

I'm looking forward to next year's BCA meeting in **Leeds** from **25th-28th March 2024**. The meeting will be organised in and around the instantly recognisable Parkinson Court building. The programme committee has begun work already and is chaired by **Peter Moody** (pcem1@leicester.ac.uk) and **Hanna Kwon** (hanna.kwon@leicester.ac.uk) from the University of Leicester. As ever, your input is valued in helping to shape the meeting and suggesting speakers.

I am delighted to welcome **Briony Yorke** as a new member of BCA Council. Briony takes over from **Hazel Sparkes** who served for five years on Council. I'm also pleased to let you know that **Ilaria Gimondi** has been co-opted as our Outreach and Education Coordinator following **Christine Beaver**'s move to the US. Thanks to **Jon Cooper** for taking over as *CN* editor from **John Finney** as of this issue. The transition has appeared painless as Jon has shadowed the publication process for the last few issues. Having seen a draft of this issue, I'm looking forward to Jon's stewardship over the next few years!

As of the next AGM, Council has vacancies for one Ordinary Member, one Outreach and Education Coordinator, and one President. There is no direct succession from Vice-president to President – anyone may be nominated for any vacancy. A quick reminder of the procedure (from BCA By-law E): Nominations may be made by any two members, accompanied by consent of the candidate to serve if elected. They must be sent to the BCA Secretary by September 30th. The nominating committee will also work to secure nominations for these vacancies.

Richard Cooper
Oxford

References:

1. https://fee.org/articles/the-great-horse-manure-crisis-of-1894.

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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 an honour to be invited to edit *Crystallography News* and to follow in the footsteps of Prof John Finney (also at UCL) who has been at the editorial helm for the last three years. John was the head of the Liquids Group in the Department of Crystallography at Birkbeck College London when I started my PhD there in 1985. He was also one of the first people to welcome me to UCL in 2007 with an interesting request for information on the work I did with Prof Tom Blundell at Birkbeck on the structure of the hexagonal form of porcine pepsin – an analysis that was initiated in the 1930's by Dorothy Hodgkin and J. D. Bernal. John has also very kindly contributed two articles to this issue. Firstly a review of John Meurig Thomas's book 'Albemarle Street – Portraits, Personalities and Presentations at the Royal Institution' and, secondly, an account of the role played by crystallographers recruited to the Special Operations Executive during World War II. This article includes a fascinating photograph of none other than the late Durwood Cruickshank (Manchester, and former BCA Vice President) at the helm of a Welfreighter, an experimental semi-submersible vessel that was developed for wartime intelligence work. As someone who used to write laboratory risk assessments, I cannot help thinking that he should have been provided with a hard hat and at least a life jacket by his employer!

We also have a review by Prof Tony North (Leeds) of the book 'The Man in the Monkeynut Coat' by Kersten Hall which is a biography of Prof William Astbury FRS (Leeds), describing the central role he played in the development of structural molecular biology of both proteins and DNA. The curious title relates to his discovery that fibrous material prepared from monkey nuts could be used to make textiles. The shortage of wool for uniforms during World War II led ICI to invest heavily in the project and Astbury regularly wore an overcoat made from this material (Ardil) at lectures.

Readers of *CN* may remember that, for some amusement in recent years, I have been researching the history of the former London-based scientific instrument manufacturer Hilger & Watts who marketed diffractometers developed by Uli Arndt, mainly during the 1960's. Uli was based at the Royal Institution and later at the MRC in Cambridge. His work at the RI was pivotal in the analysis of the first enzyme structure by Prof Sir David C. Phillips FRS, which is described in John Finney's book review. My quest to find surviving examples of these instruments has so far led to a Y290 four-circle diffractometer being located in Galway. Various clues from the internet and a very helpful tip-off from John Low (Dundee) suggested that one of the earlier linear diffractometers had been preserved by the University of Aberdeen. The covid lockdowns got in the way of confirming its existence but the exceptionally helpful library staff in Aberdeen have indeed located it in off-site storage and a short report is included in this issue.

We also have an article from Simon Coles (Southampton) featuring the new EPSRC funding award for the National Electron Diffraction Facility and reports on the YCG and BSG sessions at the 2023 BCA Spring Meeting in Sheffield as well as the student bursary winner reports. Summaries of the remaining sessions will appear later in the year, hopefully in the next issue.

Finally, Bob Gould in Edinburgh must be thanked for providing us with a crystallographic puzzle in each CN issue for as long as I can remember. However, I gather that Bob has, understandably, indicated that he would like to stop doing this and, partly as a long-time low-performer in aptitude tests, I am sympathetic, but the puzzle is something that could of course be re-instated by popular demand – just let me know. Meanwhile, I have a suggestion for a possible substitute for Bob's ingenious quizzes which was inspired by a guided tour of Bloomsbury last year, during which we were shown the home of Charles Fort (1874-1932) who became famous for his studies of anomalous phenomena. Being within a few miles of at least 10 crystallography laboratories and given the importance of such phenomena for phasing, at least in biological crystallography, it crossed my mind that a small section on ***Crystallographic Forteana*** could be a future source of digression for *CN* readers. So to start the ball rolling I have included two photographs of mine, one showing the plaque on Fort's house and another showing a quasi-crystalline lattice of starlings that I came across last Summer. Using various online 2D Fourier transform tools (not shown) one can see that this partially ordered murmur even generates some low resolution diffraction peaks! Anyone who has glanced at Fortean Times will know the type of phenomena which his followers are interested in and, although this is something that we should perhaps not encourage too much, readers are welcome to send me similar observations e.g. oddly-shaped crystals, unusual features in structures, etc. Anything that challenges the boundaries of scientific knowledge fits the bill and is most welcome. Your imagination is the limit!

Jon Cooper
UCL

Revise that diffraction theory

We know that the scattering or reciprocal lattice vector, **S**, has amplitude $|S| = \frac{1}{d}$ where d is the inter-planar spacing, or the resolution of the corresponding diffraction spot. In the excellent textbook Crystals and X-rays by the late Dame Kathleen Lonsdale FRS (Bell, 1948) on page 54, there is an interesting formula which the author describes as being "easy to remember, because of its symmetry":

$$\frac{1}{d^2} = \frac{\frac{h}{a}\begin{vmatrix} \frac{h}{a} & \cos\gamma & \cos\beta \\ \frac{k}{b} & 1 & \cos\alpha \\ \frac{l}{c} & \cos\alpha & 1 \end{vmatrix} + \frac{k}{b}\begin{vmatrix} 1 & \frac{h}{a} & \cos\beta \\ \cos\gamma & \frac{k}{b} & \cos\alpha \\ \cos\beta & \frac{l}{c} & 1 \end{vmatrix} + \frac{l}{c}\begin{vmatrix} 1 & \cos\gamma & \frac{h}{a} \\ \cos\gamma & 1 & \frac{k}{b} \\ \cos\beta & \cos\alpha & \frac{l}{c} \end{vmatrix}}{\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}}$$

From this we see that d is a function of the unit cell parameters (a, b, c, α, β and γ) and the diffraction indices (h, k, l). The boxes in the formula are, of course, determinants and their expansion is beyond the scope of this exercise. Describe succinctly the symmetry which the author mentions is present in this formula and propose a simple rule of thumb for memorising it. **Answers to the editor**.

Reports on the BCA Spring Meeting, Sheffield

YCG Satellite Meeting

The YCG Satellite meeting is an opportunity for early stage crystallography researchers, from across the BSG, CCG, PCG and IG, to present their work in a supportive and friendly environment. This year's meeting, held at the University of Sheffield, saw the second in-person meeting to be held since 2019 and was the last YCG meeting, as the section's name change to the Early Stage Crystallographer Group (ESCG) became official from the end of the meeting.

This year's meeting started with the first plenary delivered by **Mark Senn** (Warwick), having travelled directly from the 2023 BCA/CCG Intensive Teaching School in X-ray Structure Analysis, held in Durham. The plenary lecture was on the symmetry assisted analysis of functional materials and how we can use this approach in predicting behaviours of these high symmetry inorganic systems. The kind of insights achievable from these techniques are the softening of phonon modes, coupled distortions and even phase transitions. Mark went on to describe how this approach has also been used in the interpretation of the pair distribution data for more local effects, such as A or B site distortions that lead to ferroelectricity, using the archetypal $BaTiO_3$ as an example. The approach can also be used to look at interesting mechanical behaviour with temperature and how the coupled distortions give rise to behaviours like negative thermal expansion and also improper ferroelectricity. Mark referred to the work of Jeremiah Tidey and Anna Herlihy in asserting the power and flexibility of this approach on these high symmetry polyhedra containing systems. The talk was an excellent kick off to the meeting and continued straight into session 1, which featured four contributed talks from YCG members.

The first was from **Thomas Roseveare** (Sheffield) who presented his work on the dynamic behaviour of metal-organic frameworks through three post synthetic modification methods. This included showing that the ability to access the fully closed form was solvent dependent in some but not all cases. The second speaker was **Alexander Lione** (Durham) who gave us an insight into how strain engineering in $SrTiO_3$ and $ReNiO_3$ can be used to induce phase transitions through first principles simulations based on density functional theory (DFT). However, some limitations in DFT's ability to correctly identify magnetic and electric properties seen experimentally were also highlighted. This was followed by a presentation from **Erin Stark** (Indicatrix) summarising the different automated crystal centring techniques, with particular focus on image processing methods, for use in X-ray diffraction experiments. Image recognition techniques were shown to be the simplest to apply but the least accurate. However, it was shown that they could be used for initial alignment and then centring could be carried out by diffraction-based methods. The final talk of the session was given by **Suzannah Hughes** (Birmingham) who showcased her work on the structure and absorption properties of the Zn/Cd-ZIF-8 system. Flow synthesis was employed, and a non-linear relationship was observed with an increase in the Cd ratio.

YCG Opening Plenary and Session 1, left to right: ***Dr Mark Senn, Dr Tom Roseveare, Mr Alexander Lione, Miss Erin Stark, Mrs Suzannah Hughes*** *and* ***Dr Rebecca Clulow*** *(chair).*

Session 2 began with an excellent talk given by **Stephen Brown** (Warwick), discussing *in-situ* studies, using the PORTO laser on EH2 at Diamond, to investigate photo-induced single-crystal-to-single-crystal transitions in titanium-oxo clusters. Leading to further understanding of the resulting increase in disorder and highlighting the crystal site selectivity shown. This was followed by **Joshua Smith** (Sheffield) who shared his work into developing serial crystallography techniques for the

analysis of high valence-state metal-organic frameworks (MOFs). This included the development of a serial gas cell to allow analysis of these micro-crystalline materials and to start to bridge the gap between synchrotron multi-crystal crystallography and conventional single-crystal diffraction characterisation techniques for MOFs. Next to speak was **Phillippa Partridge** (Edinburgh), who detailed an investigation of the order-disorder solid-solid phase transition behaviour exhibited by (cyanomethyl)trimethylammonium hexafluorophosphate, illustrating that the change from a trigonal to monoclinic phase always caused non-merohedral twinning, with 3 domains, to occur. **Cameron Scott** (Durham) then concluded the session with his talk about directions by which to achieve magnetoelectric multiferroic materials based on the polar structure of HfO_2 through investigation, by symmetry analyses and first-principles simulations, of the effect of replacing hafnium with various magnetic cations.

YCG Session 2, left to right: Mx Stephen Brown, Mr Joshua Smith, Miss Phillippa Partridge, Mr Cameron Scott and Mr Josh Morris (chair).

The third and final speaker session of the day started with an interesting talk on the crystalline sponge method and the conformation of guest molecules by **Eleanor Soper** (Southampton). This was investigated using a DFT based approach to study the conformation of guests within the pore environment. The second speaker was **Ben Tragheim** (Warwick) who spoke about colossal magnetoresistance and the impact of Jahn-Teller distortions, orbital order and structural freedom regarding a manganite perovskite prototype system as explored using diffraction data. The third speaker was **Eliza Dempsey** (Edinburgh) who gave an interesting talk on the potential to induce negative thermal expansion by altering the fluoride composition of niobium oxyfluorides. This talk drew on *ab initio* predictions and X-ray diffraction data at extreme conditions. The final speaker for this session was **Ben Coulson**

YCG Session 3, left to right: Miss Eleanor Soper, Mr Ben Tragheim, Ms Eliza Dempsey, Dr Ben Coulson and Dr Rachael Wilkinson (chair).

(Cardiff) who described the impact of varying the functionality of an ester group distant from the metal centre, on the photoisomerism behaviour of palladium nitro-complexes. This talk focused on how bulkier ligands result in a lower temperature required to reach relaxation to ground state.

This session was followed by a series of flash presentations from conference attendees who were presenting posters. It was the first year in memory that all participants managed to keep to the 30 second time limit for the flash presentations, illustrating how high the quality was this year. The day's sessions were concluded with a poster session where attendees could discuss their recent work.

Day two commenced with the Parkin Prize Lecture, this year's recipient was **Lewis Owen** (Sheffield). The Parkin Lecture is awarded in honour of the late Dr Andrew Parkin for contributions to scientific outreach and communication, with this year's recipient focussing on the latter. By utilising his background in acting, Lewis was able to walk us through various techniques for improving scientific communication of *any* format by treating it as a performance. After a short contemplation of why science communication is performed in the first place, the forms it can take were categorised as either written or performative science communication.

By focusing on the performances, guidance on how to consider the audience, formality, structure, and one's own physical/vocal presence, the communicator can calibrate their performance to those that view it. Lewis's performance was peppered with Shakespeare quotes, linking to theatrical themes, with Reservoir Dogs receiving an honourable mention in the context of presenting the timeline of events and how this does not necessarily have to be linear. Mike Glazer mentioned humour and how this can be a handy communication tool, prompting Lewis to recount a time when things went wrong and how humour was used as a "get out of jail free."

Notable advice was that it is always better to pitch the content difficulty lower than expected, rather than accidentally too high, as this will flatter the audience and continue to keep them engaged. "Learning to love the pause", allowing time for your audience to process the information you are delivering. Producing one-line clarifications – what was the main point of the performance, and does the audience leave recalling that? Also, practising a presentation in advance should not just be to control nerves but to try out different ways of saying things and presenting the information, to help improve the overall performance and prevent it from feeling rigid and over-rehearsed.

Finally, one of the most powerful devices for science communication was claimed to be analogies to produce visual images in the audience's mind. "Tell them stories," wrote Phillip Pullman in The Amber Spyglass, narratives and visuals are all part of the performance and highlights how "All the world's a stage."

The Prize Lecture was followed by four more oral contributions from early career researchers. **Olivia Breen** (Dublin) kicked off this final YCG speaker session by presenting an impressive number of metal ammonia oxalate coordination polymer complexes with varying degrees of polymorphism. **Jessica Metherall** (Newcastle) then spoke about high-throughput Encapsulated Nanodroplet Crystallisation – a promising approach for obtaining high quality co-crystals, suitable for SCXRD. This was followed by **Jake Hill** (Bradford) who

provided some fascinating insight into UV related cataract formation. Jake's study of oxidised crystals showed that UV irradiation disrupted the covalent modification of surface cysteines, resulting in the aggregation of crystallin proteins. The session was closed by **Holly McPhillips** discussing cation order in the A-site doped multiferroic material $MnAMo_3O_8$ (A^{2+} = Fe, Co, Zn) where neutron diffraction and X-ray absorption spectroscopy was used to explore how the structure and magnetic behaviour of the parent $Mn_2Mo_3O_8$ structure is changed by doping.

The session, and the overall meeting, was concluded with a virtual plenary talk from **Lauren Hatcher** (Cardiff). Lauren gave a fascinating overview of the work that has been carried out by her and her group (specifically mentioning the work of Ben Coulson, Sam Lewis and Josh Morris), studying dynamic processes induced by stimuli such as light and electric fields, using single crystal X-ray diffraction. Lauren highlighted how much in-house diffractometers can be adapted to allow for the analysis of very fast linkage isomerism processes using pulsed LED light and electronically gated detectors in time-resolved studies. It was clear that further innovations can be expected in the development of these *in-situ* and in-house analytical techniques, which will be invaluable for the understanding and design of future smart materials.

*YCG Parkin Lecture, Session 4 and Closing Plenary: **Mr Thomas Hitchings** (chair), **Dr Lewis Owen, Ms Olivia Breen, Miss Jessica Metherall, Mr Jake Hill, Miss Holly McPhillips, Dr Anna Herlihy** (chair) and **Mr Lee Birchall** (chair). Not pictured **Dr Lauren Hatcher**, who gave her talk virtually.*

Overall, the YCG Satellite Meeting demonstrated the broad interests and high calibre of research conducted by early stage researchers within the BCA. The group hopes to continue this as it moves forward as the ESCG and looks forward to welcoming attendees to the 2024 meeting in Leeds.

By the 2022/23 YCG committee members **Natalie Pridmore, Thomas Hitchings, Rebecca Clulow, Josh Morris, Rachael Wilkinson, Anna Herlihy** and **Lee Birchall**.

MAIN MEETING

The Lonsdale Lecture

The Lonsdale Lecture celebrates the work of the late Dame Kathleen Lonsdale. It is awarded by the BCA on the advice of the YCG. Typically, this prize lecture is presented at the start of the Spring Meeting following the YCG Satellite Meeting and is an opportunity for the speaker to present on a range of topics.

This year's Lonsdale Lecture 'From Ångstroms to kilometres and back again: Science at interfaces and the importance of belonging' was given by **Dr Kate Brown** (University of Cambridge and the University of Texas at Austin) who discussed the advantages and challenges of working across different disciplines.

First Kate commented on Kathleen Lonsdale's career and how her reputation as a scientist enabled her to continue working even though she did not obtain a permanent contract for a very long time. She also highlighted how events in Kathleen's life influenced her work and actions. Similarly, Kate's work was influenced by factors in her own life, including her introduction to science through her father's own work and working as a glassware cleaner in a lab through university.

Kate illustrated the route her career has taken from her work on site directed mutants of tyrosyl-tRNA synthetase with David Blow, through second-site revertants, biocatalytic reactions, nanoclusters for potential bioimaging applications, to changing fields to work with industry on infectious diseases, computational modelling of disease spread, and helium atom scattering. She highlighted how many of these shifts in focus gave her a unique view of the topic and still built on her previously gained knowledge and skills, but applied them in different ways. Ultimately this is why multidisciplinary teams can be so innovative, when they build a sense of community too. However, Kate also discussed how her path wasn't easy and, as well as hard work, required support and people to fight for you, echoing the experiences of Kathleen Lonsdale, that she highlighted at the start of the talk.

Natalie Pridmore, Bristol

*Kate Brown (right) receiving the Lonsdale Prize Lecture certificate from **Natalie Pridmore** (left).*

Biological Structures Group

The BSG session "Complementary Methods for Structural Biology" was chaired by **Andrew Burnett** (Leeds) and began with a presentation by **Sofia Jaho** (DLS) who spoke on the subject of "Serial synchrotron crystallography coupled with *in crystallo* optical micro-spectroscopy for protein dynamics at I24." The I24 beamline has capabilities for room temperature data collection from crystals mounted on special chips with robotic scanning of up to 25,000 positions, in addition to a viscous extruder for delivering membrane protein crystals grown in the lipidic cubic phase (LCP) into the beam. I24 is tuneable with an energy range of 7 – 23 keV and high flux density, adaptable beam size and a choice of either Pilatus or Eiger detectors. The beamline also has anaerobic and rapid-mixing capabilities along with UV-visible microspectroscopy as well as laser activation facilities for time resolved studies of photocaged compounds. Then, **Adam Crawshaw** (DLS) spoke on "Assessing the qualities of different focussed ion beam sources for the preparation of protein crystal lamellae for three-dimensional electron diffraction". The speaker described how ED allows one to work with exceptionally small crystals (< 0.5 µm) and how these are inherently more efficient for fragment soaking experiments. Since ion beam milling is important for removing the unwanted matrix surrounding the crystal, the data collected by continuous rotation ED with a Dectris 1M detector from crystals treated with a range of milling sources were compared. Next, **Sofia Kapetanaki** (Pecs, Hungary) spoke on "Conformational flexibility in a photoactivated adenylate cyclase studied by solution X-ray scattering". The enzyme studied is from photosynthetic cyanobacterium *Oscillatoria acuminata* and is homodimeric with an N-terminal domain that senses blue light using flavin (BLUF) and a C-terminal class III adenylate cyclase (AC) domain. The speaker explained how modulating the cellular concentration of cAMP has emerged as the focus of modern optogenetic applications and therapeutic approaches. Recent crystallographic studies have indicated that although the light-activation of this enzyme (OaPAC) is substantial, it involves only small structural changes. The speaker explained how time-resolved SAXS and other biophysical techniques including WAXS are being used to investigate the light- and substrate-induced conformational changes of OaPAC.

Following this, the BSG networking session was an opportunity to meet other researchers and discuss research and collaboration opportunities in an informal setting. A light hearted discussion of various X-ray sources was initiated with a game of TopTrons designed by **Sam Horrell** (DLS, Twitter: @Drhorrell). This is an extension of Sam's wildly popular synchrotron mug madness competition (#SynchrotronMugMadness) which has created a global ranking of synchrotron mugs. Synchrotron TopTrons is an excellent educational opportunity for budding crystallographers and a useful resource for those wanting to compare the volume of different synchrotron sources or the energy contained within their corresponding cuppa! The tradition of scientific tea breaks is an important ritual that encourages informal discussion of new ideas and creates a space for scientists to express their creativity whilst contributing to the well-being of scientists at all levels of their career.

The session "Science for Better Research" was chaired by **Sam Horrell** (DLS) and began with a lecture by **Anna Warren** (DLS) entitled "VMXm: A new micro/nanofocus protein crystallography beamline at Diamond". Anna described how this *in vacuo* beamline allows users to work with samples as small as 0.5 µm due to its remarkably small beam size (0.4 – 10 µm). The facility has an energy range of 6 – 28 keV and offers a choice of Eiger or Pilatus detectors. The samples are mounted on cryo-EM grids and excess mother liquor blotted from the other side. Conductive cooling is achieved through the use of copper sample mounts and the beamline incorporates an electron microscope for alignment of extremely small samples! The next lecture entitled "Laser-driven X-ray photon sources and endstations at ELI Beamlines" was given remotely by **Yelyzaveta Pulnova** (ELI ERIC, Czech Republic) who described this pulsed plasma X-ray facility, based on laser excitation of disposable 20 µm thick copper tape, for time-resolved pump-probe studies of cryo-cooled crystals. The X-ray pulse-duration is less than 300 fs and the facility has an Eiger detector for time-resolved data collection by multiplexing with the Hadamard method. Next, **Caitlin Hatton** (Hamburg) gave a presentation entitled "Millisecond cryo-trapping by the spitrobot crystal plunger simplifies time-resolved crystallography." The speaker outlined the general approaches to time-resolved studies and described prior work on a number of enzymes. Caitlin described the approach of plunge-freezing samples prepared with a liquid application robot which loads crystals as small as 20 µm and substrates onto micromeshes at precise time points with millisecond resolution. Studies of glucose isomerase and tryptophan synthase have been successful. The final talk in this fascinating session was given by **Jeney Wierman** (CHESS, Cornell) and was entitled: "Under pressure: structural biology meets high-pressure capabilities at the Cornell High Energy Synchrotron Source". The speaker described SAXS and MX studies of proteins such as cytochrome c peroxidase and tryptophan synthase from deep sea fish, such as comb jellies, using a diamond anvil cell to reach pressures of 400 mega Pascals.

The X-ray source TopTrons card game devised by **Sam Horrell** *(DLS), as played in the BSG networking session.*

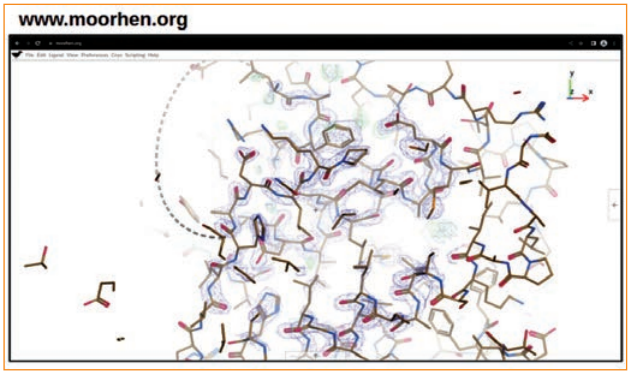
The BSG early career prize lecture this year was given by **Tiago Costa** (Imperial) and chaired by **Helen Playford** (ISIS). Tiago's presentation was entitled: "Architecture of an antimicrobial resistance propagator" and covered cryo-EM studies of the bacterial type-IV secretion system (T4SS), in particular the F-pilus which is involved in DNA transfer from one cell to another during bacterial conjugation. The structure of the pilus protein monomer is a helical hairpin which was found to have additional electron density at the inter-helical loop, probably for a phosphatidylglycerol molecule. Simulation studies suggest that the phospholipid molecules, which occupy the central cavity of the pilus, are essential for its stability. The speaker concluded with some impressive pictures of the 2.1 MDa T4SS complex solved by EM at 3.2 Å resolution. This session was followed by an exhibitor forum chaired by **Tony Bell** (Sheffield Hallam), beginning with a presentation by **Patrick Shaw-Stewart** (Douglas Instruments). Patrick demonstrated that seeding dramatically increases the success rate in crystal screening and that *in situ* dynamic light scattering is a useful tool to detect those crystallisation droplets in which the protein remains monodisperse.

The session "Science for Better Health and Wellbeing" was chaired by **Stephen Muench** (Leeds) and began with a lecture by **Andrea Thorn** (Hamburg) entitled "COVID-19: The pandemic response in structural biology." The speaker highlighted the fact that errors within structures in the PDB are normal and are potentially inevitable with the current effort and skillset required to solve a structure. Andrea described the rapid formation of the Coronavirus Structural Task Force (CSTF) at the start of the COVID-19 pandemic and how it grew to an impressive collection of 29 scientists. The CSTF worked on improving the accuracy of the SARS-CoV-2 structures as they were being solved at a rapid pace by designing a pipeline using automated and manual evaluation of new structures. Andrea went on to describe how improved structures were offered as feedback to the authors without a request for acknowledgement and consequently these corrections were made and deposited. It was a really lovely example of how science is improved by the collaborative effort of multiple experts. Without a means of acknowledgement in the current system, however, this cannot be sustained, posing the question of the way we acknowledge collaborations in this context. Recent developments include the application of AI in diagnosing problematic data. The speaker described how proteases play keys roles in the viral life cycle including ACE2 which acts as the receptor, cell surface proteases which cleave the spike protein leading to endocytosis and the viral 3C protease, which is essential for covid replication. The other aspect of CSTF which the speaker referred to throughout her talk was public engagement and outreach in all forms and guises. The pandemic highlighted the importance of communication between scientists and the community, and it was very impressive to see this so well embedded into a project. The second speaker within this session was **Doryen Bubeck** (Imperial) who gave an insightful talk entitled "Controlling MAC pore formation." Doryen's lecture covered how activation of the complement system leads to formation of a large membrane attack complex (MAC), and how structural techniques such as cryo-EM can inform on the complement system, particularly the MAC. The speaker gave a whirlwind tour of how her research has focused on understanding how MAC forms pores within the bacterial cell membrane, how human cells are protected against this, and how this can be used to develop therapies for aberrant complement activation. An impressive combination of crystallography and cryo-EM analysis allowed the stoichiometry of protein components in these complexes to be established. In addition, structural insights demonstrated the controlled transition of complement proteins from helical bundles (in soluble forms) to β-hairpins (membrane bound form). The speaker went on to describe how structural information about the 10 kDa CD59 obtained from EM studies of lipid nanodiscs allowed insight into how it was able to protect human cells from MAC-mediated lysis. Complement proteins C8 and C9 were shown to interact with CD59 and result in altered orientation at the plane of the membrane, inhibiting the assembly of the pore-forming proteins. This insight has resulted in the development of a cyclic peptide which could provide a future therapeutic solution to MAC-related disease states. This talk was a great example of how structural biology can help inform the development of future treatments. The final speaker within this session was **Clinton Lau** (Oxford) who gave a talk entitled "Lis1 bridges dynein to dynactin to regulate complex assembly and motility" covering his work on dynein complexes and migration on microtubules. The motor protein dynein, which is responsible for moving lysosomes, mitochondria and RNA along microtubules, forms a complex with the co-factor protein dynactin. The Lis1 protein, which is implicated in the rare smooth brain disorder lissencephaly, is required for the assembly of the dynein-dynactin complex. Clinton described his use of total internal reflection fluorescence (TIRF) assays and cryo-EM to elucidate key residues involved in the activation of the complex. This talk focused primarily on the cofactor Lis1 and cargo adapter Jip3. Cryo-EM analysis of complexes demonstrated a structure more confined than previously predicted due to long flexible regions. Lis1 was shown to bridge between dynein and dynactin in the complex and a number of lissencephaly-associated mutations occur at its dynein-binding surface. Interestingly, Clinton described an unexpected interaction between the dimerization domain of Lis1 and the p150 domain of dynactin. This was further explored using AlphaFold which provided an unusual fold and was able to highlight potential key residues for interaction. The importance of these residues was then experimentally tested using mutagenesis and TIRF assays which showed mutation of these residues prevented activation of dynein. The speaker described further success with AlphaFold in highlighting potential key residues in Jip3, which predicted interactions showing a further two phenylalanine residues, similar to those observed for Lis1, with their importance subsequently being confirmed by mutations and TIRF assays. This talk posed the question of how useful AlphaFold could be in helping constrain experimental questions.

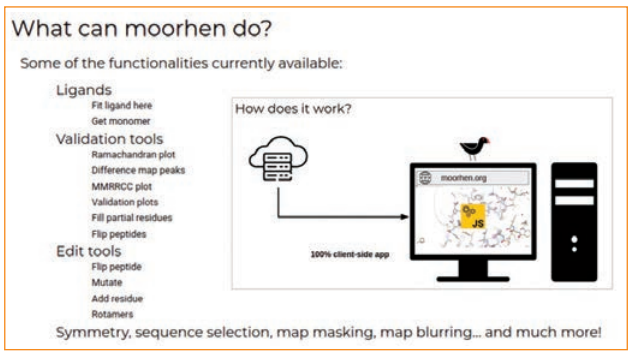
The BSG plenary lecture, chaired by **Briony Yorke** (Bradford), was given by **Simon Newstead** (Oxford) and was entitled "Decoding the role of solute carrier membrane proteins in health and disease." Simon described the role of these cellular gatekeepers which transport nutrients across the plasma membrane in a Na^+, K^+ or H^+-dependent manner and how their flux is regulated in different cell types. Simon then moved on describe the proton-coupled PepT1 transporter which is encoded by the SLC15A1 gene and is abundant in the small intestinal epithelium where it is involved in bulk dietary nitrogen uptake. It can also transport antibiotics and potentially other drugs if we can improve our understanding of its mechanism. The speaker went on to describe in detail studies of the mammalian K^+-transporter and the proton-coupled folate transporter CS2, both of which were analysed structurally by cryo-EM of nanobody complexes and by molecular dynamics. The folate transporter is a potential anti-cancer drug target and has been analysed in complex with a new-generation antifolate drug pemetrexed.

*Speakers in the Computational Crystallography session: **Filomeno Rodriguez** (York), **Elspeth Garman** (Oxford) and **Jordan Dialpuri** (York) along with the chair: **Keitaro Yamashita** (MRC Cambridge). Photo: Claire Naylor (SPT Labtech).*

The session entitled *Computational Crystallography* was chaired **Keitaro Yamashita** (MRC, Cambridge) and began with a presentation by **Elspeth Garman** (Oxford) entitled "Dose estimations for a variety of X-ray diffraction and scattering experiments: extensions to RADDOSE-3D". Elspeth described how the dose at the crystal can be calculated from the physics of the incident beam and the chemical composition of the sample. Recent developments in the RADDOSE-3D software aim to model the absorbed dose in situations where the beam is considerably smaller than the crystal. It can also be used for XFEL and SAXS applications. The next speaker was **Jordan Dialpuri** (York) whose presentation on "Analysis and validation of overall N-glycan conformation in Privateer" covered the range and occurrence of geometric errors in the N-linked glycosylations in the PDB. The program Privateer is able to detect and correct many of these errors based on cluster analysis of various known glycan linkages and torsion angle refinement. Next, **Filomeno Rodriguez** (York) gave an interesting talk entitled "Moorhen: a web molecular graphics program" and described a web application which aims to replicate much of the functionality of Coot. The program is written in javascript, can be accessed at **moorhen.org** and runs as a client-side script on any device with a web browser. The aim is to make model-building easier for new users and this was emphasised in a live demonstration of the program's capabilities. Last but not least, the final speaker of this session



*A screenshot of the new web-based macromolecular graphics program moorhen, presented in the Computational Crystallography session by **Filomeno Rodriguez** (York).*

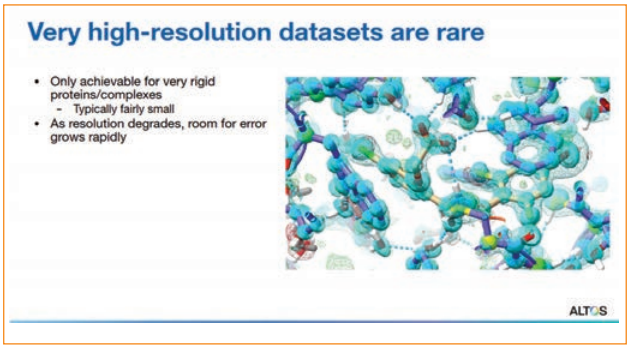


*Some more capabilities of moorhen from the presentation by **Filomeno Rodriguez** (York).*

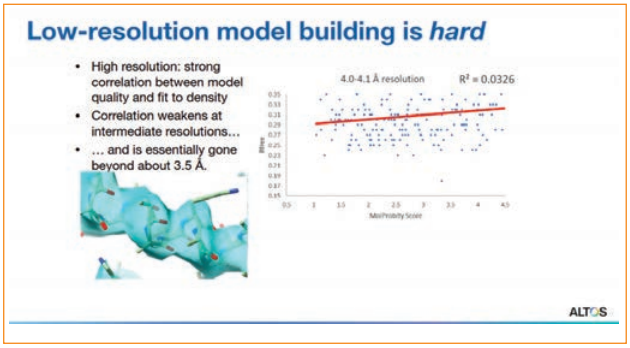
was **Anton Cleverley** (Warwick) whose talk was entitled "The optimisation of Bloch-wave modelling of cRED data, helping to close in on the *R*-factor gap." The speaker covered the two main theoretical approaches for analysing dynamic electron scattering, namely the multislice and Bloch-wave models, as well as corrections based on the Bloch-wave model to improve the refinement *R*-factors of electron diffraction structures.

***Briony Yorke** (Bradford) and **Tristan Croll** (Cambridge) at the "Difficult Density" workshop. Photo: Claire Naylor (SPT Labtech).*

On the final day of the meeting a "Difficult Density Workshop", chaired by **Briony Yorke** (Bradford) was given by **Tristan Croll** (Cambridge) whose keynote presentation was entitled "Modelling into low-resolution crystallographic datasets with AlphaFold and ISOLDE." The speaker gave a live demonstration of this impressive program which is an extension of UCSF ChimeraX. This proved to be a very interesting tutorial, showing how ISOLDE allows the maps to be updated on the fly as you do the model building while sophisticated force fields are used to keep the chemistry sensible.



Tristan Croll (Cambridge) demonstrated the capabilities of his molecular modelling program ISOLDE.



ISOLDE caters specifically for the challenges of building into low resolution electron density maps.

Finally, we must mention that the BSG poster prize (the Blue John crystal or David Blow Prize) was awarded to **Jake Hill** (Bradford) for the poster entitled "UV related cataract formation: insights from serial synchrotron crystallography." Jake also gave a lecture on this subject in the YCG satellite meeting.

Rachael Wilkinson (Swansea, bursary awardee), **Briony Yorke** (Bradford), **Jon Cooper** (UCL) and **Mark Montgomery** (Syngenta)

The following day started on a high with the Parkin Lecture given by **Lewis Owen** (Sheffield), who instilled into his talk theatrical flair and moreover the importance of science communication as a skill that can be honed. Followed by more talks including **Jake Hill** (Bradford) who showed how serial crystallography coupled with UV irradiation elucidates an important mechanism in cataract formation. The YCG satellite meeting concluded with **Lauren Hatcher** (Cardiff) who was able to give her talk remotely thanks to hybrid meeting technology – a boon from remote working during covid. She covered the development of a time resolved pump-probe technique to study photoswitchable crystals *in situ* and the complementarity of synchrotron and home-lab techniques.

The main meeting commenced with the Lonsdale lecture given by **Katherine Brown** (Cambridge) and was an excellent discussion of a non-traditional career path and the barriers still faced by many in the scientific community. With the conference started in earnest, the busy schedule of plenaries and parallel talks got underway. My highlights were **Hanna Boström** (Max Planck Institute for Solid State Research) on the difficulties in achieving reproducibility in a Zr-porphyrin MOF, highlighting the importance of considering and reporting all synthetic parameters. The evening concluded with a bustling poster session with plenty of discussion which carried on after we were turfed out into the bar upstairs and then for some time afterwards.

Wednesday's highlights included CCG prize lecture by **Lucy Saunders** (DLS) on proton transfer in molecular crystals and the use of an electric field cell for *in situ* diffraction experiments. Additionally, the central facilities panel discussion, showcased a wide range of techniques available to the crystallographic community.

The evening concluded with the conference dinner, a celebration of the community's work and to thank those who worked tirelessly to make the conference a success, the evening was capped-off with a cèilidh, a type of highly symmetric folk dancing. To our credit we did our absolute best to showcase symmetry breaking, our dance moves demonstrating all kinds of disorder; positional, substitutional, and twinning were the ones I noticed!

Stephen Brown
Warwick

Spring meeting reports from the bursary winners

I arrived in Sheffield on Monday for the YCG satellite meeting, the mood was friendly and welcoming. The opening speaker was **Mark Senn** (Warwick) who spoke on using symmetry to transform the models of crystal structures into a symmetry derived basis that allows for novel insights. That afternoon we had a range of talks from a diverse background of speakers, particular highlights for me were **Tom Roseveare** (Sheffield) on a 'wine-rack' mechanism in a flexible MOF. It was also time for my talk, an opportunity to talk about the work I'm enthusiastic about to my peers.

As well as talks, the YCG AGM took place where the name change to the ESCG Early Stage Crystallographer Group was agreed and cemented the group's aim to help all who are new to crystallography. This was followed by a poster session, not only an opportunity to speak to others about their work but also to network. Specifically, it was so great to catch up with so many from the crystallography community.

This conference was to be the first of many that our research group would attend together and, my first at which I would present a poster. Excitement coupled with a hint of nerves was heavy as we took the train to Sheffield on the sunny day to mark the start of spring. On the way, we deliberated on the topics to look out for during the packed parallel sessions on the scientific program as well as pointed out notable names in the exhilarating line up.

Upon arriving, we hung up our posters and I quickly became acquainted with fellow students doing the same around me. The fact that our topics were almost completely unrelated to each other and yet we met at this very conference was very amusing and I took my time exploring the research of others until the sound of a bell echoed through the room, signalling the start of the YCG meetings. It was a pleasant beginning to what was 4 days of intense information reception, and greatly inspired me to present my work to the same calibre. The day concluded with a lovely warm dinner and networking around the hall of posters with a glass of wine in hand.

The main meeting commenced on day 2 with a memorable talk from **Lewis Owen** (Sheffield) on outreach and scientific communication. As a keen scholar who regularly participates in outreach projects, this talk resonated with me and I had learnt so much on how I can present my ideas and myself in a manner that can capture the audience, just like how Dr Owen captured the attention of all the attendants in the room. I believe this day was most memorable to me due to the talk from **Kate Brown** (Cambridge). The science aspect was undeniably fascinating but it was the insights into the hardships of being a woman in science and the unjustifiable challenges she had to overcome due to out-dated preconceived social expectations that touched me. It made me realise how lucky I am in my position as well as aspired me to stand up for equality movements in the field. The conference dinner was a fun affair where I got to chat to the attendees in a more casual setting and got to know more about their work and the ups and downs of it. Both of the post docs in my group were able to win the poster and flash presentation prize, marking a happy and triumphant day for the Hobday group. Then, the rest of the meeting flew by, each talk encouraging me to take new approaches to my project and by the end of it, I was brimming with new ideas and a new drive to work hard.

Coming into this, I was unaware of the excitement and inspiration this conference would bring and now that it has ended, I can only look forward to our next, hopefully with new results of my own to present!

Cecilia Hong
Edinburgh

The BCA spring meeting was held in Sheffield this year, the theme of which was 'Teaching Crystallography'. The parallel sessions spanned many topics, such as sustainability, computational crystallography and crystal structure prediction. Following on from the Lonsdale lecture and the PCG plenary talk on the first day of the main meeting, the YCG/CCG joint session on 'Crystal growth' got underway. The keynote speech was given by **Katharina Edkins** (Manchester) who gave a succinct overview of the fundamental principles behind growing crystals. In her talk, Katharina covered the foundational theory behind crystal growth and highlighted the complexity of solubilities and other crystallisation conditions, which can have profound effects on the success. She also supplied an excellent overview of some of the most commonly implemented techniques used by synthetic chemists to grow crystals.

The second speaker, **Michael Hall** (Newcastle) added to the discussion of crystallisation methods by presenting recent advances in high-throughput crystallisation of small molecules via encapsulated nanodroplet crystallisation (ENaCt) protocols. This technique is based on classical protein crystallisation protocols which have been adapted to suit small molecules that are supplied in very small quantities. Michael went on to demonstrate the reach of the ENaCt technique, such as the crystallisation of natural products, the growth of co-crystals and polymorph screening protocols.

ENaCt was mentioned later in the session by the next speaker **Rhona Lonergan** (Kent) who spoke about her search for solvates, polymorphs and co-crystals of spin crossover (SCO) materials. Rhona gave an interesting overview of her PhD research which aims to understand structure-property relationships in SCO complexes, since a current practical impediment is the inability to rationally design such functional materials at present. By systematically changing certain aspects of the solid-state structures, Rhona presented her key results, which included the synthesis and characterisation of several solvatomorphs and co-crystals.

The session concluded with a talk from **Hanna Boström** (Max Planck) with her presentation on synthetic reproducibility in porphyrinic zirconium metal-organic frameworks (Zr-MOFs). Hanna provided an account of how the 'round robin' approach – where several different groups were sent the two Zr-MOF samples – was used to produce different phases of two different samples. This talk highlighted the difficulties that can be encountered when trying to produce a phase pure sample and how it is important to note the effects of the solvent and water content used to reproduce these materials (for example, details such as the age of the bottle and the supplier would be useful to record). As a whole, the session on crystal growth gave a well-rounded view of the variety of factors that must be considered when trying to crystallise a range of different compounds.

Alexandra Longcake
Newcastle

I arrived at the University of Sheffield on the Monday morning ready for the annual conference to begin, this was my first time attending a non-school conference, so I was very nervous and unsure of what to expect. The conference consisted of two meetings, the YCG satellite meeting, followed by the main meeting which started at midday on the Tuesday. The whole conference covered a large variety of topics on research I previously never knew much about. It was great to get exposure to these methods and techniques as an early stage crystallographer and has opened doors for future project developments.

The YCG meeting kicked off with **Mark Senn** (Warwick) who gave a talk on symmetry decomposition analysis. The meeting then continued with talks from early stage crystallographers covering a diverse range of areas in the crystallography industry including MOFs, perovskites and phase transitions.

Some highlights that were of great interest on Monday included **Phillipa Partridge** (Edinburgh) and **Eliza Dempsey** (Edinburgh). Phillipa explained her research of the disorder-to-order reversible phase changes that occur as a function of temperature changes. Later in the day, there was another talk by Eliza about how fluorine doping of the niobium complex can induce negative thermal expansion. The YCG meeting was brought to a close with a virtual talk with **Lauren Hatcher** (Cardiff) who gave an overview of photoswitchable linkage isomers and updates on a new time-resolved diffractometer, currently being developed at Cardiff University.

The main meeting started on the Tuesday afternoon, with parallel sessions running for most of the time. I attended the Crystal Growth Session where there was a really interesting talk by **Katharina Edkins** (Manchester) explaining the fundamental theories for high quality crystal growth. Another interesting talk I attended, which aligned with work I am currently completing, was from **Cameron Wilson** (Edinburgh) where he discussed his CellVol code which can help detect subtle pressure induced phase transitions, by changes in void volumes. These phase transitions can be identified by data from Raman spectroscopy and diffraction experiments complementing each other.

The breaks between the talks and the poster sessions gave me the opportunity to network with fellow researchers from lots of different universities, discussing their work and discovering what their next steps are. It was an amazing environment to engage with other students and discuss the work that I have been completing recently. Moreover, I really valued the feedback and ideas on my project that I was given to allow me to work on in the future.

The whole conference was a great experience, it was lovely to engage with the crystallographic community and to put faces to the names of papers I have read so many times. I thoroughly enjoyed the whole experience of learning about other people's research and communicating mine. I am very fortunate to have had the opportunity to attend.

Freya Palmer
Newcastle

I arrived in Sheffield on the morning of Monday the 3rd of April for 2023's BCA and YCG spring meetings. I travelled on the train with nervous energy as I had been invited to present my research as a talk for the first time during my PhD. I made my way to the Edge building where people were starting to gather for the YCG meeting. It was a particularly sunny day for England, bringing smiles and excitement all around.

Throughout the YCG, it was incredibly encouraging to hear talks from other PhD students. My talk itself led to some fun scientific discussions, advice, and additions to my PhD's ever growing to-do list. I felt grateful to be a part of such a supportive community as an early stage crystallographer.

As members of the YCG committee, **Julia Gasol Cardona** (Strathclyde) and I chaired the flash presentations for those presenting posters that following evening. It was great to see so many people participate in this session and everyone did a fantastic job advertising their posters.

The BCA spring meeting itself ran over three days with lectures and plenaries. On top of this, three parallel sessions took place, allowing you to choose sessions relating to chemical, industrial, biological, and physical crystallography. I found it difficult to choose between these sessions and it was exciting to get a snapshot into the breadth of the field of crystallography by attending those sessions outside of my field of research.

The PCG session on phase transitions was one of my favourite sessions that I attended. I thoroughly enjoyed every talk in this session and in particular I left the talk by **Siân Dutton** (Cambridge) on Jahn-Teller distortions in $NaNiO_2$ feeling inspired to try some new techniques to quantify the disorder within my own systems. This was exasperated throughout the session on Powder Diffraction for Chemical Crystallography where **Charlie McMonagle** (ESRF) gave an interesting talk on a sapphire capillary cell at the ESRF, sharing some high pressure results collected with this in-situ set up.

The poster session was the biggest highlight of this meeting for me and an aspect of in person conferences I always look forward to. I thoroughly enjoyed catching up with people I had met at last year's conference and meeting some new faces. Talking to other crystallographers about their work, I was so encouraged to see everyone's projects progressing and the wide variety of research topics throughout the room. There's so much impressive research being carried out!

The last evening, we all gathered at the Student Union building for the conference dinner and cèilidh. Prizes were awarded, wine was drank, and a well deserved thanks given to the organisers of the BCA spring meeting. I look forward to next year's meeting already!

Phillippa Partridge
Edinburgh

I arrived in the University of Sheffield, one hour train from Manchester, for the BCA Spring Meeting 2023. It was my second time to attend the BCA meeting and I had fantastic experience there again, not only because of the thrilling presentations of the cutting-edge science and technology, but also the old and new friends that I met and made there.

The conference contained two meetings and the first was the YCG Satellite Meeting, starting in the afternoon of Monday 3 April. **Mark Senn** (Warwick) gave a wonderful talk on symmetry assisted insights into ferroic materials, as an opening lecture. On Tuesday morning, the plenary talk which impressed me most was given by **Lewis Owen** (Sheffield) who spoke on how to give a good science communication and presentation. The YCG meeting provided an amazing opportunity for young crystallographers to give a presentation of their work to peer researchers and the coffee break and poster session were good opportunities to communicate and make friends with others.

The main meeting programme ran for the next three days, with different parallel sessions. A particular highlight for me was the presentation given by **Colin Seaton** (Bradford) about caffeine-benzoic acid co-crystals, which was the system that I had researched on. It was fascinating research and the methods they had used were very inspiring.

I was very honoured to have a poster presentation during the conference to introduce my work. I was also pleased that many researchers especially those working on co-crystals were interested in my research and came to talk with me.

There was plenty of time for well-scheduled networking events such as a grand conference dinner and cèilidh on the last evening of the conference, providing larger space and relaxing atmosphere for social work. Additionally, the exhibition and the networking events were great opportunities to learn about the new equipment from the sponsor companies.

The conference closed on 6 April, and it was a wonderful event to attend. It widened my research horizon on crystallization in many different fields and I was inspired by the researchers and their ideas and research methods. Since I am in my final year, it was a great event to attend to help my decision on what I am interested in and would like to do in the future.

Yichun Shen
Manchester

A new national facility for crystal structure analysis by electron diffraction

FOR over 100 years we have been using X-rays for crystal structure analysis to the point that the technique is fundamental to chemical characterisation, ubiquitous and relatively routine for many samples. However, there are still limitations – you need to be able to grow good micron-size crystals. For those systems which only produce crystalline powders it is not possible to access the same level of atomic resolution, structure and bonding information as those which grow single crystals more easily. Using electrons as the radiation source for these experiments gives the best possible answer to this problem, as they interact with solid material 10,000 times more strongly than X-rays do! For decades, diffraction experiments have been possible in transmission electron microscopes, but technical limitations meant that it was extremely difficult to use this information to go as far as solving crystal structures. The necessary technology, mainly around detectors and control software, has recently moved on and is highly complementary to what we can achieve with X-rays. This has recently made electron diffraction a viable technique for routinely obtaining single crystal structures from *nanocrystals* i.e., an order of magnitude smaller than those we can currently measure, even using synchrotron radiation. This is a game-changer for solid-state inorganics, pharmaceuticals, and MOF chemistry, but also for any compounds which stubbornly refuse to grow larger crystals!

Recent funding awarded via the EPSRC Strategic Equipment programme will now enable the universities of Southampton and Warwick to partner with Rigaku to build a **National Electron Diffraction Facility** which will be part of the UK National Crystallography Service (NCS, www.ncs.ac.uk). It will be the first dedicated instrumentation of its type in the UK – Warwick and Southampton will each get a Rigaku XtaLAB Synergy-ED instrument (https://www.rigaku.com/products/crystallography/synergy-ed). The facility will build on existing expertise, with national service delivery in Southampton, complemented by technique development in Warwick.

As well as determining the structures of hitherto intractable samples, over time we will be developing other techniques already well established in electron microscopy to answer bigger scientific questions. For example, energy dispersive X-ray spectroscopy will be incorporated to simultaneously assess chemical composition of the sample and enable coupled structure – chemical mapping. From the first days of operation, we will be able to collect low temperature data, which improves the quality of data collected and will mean that we can manipulate and then study highly volatile compounds/materials at liquid nitrogen temperatures. But as the facility matures it will also explore a number of other sample environment options: such as high temperature and gas cell to complement and drive existing X-ray based dynamic crystallography via electron diffraction.

*NCS Coordinator, **Dr Robert Bannister**, gets hands-on during a XtaLAB Synergy-ED demo!*

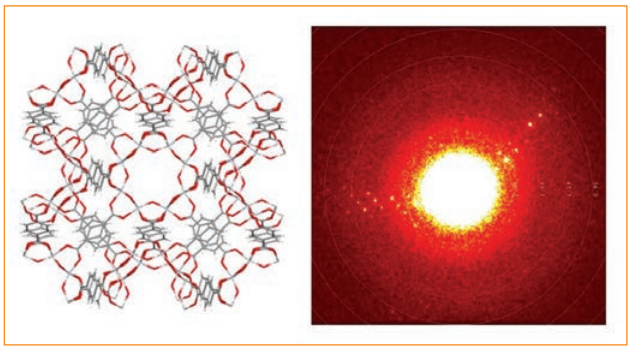
***Simon Coles** and **Richard Beanland** finally meet the XtaLAB Synergy-ED 'in-person' during a Rigaku Oxford Diffraction User Meeting (October 2022)!*

The success of the NCS is based as much on the expertise of its staff as the advanced instrumentation it uses. The facility will benefit from the expertise of Research Technical Professionals (RTPs), both through a dedicated RTP recruited to each site, and from the leadership of Dr David Walker as the Warwick lead. Amongst many activities, these RTPs will be critical in developing the technology, sample protocols, running experiments, training new users and data analysis.

Over this summer, we anticipate installing and commissioning instruments at both sites – in fact by the time you read this we hope to have completed our first experiments. A significant proportion of the available instrument time over the two sites will be dedicated to use by the whole UK research community. Access to the facility will be managed via the existing NCS application process, which runs biannually for the January-June and July-December periods. Short applications will be accepted, and we will provide a mail-in service for a small number of samples of a one-off or urgent nature. You will also be able to apply for a 'shift' on an instrument, which we see as supporting project-like activity where larger numbers of samples can be examined for departmental crystallographers, big research programmes, etc. As this is a relatively new technique, we will establish a training programme and eventually support online monitoring/control of experiments. Industry access is also very much supported – please contact us for a more detailed discussion of what can be achieved.

Initially we expect demand to be high and so it will be necessary to be selective about what work can be undertaken in order to provide equitable access to as many of the UK research community members as we possibly can. Applications for use will be reviewed and moderated by our Strategy and Allocations Panel who will produce a ranked priority list for us to work through. We intend to begin offering national access use from 1st July, beginning at low levels as we establish the equipment as a full facility and ramping up to be at full capacity by January 2024. Up-to-date information about this process can be found by visiting www.ncs.ac.uk/NEDF.

University of Southampton:
Robert Bannister, Simon Coles & Mark Light
University of Warwick:
Richard Beanland, David Walker & Richard Walton
Rigaku:
Mark Benson, Robert Bucker & James Gordon



The nano-crystal electron diffraction pattern and resulting structure of a Ti-MOF used as a test sample.

Robert Bannister and Simon Coles, during a XtaLAB Synergy-ED demo in February 2023.

What did you do in the war, Prof?

THIS phrase came to mind last summer when I was trying to get away from it all in Western Scotland. The prime reason for the trip was to 'assist' in celebrating the 'formal' reopening as a community pub of The Old Forge – an isolated pub in Knoydart accessible only by a long hike from Kinloch Hourn or a boat ride from Mallaig. Following a very successful 'assisting' at the opening, we retired back across Loch Nevis and down to nearby Arisaig for a couple of days pottering about.

As there was a 'visitor centre' in Arisaig (the 'Land Sea and Islands Centre' https://www.arisaiginfo.org.uk/), we popped in to see what was on offer there. In addition to the kind of exhibits you might expect, such as on local history and wildlife, there was also a strange collection of odd pieces of kit and photos of guys in military uniform. It turned out that nearby Arisaig House was requisitioned during World War II for use by the Special Operations Executive (SOE) to train agents that would be inserted 'behind the lines' to carry out sabotage operations or assist local resistance movements.

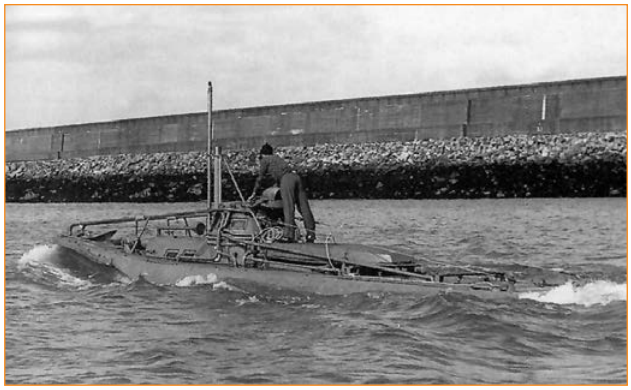
So what's this got to do with Crystallography? Nothing obvious, but then, browsing over a set of bookshelves I noticed one[1] with a name on the spine that I recognised: Douglas Everett' He was Professor of Chemistry at Bristol in 1967, when I gave my first conference talk at a Faraday Society Discussion on Liquids that year. At that meeting, Everett responded very positively to my talk, not only encouraging me in my Ph.D. work, but also made the first attempt in the discussion to estimate the configurational entropy of the random close packing of hard spheres[2] that was the core of my thesis.

Intrigued, I picked the book off the shelf and started browsing through it. Clearly Everett was a major figure in the SOE, but also two other names stood out – two eminent crystallographers who were also deeply involved in these clandestine operations.

The first was Gordon Cox[3], who the oldies amongst us will remember joined William Bragg at The Royal Institution in the early days of crystallography where he tackled the structure of benzene. He moved on, via Birmingham (where he worked on the structure of vitamin C, and of explosives!), to Leeds, from where a stream of structure determinations followed. In 1932 he was recruited to strengthen the scientific basis of the research work of the SOE at 'Station IX' in Welwyn – as he had led an Advisory Group of the Ministry of Supply where he was involved in problems of explosives production[4], this seemed to be an appropriate appointment. As Director of Scientific Research, he chaired weekly meetings of senior staff to assess ideas and proposed projects. Later in the war, he went to France for liaison meetings with the Underground on V2 rocket sites and counter sabotage activities, revealing valuable evidence on a Belgian resistance group's highly successful sabotage work during the occupation.

From my (admittedly limited) interactions with him when a young lecturer, I don't think he would have appreciated being called by his SOE nickname of Pippin!

The other name in the book that rang a loud bell with me was that of Durward Cruickshank. He was recruited straight from an engineering course at Loughborough during one of C.P. Snow's travels round the universities looking for talent to strengthen the Allied war effort. Known within SOE as Dagwood (!), he was involved in the design and testing of the 'Welfreighter' (Wel- from Welwyn, the location of Station IX), a semi-submersible vessel that was intended for transporting up to a ton of stores close in to a secluded enemy-held shore. According to Everett[1], who was Chairman of the Trials Committee, the sea trials of Welfreighters that were undertaken at Fishguard (see figure) were not without their hazardous – and light-hearted – moments: copies of the book are still available on Abebooks if you want to follow these up (or drop me an email!). I only wish I had known about Durward's war exploits during our meetings to get his side on these stories, which I suspect would have been even more amusing!



Durward Cruickshank during a Welfreighter speed trial in Fishguard Harbour.

Continued overleaf

1. Fredric Boyce and Douglas Everett. 'SOE the scientific secrets'. Sutton Publishing, Stroud, 2003.
2. D.H. Everett, *Discuss. Faraday Soc.*, **43**, 82-83, 1967.
3. https://www.iucr.org/people/crystallographers/ernest-gordon-cox-1906-1996.
4. Apparently he was intrigued by the fact that in the then recently discovered explosive PETN (pentaerythritol tetranitrate), the four arms of the molecule were arranged in the form of a swastika. Apparently, he commented that this might symbolise the role of PETN in the fight against Nazism!

There are many other scientists mentioned in the book, but I picked out only two others with apparent crystallographic interests. Gordon Claringbull (after whom the mineral Claringbullite was named), was called in from his position as Assistant Keeper at the Natural History Museum for his interest in explosives. And Francis Arthur Freeth, an industrial chemist who applied the phase rule to predict the ideal conditions for the crystallisation of ammonium nitrate from a solution of ammonium sulphate and sodium nitrate, and so improve the production of this – obviously very important – material.

I don't know about you, but my father wasn't very keen to answer the question: 'What did you do in the war, dad?'. Now of course it's too late to push him further on this. And also sadly too late to talk with Gordon Cox and Durward Cruickshank about their work during the war. But reading just a little something about the work they did in SOE did shed some light on the contributions made by these two eminent crystallographers.

John Finney
UCL

Locating a surviving Hilger & Watts Y190 linear diffractometer

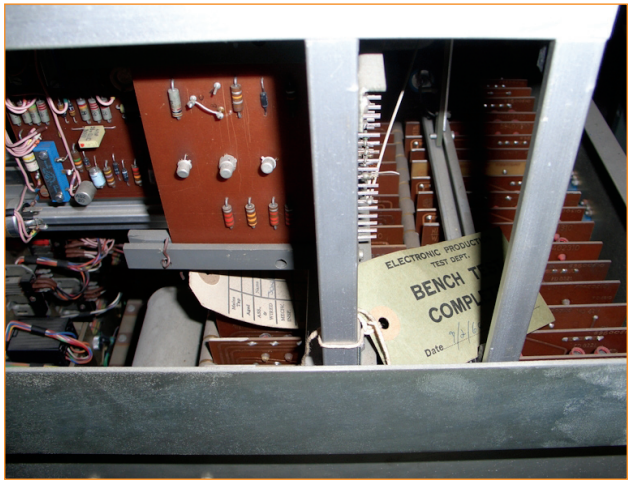
AROUND 2 – 3 years ago I started compiling some history of the diffractometers designed by the late Dr Uli Arndt (Cambridge) which were manufactured by Hilger and Watts (H&W) Limited in Camden, London during the 1960's (J. Cooper. 2020. *Crystallography News* 153, 20-22). This generated some interest from members and led to a surviving Y290 four-circle diffractometer being located at the University of Galway (P. McArdle. 2021. *Crystallography News* 156, 22-23). This instrument is one of the later, more automated diffractometers which were made from the mid-1960's to early 1970's, having superceded the earlier linear diffractometer that H&W marketed as the Y190 model. John Low in Dundee very kindly pointed out that a Y190 at the University of Aberdeen had been placed in the University Museum during the late 1970's and a search of the web suggested that a Y190 operation manual was in their collection. Hannah Clarke, Assistant Curator of the Museums and Special Collections at the University of Aberdeen, has since very kindly assisted in locating the instrument, which is now in off-site storage, and has sent the accompanying photographs, confirming that it remains in very good condition. I am very grateful to Hannah for persisting with the task of locating the instrument in spite of the numerous difficulties caused by the Covid-19 lockdowns over the last two years.

Quoting from **Derek Coggrave**, a former H&W engineer: *"The electronics for the Y190 was very basic stuff and the positioning of the axes was controlled by uniselectors – they were the devices used in telephone exchanges to select phone lines. If I remember correctly the ones used had fifty connections and they clicked round to select the amount of movement on the axes. They had to be lubricated regularly otherwise a poor connection could result in the stepper motors finishing up in the wrong place. They were a nightmare to install as one had to test for such errors over several hours. The machine might work for several hours or even a day and then suddenly start misbehaving. And, of course, there were thousands of soldered joints and any one of those could be dry. They could work for hours or days and then go intermittent. Those were the days of germanium transistors. They were very unstable and very sensitive to overheating. In many cases they were borderline between working and blowing up."*

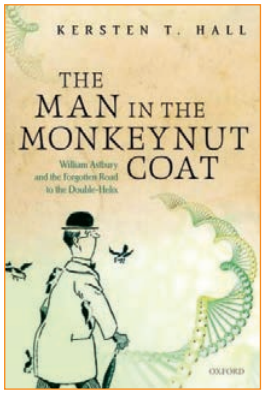
"What is surprising is that with the very limited technology available at that time - valves were still present in much of the electronics - a quite extraordinary mechanical computer and a bagatelle of electronic components resulted in a machine that collected a great deal of useful data. All down to some inspirational thought by the designers."

Thus to conclude, it seems to me to be very fitting that a surviving example of each of the two diffractometer designs which Uli Arndt conceived has now been found.

Jon Cooper
UCL.



A surviving Hilger & Watts Y190 linear diffractometer emerges from under the dust sheets in the University of Aberdeen Museum. The images are courtesy University of Aberdeen Museums and are reproduced with permission.



The Man in the Monkeynut Coat

by **Kersten T Hall**

Oxford University Press, 2014.
Pp ix+256.
ISBN: 9780198704591

THE amusing picture on the book's cover of the puzzled man afflicted by birds and a wandering helix may attract attention in the bookshop, but perhaps risks failing to attract readers to an extremely well-researched book about William Astbury and the central role he played in the development of the field of molecular biology. Among the earlier scientists who laid the foundations of the studies of molecular structure were William Henry Bragg and his son William Lawrence, who showed how X-rays could be used to determine the arrangement of atoms in molecules; the father (later Sir William) was Professor of Physics in Leeds and later became Director of the Davy Faraday Laboratory of the Royal Institution in London, where Astbury became a research fellow; later, Astbury himself moved to Leeds and the younger Bragg, now Sir Lawrence, to Cambridge. However, the development of 'molecular biology' required not just basic physics, but also an understanding of biological processes and of the chemistry that underlay the assembly and functioning of complex molecules. This involved a number of strands of information – Kersten Hall gives a thorough account of these sources and interesting information about the scientists who provided them, often with details about their personalities. A number of false trails, misunderstandings and clashes of personality impeded the development of the field and, rather sadly, Astbury who had played a central role was not among the fortunate few who were rewarded with Nobel prizes to celebrate the explanation of the functioning of living organisms through knowledge of the 3-dimensional structures and properties of proteins and nucleic acids.

Astbury came from relatively humble beginnings in the Staffordshire Potteries. His schooling led to his love of both science and music, and he started on a degree in Cambridge. However, this was at the start of the First World War and after just two terms he was called up for military service. He was sent to join the Royal Army Medical Corps in Ireland – and this resulted in his first acquaintance with X-rays, in their use for diagnosis of injuries. He also met his future wife while in Ireland.

After the war, he finished his university studies in Cambridge. By this time, both Braggs had moved from Leeds; William to the RI in London, where he initiated studies of organic molecules and Lawrence to Manchester, where he concentrated on inorganic substances. Astbury was appointed to a research post in Bragg's group at the RI, another post there being filled by Kathleen Yardley (later Lonsdale) and the two collaborated, one notable achievement being what became the International Tables for Crystallography, a compendium of the possible spatial and symmetrical arrangements of atoms in crystals.

Preparing for a lecture on the 'The Imperfect Crystallisation of Common Things', Bragg asked Astbury to take X-ray photographs of a number of naturally-occurring fibres such as human hair and cotton; these showed that their molecules had regularly repeating order along their lengths. This stimulated Astbury to believe that the molecular architecture of life itself could be studied by X-rays. The opportunity for him to do so arose in Leeds, where, following the establishment of the Wool Industry Research Association's laboratory to develop improvements in textile production, the University's Department of Textiles decided to appoint a physicist to conduct basic research in the field and Bragg was pleased to continue his relationship with Leeds by nominating Astbury for the post. Having arrived in Leeds, Astbury found it was a tedious business to set up the X-ray equipment, but eventually he and collaborators studied a variety of fibrous proteins, initially of the keratin family. Although these structural proteins are important components of all living systems, made up from a chain of amino acids, it was unclear how they utilised the different amino acids from which they were formed.

However, an important property of wool is that it can be stretched or shrunk, and Astbury found that this resulted in a change to the pattern of X-rays diffracted by the fibres; he deduced that this indicated the chains could be folded in two different ways, alpha (folded) and beta (stretched). Another biologically important fibre is silk, which showed an X-ray pattern like stretched wool. It was a vitally important deduction that the properties and functions of biologically important molecules could be affected by changes in their shapes. It was also known that soluble proteins such as haemoglobin could be 'denatured' into linear forms which were non-functional; Astbury toyed with the idea of studying them, but agreed to concentrate on the fibrous materials, leaving his former RI colleague J D Bernal to study them in Cambridge.

Astbury's view of the importance of molecular structure in biological organisms led also to the realisation that, as similar structures were found in different organisms, this implied that the evolution of different species was effected by the copying of fundamentally important functional molecules. Following from Miescher's work in the mid-19th century, it was known that another type of long polymeric molecule was a fundamental component of living systems: nucleic acids. They seemed rather boring substances, composed of just 4 monomers with similar properties, unlike proteins with their 20 amino acids having a variety of properties. Astbury decided that it would nevertheless be worth studying nucleic acid structure by X-ray diffraction and he was fortunate to be able to offer a post to a physicist from Lawrence Bragg's group in Manchester, Florence Bell, who obtained X-ray photographs having a very

strong reflection on the vertical axis, implying that atoms in the fibres tended to be spaced regularly from their neighbours 'like a pile of pennies'. The other features in the photographs were rather blurred, so it was not possible to work out how the atoms were connected. Astbury and Bell were however 'ecstatic' in finding that the regular repeating distance between atoms was exactly the same as the repeating distance as that in one of the forms of wool keratin, suggesting a structural relationship between nucleic acids and proteins. Unfortunately, Astbury and Bell were unable to show what this might be. Sadly, the World War now intervened, with a variety of consequences. Bell was called up for war service and eventually married an American.

During the war, the American Oswald Avery proved that it was nucleic acid that was the 'transforming principle' responsible for heredity and Astbury pondered about the possible structural relationships between nucleic acids and proteins that might lead to nucleic acids directly determining the structures of proteins. He had by then become recognised internationally, nationally and in his own University, which appointed him as 'Professor of Biomolecular Structure'. But he then found difficulties in getting the funds required to support a research programme in his new department. Despite some initial encouragement from the head of the Medical Research Council (MRC), there were now new entrants into the field, including some with physics backgrounds who had contributed to the war effort, but now wished to apply science to peaceful research. They included John Randall, who was establishing Biophysical Research at King's College, London. In addition, Lawrence Bragg had obtained support from the MRC in Cambridge, where he had moved from Manchester. The upshot of their applications for MRC funding was that Randall obtained funding, but Astbury failed to do so. It's unclear whether Astbury was over-confident and had not presented his case well enough. Astbury's disappointment by his failure to obtain funding would undoubtedly have been compounded by Linus Pauling's deduction that the alpha keratin model that Astbury had proposed was incorrect, with the protein chain actually folded into a hydrogen-bonded helix.

Although the facilities of his building in Leeds were rather inadequate, Astbury nevertheless did eventually obtain funding, leading to the acquisition of one of the first electron microscopes in the country. At a meeting in Naples in 1951, Astbury met Maurice Wilkins, Assistant Head of Randall's laboratory, who in the meeting had shown X-ray photographs from nucleic acid fibres that he and his student Raymond Gosling had obtained; Astbury congratulated him on their better quality than Florence Bell's. What is strange is that later the same year, Astbury received some nucleic acid samples from Erwin Chargaff and he asked his research assistant Elwyn Beighton to obtain X-ray photographs from them. Beighton's diagrams were much better than those of Bell but, inexplicably, Astbury neither published them nor presented them at a conference. Had he done so, the name of Astbury might well have become associated with the 3-dimensional structure of DNA and its biological role.

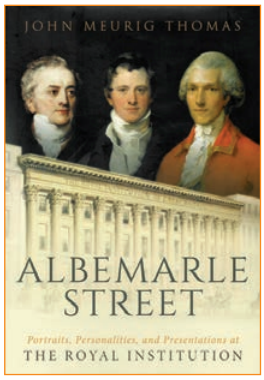
He did, however, become interested in another biological phenomenon – the wave-like movements of bacterial flagella. He remained convinced of the importance of structural changes as playing a vital role in biological function but he was unsuccessful in finding direct physical associations between nucleic acid and protein molecules, such as occurred in the sliding filament relationship between the polypeptides in muscle function.

Although Hall devotes considerable space to the competitions and collaborations that finally led to the establishment of the 3-dimensional structure of DNA and the role of the molecule in living systems, Astbury had played little part in them and with his love of music, he wrote that "above all molecules, the thread molecule is the chosen instrument in the symphony of creation" and our knowledge of biological molecules could help us to "build our world anew, perhaps through the rise of novel industries based upon the deliberate manipulation of these giant molecules", giving as an example the overcoat made from Ardil, a protein extracted from monkey nuts (pea-nuts) following his collaboration with scientists at ICI (Imperial Chemical Industry) in the 1940s.

Hall's book closes describing the concerns of some scientists that molecular biology, developed by people with a love of gaining an understanding of the evolution and properties of our constituent molecules, might result in the value of human life just being reduced to complex chemistry. But Astbury's words were "I feel that there is something much greater behind it all – don't ask me what. I don't know."

Hall has provided extensively researched accounts of the many scientists who contributed to the development of the field that Astbury termed 'molecular biology', though surprisingly there is little about his 'domestic' environment, apart from his love of music. Indeed, rather oddly, the first chapter of the book includes a brief account of the personalities of the scientists who carried out the successful structural studies of DNA which resulted in Astbury not receiving a share of a Nobel prize in the field that he had initiated. But this is an excellent account of molecular biology and Astbury's role in its history.

Anthony C T North
Leeds



Albemarle Street. Portraits, Personalities and Presentations at The Royal Institution

by **John Meurig Thomas**

Oxford University Press, 2021.
Pp xix + 263.
ISBN: 9780192898005
DOI: 10.1093/oso/9780192898005.001.0001

THE *Crystallography News* Editor regularly gets emails from publishers offering review copies of recently published books. When one of crystallographic interest turns up, after sometimes asking around for suggestions, I usually contact a BCA member who I think would be interested in reviewing it. This time, however, knowing a fair bit about The Royal Institution (the RI) – not only through attending their famous Discourses since the 1960s (yes – I really am that old…), but also being aware of its important role in the development of crystallography – I thought I might find it interesting to look at it myself.

Indeed I did find it interesting. Perhaps not primarily because of the crystallographic content – which I think the author Sir

John Meurig Thomas (the RI's Director between 1986 and 1991) could have made more of – but for much of the other material from which I learned a fair amount relating to wider scientific issues and some of the people concerned since the RI's foundation in 1799. Moreover, it was particularly interesting to read John's views on the current state and the future of the RI, which as many of us know, has been through very difficult times since the 1990s.

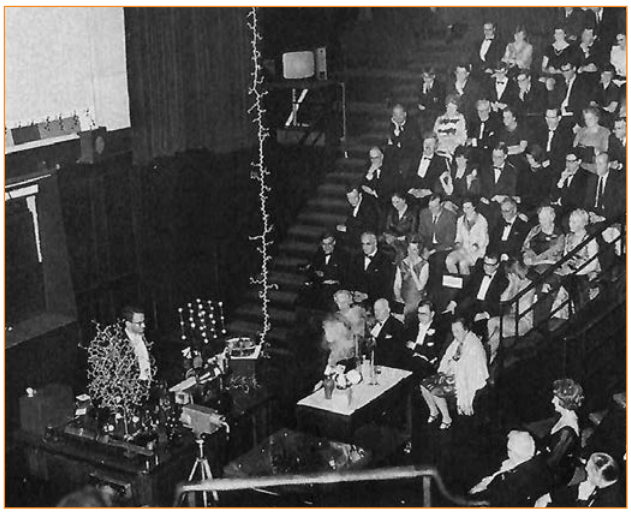
The subtitle of the book calls it a personal selection of 'Portraits, Personalities and Presentations at The Royal Institution'. The Preface casts the book as '...a collection of vignettes… laced with some personal reminiscences'. While much of the material indeed does focus on things that have happened at the RI, some of the issues, people, events and the science chosen hang only loosely on the RI peg, and often move far away from Albemarle Street. But no matter: many of the anecdotes are indeed interesting, informative, and illuminating – and from time to time amusing.

As one might expect, the main part of the book starts with the foundation of the RI by Count Rumford, following a meeting in 1799 hosted by the then President of The Royal Society, Joseph Banks. John tells us a great deal about Rumford and his non-scientific escapades which makes for a good read, though your respect for Rumford is likely to be considerably reduced after reading chapter 2 (I certainly didn't know he'd married Madame Lavoisier a decade after Lavoisier's execution – or that following 'marital difficulties', she had sabotaged his garden!). What did hit home to me was that the founding principles were 'diffusing the knowledge and facilitating the general introduction of useful mechanical inventions and improvements' and 'teaching by courses of philosophical lectures and experiments the application of science to the common purposes of life'. Yes – the Discourses are there, but the stress on 'applied science' was new to me. As John Thomas underlines, there was no mention of pure science in Rumford's vision – he saw the science done at the RI as being primarily intended to be useful.

Unsurprisingly, early chapters go into detail on Davy, Faraday and Rayleigh, which cover not only their most famous work but also demonstrate the breadth of their scientific interests and experiments. Following some accounts of some less famous scientists – for example the Welsh physicist William Robert Groves, who we learn invented the fuel cell in the 1830s. The link to the RI here is a bit tenuous – Groves didn't do the work there, but wrote to Faraday to tell him of his invention, and subsequently gave a Discourse at the RI in 1843. Similarly, the only connection to the RI of the early development of MRI is a Discourse by Raymond Andrew. And with respect to positron emission spectroscopy, there isn't even an RI Discourse mentioned. Noting that we can't really ascribe to the RI the work of people who give lectures there, nevertheless, these discussions are of general interest – though the explanation of MRI is not for even the strong-hearted non-scientist!

When we come to crystallography and the RI, I think Thomas both underestimates and overestimates the part the RI has played in its development. Though there are brief mentions of eminent crystallographers in a number of chapters, the main crystallographic discussion is in chapter 7. That chapter's title: 'Molecular Biology and the Crucial Role Played by the Davy-Faraday Research Laboratory in its Birth', alerts us to what is to come – that Thomas writes as if molecular biology was born in the RI. Sure – William Lawrence Bragg, when Director of the Davy-Faraday Research Laboratory (DFRL) at the RI, may have assembled the team under David Phillips that was the first to solve the structure of an enzyme (see figures). I'm old enough to remember the occasion when I was a Ph.D. student at Birkbeck, and it was indeed one of the key early advances in structural biology. But to claim – as the author implies – that this was the beginning of molecular biology seems to me to be going too far. Also I think implying that Kendrew's and Perutz's positions as being Visiting Readers at the DFRL was instrumental in their successes with myoglobin and haemoglobin is overdoing it! Though it is true that Uli Arndt, working with David Phillips at the RI, did design the linear diffractometer that Phillips's group used to collect the lysozyme data. I also found it interesting that Rosalind Franklin and Aaron Klug – then at Birkbeck – needed to use a rotating anode source at the RI to collect diffraction data on the viruses they were working on.

The team that solved the structure of lysozyme at the RI. L-R: ***Gareth Mair, Colin Blake, Louise Johnson, Tony North, David Phillips*** *and* ***Raghupathy Sarma****. Credit: Tony North.*



David Phillips *presenting his Friday Evening Discourse on the structure of lysozyme in November 1965. Credit: OUP.*

This chapter ends with Thomas arguing – as Rutherford and the Braggs had done – that it's vital for a centre of excellence to have expert technicians in a well-equipped workshop. He also relates Perutz's account that one of the secrets of the success of his and Kendrew's work at the Cambridge Laboratory for Molecular Biology (the LMB) was "the well-equipped workshop, manned by disciplined, dextrous, and gifted technicians, who could be approached readily by the research staff. The

research teams dined and drank tea and coffee together with the technical staff.". Memories of Birkbeck Crystallography in the 1960s come to mind.

Where I think Thomas understates the role of the RI is in the very early development of crystallography. In the early days under William Henry Bragg (Director of the DFRL from 1923 to 1942), major steps forward were made. For example, as well as developing both an early rotation camera from brass tubing, bicycle clips, an alarm clock and a bent nail (see *Crystallography News* September 2021 page 10), Bernal developed the Bernal Chart which was still being used to index rotation pictures in the 1960s. His solution of the structure of graphite was a significant breakthrough, explaining why graphite and diamond had very different physical properties. While Kathleen Lonsdale was at the RI, she solved the structure of benzene, showing it was a planar structure. These may seem simple problems today, but then they were at the forefront of structural science – and the RI was where they were solved. Gordon Cox (who, Thomas relates, took him to his first Friday evening Discourse in the 1970s and thereby introduced the future Director to the place!) was also there in the 1920s, taking data on aluminium acetylacetone. John Monteith Robertson spent two periods at the RI – in the 1920s when he initially crystallised and worked on sesquiterpenes and in the 1930s, during which period he solved the structures of many small organic molecules, several novel phthalocyanines, and used heavy-metal derivatives to solve the phase problem by isomorphous replacement, paving the way to determine novel structures. While some of these matters are mentioned in various parts of the book, it would have been good to have them brought together to demonstrate the importance of the RI in the early development of crystallography.

What we DO get in this chapter, as well as generously scattered elsewhere in the book, are some really interesting pictures of some of the actors – in their younger days. It's worth looking at the book just for both those and images of historic documents from the earliest days of the RI (though some of the image credits leave something to be desired).

The following chapters are rather bitty – though not necessarily uninteresting. Through famous Egyptologists such as Flinders Petrie and Howard Carter giving Discourses, we learn interesting things about Egyptomania at the RI. We learn that Roget (of Thesaurus fame) was Fullerian Professor of Chemistry and Physiology (and incidentally are told things that the professorship's founder, John Fuller MP, may not want to be in the public domain), and also about some of the contributions of T.H. Huxley and Peter Medawar. Chapter 11 discusses the author's candidates for 'The Most Beautiful Experiment in Physics'. Not surprisingly, the double slit experiment of Thomas Young (once Professor of Natural Philosophy at the RI) is up there, as is Faraday's demonstration of lines of force using iron filings together with several of Davy's experiments – all experiments first performed at the RI. Ewald's 1912 zinc blende and beryl X-ray diffraction patterns also get into Thomas's top ten – as does Eratosthenes's measurement of the circumference of the Earth in the third century BC!

The final chapter is very personal, filled with John Meurig's reminiscences of his days at the RI. This includes a page on Kathleen Lonsdale (with a picture of her and the late 1920s research team at the DFRL), as well as pen pictures of Margaret Gowing and Michael Atiyah. This latter item – which includes a great picture of Lord Kelvin's diagram of 'The First Seven Orders of Knottiness' – is followed by the text of the part of Atiyah's 1992 Anniversary address as President of The Royal Society on the responsibilities of scientists. John echoes those remarks. Other reminiscences follow on people (not all of them scientists) and aspects of RI operation (including entertaining Discourse speakers).

The book ends with an 'Afterword' which discusses a wide range of things, with more interesting photographs and historical images (one of them of a teenage Mike Glazer at a 1958 schools lecture given by Lawrence Bragg!). The final section is a brief statement of John Thomas's views of the present status of the RI. He starts by setting out the things the RI was renowned for over more than two centuries:

1. Original scientific research.
2. Dissemination of scientific knowledge among the general population.
3. The retention of the historicity of its ancient buildings, as the home of some of the greatest scientific discoveries in the world.
4. The maintenance of a high standard and genuinely popular series of Christmas Lectures.

As he says, it's no secret that many significant changes have been introduced at the RI from the early 1990s. He is happy that the RI retains an outstanding reputation insofar as popular lectures are concerned. He is less happy with the Christmas Lectures. Whereas previously there were six lecture-demonstrations in each series, this is now reduced to three or four, a number which he thinks means the detailed science that can be conveyed to the general audience is limited. With respect to original research, in his view this is a "mere shadow" of what the DFRL did from the 1900s until ca. 1995. To quote him: "It is no longer the cradle of discovery and innovation. This saddens me." The workshop no longer exists, and offices which "hitherto were occupied by scientists are now rented out for other purposes.". His final words: "Unless major changes of policy are made in the near future, I believe that there is little prospect now of regenerating the DFRL as a world-class stand alone centre of scientific research."

How science is done has, of course, changed over the last few decades, in ways which raise problems for a stand-alone institution like the RI. But part of me is still sad that a better 'solution' to the present one cannot be found.

Whatever our views on this issue or the book's author (who died just after its completion), every scientist should get something really interesting and enjoyable from reading what must have been one of the last things John Meurig Thomas wrote.

John Finney
UCL

Celebrating Dr Olga Kennard OBE FRS, Founder of the Cambridge Structural Database, 1924 – 2023

It is with great sadness that we learn of the passing of Dr Olga Kennard. Her long, successful life was full of many achievements, including founding the Cambridge Structural Database (CSD) that is now a fundamental resource that supports the global development of new drugs and materials that benefit us all, is used in chemistry education, and the advancement of science. In this obituary for Dr Kennard we celebrate and recognize her many achievements in the scientific community.

Dr Jürgen Harter, CEO, CCDC, expresses his condolences and gives thanks for Dr Kennard's vision: "Our thoughts and condolences extend to Dr Kennard's family and friends at this time of great sadness. Not only is it a time for mourning, but it is also a time for celebration by everyone connected to the CCDC and the wider structural science community of Olga's many achievements, including the foundation of the CSD. This was made possible by her drive and determination to overcome the status quo with visionary foresight. I am sure many pharmaceuticals and materials that we all benefit from today would not have been discovered if it wasn't for Dr Kennard."

Born in Hungary, Dr Kennard moved to the UK in 1939 just before the outbreak of the second world war. After graduating from the University of Cambridge in 1944 she joined the Cavendish Laboratory under Lawrence Bragg as an assistant to Max Perutz in the Department of Physics. After completing the first X-ray structure at the Laboratory (albeit on a very small structure), Dr Kennard moved to London in 1948, and then to the Chemistry Department at Cambridge University in 1962. At this point it was difficult to solve larger structures with crystallography, and very unusual for crystallographers to be in a chemistry department. Crystallographers often experienced suspicion from more traditional chemists who thought this 'upstart subject' was taking over their territory.

Dr Kennard persevered and persuaded the department to purchase a diffractometer, the first to be used for small molecule studies. Working with a small but gradually increasing group, supported by the Medical Research Council, Dr Kennard and colleagues worked on a variety of medical compounds including antibiotics and (excitingly) the structure of adenosine triphosphate (ATP). As the volume of structural data increased, Dr Kennard along with Prof J. D. Bernal had a vision that the collective use of data would lead to new knowledge and generate insights: "We (sic. J. D. Bernal and I) had a passionate belief that the collective use of data would lead to the discovery of new knowledge which transcends the results of individual experiments."

Dr Olga Kennard giving opening remarks at the CCDC's CSD 50th celebration.

This vision led to the founding of the the CSD in 1965. From its humble beginnings, the CSD now contains over 1.2M small-molecule organic and metal-organic crystal structures. Continually growing, big-data learnings from the collective results are used globally to advance scientific research into pharmaceuticals, functional materials, catalysts, and more in both commercial and academic research. During her 1995 J. D. Bernal lecture, Dr Kennard had no doubt as to the future value of the database: "I think that the great ocean of truth is still in front of us and we will continue to discover new aspects of this truth."

Dr Kennard went on to lead the CCDC until 1997 and authored over 140 structures during her career. One of her first structures with coordinates was published back in 1963 and was a chlorobenzoate salt (CSD refcode MSCBZO). Her more recent examples include a uridine structure, which was published in 1991 (CSD refcode JOSCAV). Dr Ian Bruno, now Director of Data Initiatives at the CCDC, remembers meeting Dr Kennard on his first day at the CCDC in 1993: "I first met Dr Kennard in 1993 when I came to the CCDC to interview for what became my first job following my PhD. Frank Allen, then Deputy Director of the CCDC, led me to Dr Kennard's office and introduced me. I was immediately struck by her formidable sense of presence. In the years that followed, I came to appreciate her commitment to achieving the best for the CCDC and her consideration for those helping to deliver on its mission. She had a wit that could be as disarming as it was sharp and a curiosity that was still evident when I encountered her again much later in life."

"The Cambridge Structural Database preserves the legacy of a community, enabling data generated by crystallographers worldwide to be reused and applied by future generations. This lives on as Dr Kennard's legacy and as a testament to her determination and drive to establish the CSD as a respected and lasting resource much valued by the scientific community and benefitting wider society."

Dr Kennard's huge contribution to crystallography was recognised by many prestigious awards, prizes, and elections to learned societies. In 1987 she was elected a Fellow of the Royal Society and, in recognition of her work, there is the Royal Society Olga Kennard Research Fellowship in crystallography. An OBE for 'Services to Scientific Research on the Structure of Biological Molecules' followed in 1988. In 1993 Dr Kennard was elected a member of the Academia Europaea and a Doctor of Law honoris causa was awarded to her by the University of Cambridge in 2003. She won the Gmelin-Beilstein Memorial Medal in 2007, awarded by the German Chemical Society for scientists and scholars who have made an outstanding contribution to the history of chemistry, chemistry literature or chemical information. In 2020 Dr Kennard was awarded the twelfth Ewald Prize by the IUCr for "her invaluable pioneering contribution to the development of crystallographic databases, in particular the CSD." Recognition for Dr Kennard's huge contribution to structural

science continued right to the end of her life with the award by the Royal Swedish Academy of Sciences of the Gregori Aminoff Prize for 2023 for establishing a crystallographic database. Dr Kennard was due to receive the award at the Aminoff Prize Symposium at the end of March.

To commemorate Dr Kennard's passing and celebrate her life, a previously unpublished interview with her that was recorded in 2011 by William Town, former Chair of the Governing Board of Trustees, CCDC, has been released on the CCDC website as part of a Living History series.

Michael Francis
CCDC

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Alexei Vagin (1944–2023)

Doctor Alexei Vagin, who died on 25 March 2023, contributed greatly to the practice of X-ray crystallography for over 50 years. He organized the (sparse) computing services of the protein group at the Moscow Institute of Crystallography during the 1970s and 1980s, then after his move to Western Europe in 1994, made major software contributions for macromolecular structure solution, all now distributed through CCP4.

Alexei was born in 1944 in Perm, the most easterly city in Europe, located in the Urals near the natural borderline between Europe and Asia. His family had been evacuated there during the war, but they returned to Moscow for his education. For his degree he studied applied physics at the prestigious Moscow Engineering Physics Institute, specializing in mathematical techniques and computer programming. He started his scientific career in material science – his first publication in 1966 was concerned with the design of blast furnaces, but soon he became more interested in crystallographic method development and moved to the protein group of the Moscow Institute of Crystallography. He was part of the team that solved the structures of bacterial ribonuclease in 1977, catalase in 1979 and was the key player behind the computational part of the latter project where he applied non-crystallographic symmetry (NCS) for phase improvement. From then on, he was involved in almost all the protein structure analyses in the laboratory, developing and implementing many tools. Unfortunately, most of these developments were never written up as Alexei always considered this part of science too boring, a sentiment to which he was loyal for the most part of his life. His PhD thesis, awarded in 1982, described an improved and faster translation function for use in molecular replacement calculations. He organized the software into *BLANC*, a comprehensive package with almost all necessary programs and libraries for crystallographic calculations, from experimental phasing to molecular replacement and map calculations. Considering that there was an embargo on computing resources for all of the Soviet Union, and those available to the institute were scarce, he had to come up with and implement clever algorithms that were both fast and used limited amount of RAM.

In 1990 the scientific scene in Moscow changed dramatically. Funding there became tighter and as the Iron Curtain dissolved it was possible for Russian scientists to move to laboratories in the West with better funding and equipment for science. Many laboratories worldwide benefitted greatly from this influx of well trained, motivated young people from the Moscow Institute (especially the York Structural Biology Laboratory!) but it meant Alexei was witnessing the decline of a great institute. In 1994 he joined the exodus, taking an EU-funded position in Brussels as a member of the team working on *CRITQUAL*. The Biotech contract he joined was entitled: 'Integrated procedures for recording and validating results of 3D structural studies of biological macromolecules'. It brought together in a complementary manner several established European laboratories working in the field of macromolecular 3D coordinate provision and analysis. The insights provided into each other's practices, working approaches and problems proved invaluable. This contract was a delight – all the participants were excited by the challenge and the six-monthly face-to-face meetings positively 'fizzed'. Atomic resolution structures solved in Hamburg revealed that some of the underlying assumptions about protein conformation derived from the existing databases developed in the EBI and Uppsala were sometimes too restrictive, and Alexei in Brussels was able to quickly recast the new insights into a well designed computer readable form to be used within the refinement program framework being developed in York. He found an elegant solution to the problem of describing 'LINKS' – between peptides, nucleic acids, and to covalently linked ligands. The restraint formats (mmCIF) he helped design are now accepted as standard.

In 1998 when the Brussels funding was exhausted, he moved to York and re-joined an active crystallographic laboratory, where he stayed until his retirement in 2010. This was a wonderfully productive period for him, and the community of structural biologists continue to benefit from his work. The program *SFCHECK* developed in Brussels to assess the quality of the agreement between model and experimental data was modified for inclusion in the *CCP*4 suite. He contributed to further developments of *REFMAC*, advised laboratory members on programming problems, structure solution and partying. He was a highly sought-after tutor for training workshops, guaranteeing excellent teaching and good fun for all. But his life-long passion was for improving the methodology of molecular replacement. At one period when both Alexei and Jorge Navaza, the author of the *AMoRe* package, were working in York, it was tremendous fun to hear their on-going debates ranging from 'what are the best scoring functions?', to 'why my fast Fourier routine is faster than yours . . . '. In 1997 he published a description of a 'new' package, *MOLREP*, in the *Journal of Applied Crystallography* before releasing it through CCP4. It was in fact partly a re-issue of much work he had done in Moscow, dating back to his 1982 PhD thesis, and partly described in the Russian journal, *Kristallografiya*.

MOLREP contained many innovative features that exploited information easily obtained from the experiment. For example, the package was able to analyse the model-free Patterson maps to consider non-crystallographic symmetry (NCS) and pseudo-translation if present. Once a search model was selected, *MOLREP* then analysed its shape and modified the search procedures to take this into account. In this package, Alexei introduced a translation function which considered all possible symmetry equivalents together. He also improved

methods for searching for multiple copies and checked any solutions against the known NCS. Once a possible solution was found, the program checked whether it would pack, and positioned the symmetry copies to give optimal contacts for an assembly. One distinctive feature of Alexei's approach to software development was a user-centred perspective and he took pains to report results and data analyses with informative graphs and extensive text. *MOLREP* was an instant hit and is still widely used by crystallographers and electron microscopists. Searching the Protein Data Bank (PDB) for references to it yields the amazing score of 36 223 entries.

Once Alexei was reasonably satisfied with the software, he turned his attention to model selection. A search to match a new sequence against the many structures available in the PDB will often produce many closely related hits. Alexei designed a database, distributed first in the package *BALBES*, and later as *MorDa*. This weeded the hits to include only the best model, and then catalogued whether the model structure existed as an oligomer, whether it could be split into flexible domains, and then used this information to design an optimal search strategy.

Alexei will be remembered for his innovative science, and for his interest in and kindness to his many colleagues, both in Moscow and Europe. But of course, he was not just a scientist and the many friends who mourn him remember his humour, his generosity both at work and play, and his wide-ranging conversations. While still in Moscow, he was one of the very few laboratory members with a car, and he was the one who took his colleagues to the airport for their departure to join various crystallographic laboratories in Europe, USA and Australia. He had no children of his own but was very good with those of his friends – one of whom, a grown up artist now, designed the *MorDa* icon, a wise friendly cat face. He loved Russian culture and his Russian friends, but never Russian politics. He was rather a citizen of the world with a passion for French chanson and movies, and deeply in tune with British black humour which matched his own. He was also profoundly grateful to the NHS which cared for him until his last moments. But his real homeland was the international community of protein crystallography, and that is where he will be remembered with love and gratitude.

Eleanor Dodson
University of York

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Meetings of interest

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

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

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

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

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

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

23rd Jul 2023 - 29th Jul 2023
18th International Summer School on Crystal Growth
Parma, Italy.
https://isscg-18.unipr.it/index.php

30th Jul 2023 - 4th Aug 2023
20th International Conference on Crystal Growth and Epitaxy
Naples, Italy.
https://www.iccge20.org/

22nd Aug 2023 - 29th Aug 2023
26th Congress and General Assembly of the International Union of Crystallography (IUCr2023)
Melbourne, Australia
https://iucr2023.org/

5th Sep 2023 - 12th Sep 2023
EMBO practical course: Image processing for cryo-electron microscopy
London, UK.
https://meetings.embo.org/event/23-cryo-em-image-processing

9th Oct 2023 - 12th Oct 2023
JCNS Workshop 2023. Trends and Perspectives in Neutron Scattering: Future Instruments at Pulsed Sources
Tutzing, Germany.
https://www.fz-juelich.de/en/jcns/expertise/conferences-and-workshops/jcns-workshops/jcns-workshop2023

16th Oct 2023 - 31st Oct 2023
Cold Spring Harbor Laboratory Course on Macromolecular Crystallography
Cold Spring Harbor, US.
https://meetings.cshl.edu/courses.aspx?course=C-CRYS&year=23

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