Crystallography News

British Crystallographic Association

Issue No. 152 March 2020
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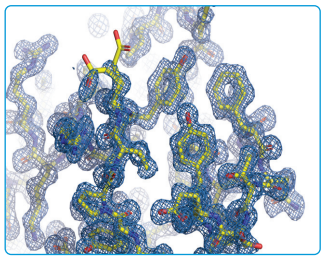

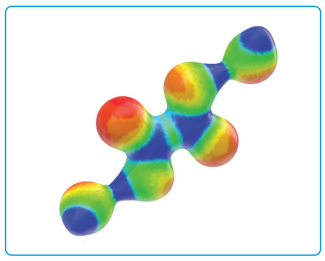

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British Crystallographic Association

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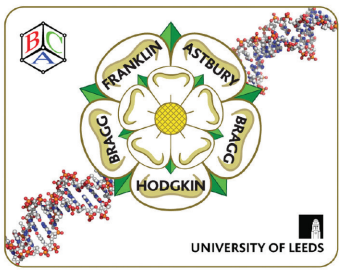
BCA members who are students/post-docs/junior or non-permanent staff are eligible to apply for bursaries to attend BCA Spring meetings and other crystallographic meetings. Applications should be made via the website: https://crystallography.org.uk/prizes/bursaries

Additional carers grants are available to BCA members at any career stage.

https://industrial.crystallography.org.uk/bursaries-and-awards/

Applications can be made now at the BCA and IG websites. For the IUCr 2020 please apply before 10th July.



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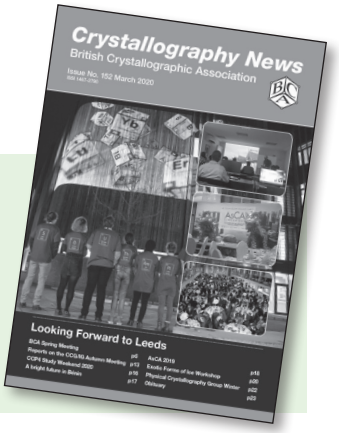
This month's cover:

The International Year of the Periodic Table draws to a close and numerous autumn and winter meetings reported.



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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 June 2020 issue are sent to the Editor to arrive before 25 April 2020.

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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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From the President

I was in Leeds before Christmas to give a lecture to the Leeds Philosophical and Literary Society in its bicentennial year. It was nice to be back at the institution where I spent over 20 years solving crystal structures, giving lectures and enduring the associated administration. The Leeds 'Phil and Lit' has a distinguished history, beginning with its founding in 1819 by 80 leading citizens of the city from various walks of life. These included local industrialists, bankers and merchants, immersed in the commercial life of the city, but also artists, clerics and doctors. In its early days, John Dalton came over from Manchester to give half a dozen lectures on his theory or atoms, molecules and chemical reactions. It supported the foundation of the Yorkshire College, the origin of the University of Leeds and founded an interesting museum, recently rehoused in the former Leeds Mechanics' Institute in Millenium Square. The collection is well worth a visit, and includes the 'Leeds Mummy'. The mummy of Nesyamun is one of the most remarkable in the UK.

Leeds is, of course, the home of crystallography, where **William and Lawrence Bragg** solved the first crystal structure. It is also where **Kathleen Lonsdale** showed that the benzene ring is planar, **Durward Cruckshank** pushed forward structure refinement and **William Astbury** championed the application of X-ray diffraction to biological materials. It is a perfect site for the 2020 Spring Meeting of the BCA.

Have you ever been scooped on a publication by another group, and does it really matter publishing second rather than first? I have had many conversations over lunch or coffee on this subject. The outcome of these discussions was frequently that being first is good, but with a feeling that a second paper close on its heels may still make an impact, and may even have advantages in building on the initial result. It was always a worry as a group leader that postdocs and PhD students need to work on high impact problems to get their careers off to a good start, but this often means 'hot' projects with the threat of the competition beating them to it.

Single-crystal crystallographic structure determination is particularly susceptible to this danger, because 'hot' structures can be targeted by several competing groups independently, and projects tend to have an unusual trajectory compared to many studies in the physical sciences, changing suddenly from 'zero to hero' in a very short time. Long periods spent in sample preparation, i.e. making crystals that diffract well enough, without awkward crystallographic complications, to solve the structure and construct an atomic model. The actual transition though data collection on a suitable sample to the model can be extremely fast these days, suddenly changing from a project with little in the way of publishable results, to the goldmine of chemical and physical data that a new structure can offer. There were a number of occasions during my career as a group leader, where another group published the structure that one of my postdocs or students was working on. If they were not progressing well towards a publishable result, I usually shifted them to a back-up project with better chances of success, but perhaps not such a hot topic.

It was because of this 'scoop anxiety' that a study by **Ryan Hill** and **Carolyn Stein**, *"Scooped! Estimating Rewards for Priority in Science"* available on the MIT website, caught my eye. They chose to use crystallography, and specifically the PDB, to study the value of being first to publish, based on paper citations and journal quality. They conclude that it is not winner-takes-all. Scooped teams are only slightly less likely to publish, and often in less prestigious journals, but if they do the papers pick up a 42% share of the total citations, and the effect on academic careers is only modest. Hill and Stein suggest that the obsession with priority in science reinforces inequality, and perhaps we should re-evaluate our attitudes and policies to take this into account.

The General Assembly and Congress of the IUCr takes place in Prague this August, so make sure you catch the early bird registration deadline of 15th May to avoid higher fees. The programme is typically wide and varied, with over 100 microsymposia and 36 Keynote lectures, covering aspects of crystallography from hard materials to biological macromolecules, quantum crystallography to social media, and combinations of techniques from neutrons, electrons, X-rays to NMR and direct imaging techniques. The cast of speakers is impressive, and the main problem promises to be how to choose which parallel sessions to attend. There is additional competition for delegates' attention outside the hall, where the sights of Prague beckon. Prague is a very attractive and interesting city to visit, with the castle as a 'must see'. I expect to see a strong cohort of UK crystallographers there.

As I write this column, voting is well under way for the elections to the Treasurer and Ordinary Member positions on Council. I hope all members have used their votes, recent political events having shown us that voting, or failing to vote, can have a serious impact on all our futures. The BCA election results will also be known by the time you read this.

The importance of voting is amply demonstrated by the landslide general election result gained by **Boris Johnson** just before Christmas. The now inexorable trajectory to BREXIT has worrying implications for many of us in the research community, with the changes to freedom of movement and access to EU funding programmes that this implies. We do not yet know what these changes will be, and will have to await the outcome of what are bound to be complex negotiations. The issue of Nature published on election day carried an analysis of the Conservative Party manifesto, concluding that the words 'research' and 'science' appeared more times than ever before, and there was a pledge to increase research and development funding from 1.7% to 2.4% of GDP. Our political masters are giving the impression that they understand the problem, but it remains to be seen if they can be trusted to deliver on their promises.

Finally, I look forward to seeing you all at the BCA 2020 Spring Meeting in Leeds.

Simon Phillips

BCA Council 2020

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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

WELCOME to another issue of Crystallography News! I'm afraid you are still having to make do with me in charge, but don't worry the end is in sight…!

I am delighted to note here that a worthy successor (I mean to Carl, not me!) has been found – and so we can get back to some semblance of stability and continuity! As of the next (June) issue, Emeritus Professor **John Finney** (UCL) will take over the reins. John tells me he has some experience of being a magazine editor and given his long standing in the community, it is clear he is eminently suitable for the position. I'll let John introduce himself in due course, however if you havn't bumped into him in the past I can reveal that early in his career he worked with one of the crystallographic superheroes, Professor **JD Bernal**, in the Crystallography Department at Birkbeck College. John has spent many years working in London, both at Birkbeck and latterly in Physics and Astronomy at UCL, but is also well known for the very significant positions he held at the ISIS Central Facility as it was being developed. So, John is therefore not only well linked in to the BCA community, but also has connections into several others.

I believe John has some thoughts on how our great magazine can be taken forward and while I leave it to him to stamp his mark as it were, I thought I would reflect a little on what I have learnt during my brief time at the helm. **Carl Schwalbe** took this job on whole heartedly – and essentially did it all on his own. This involved attending all Spring Meetings, at least two international conferences a year and autumn meetings – as a minimum. It's not just about meeting reports however, he saw opportunities for articles and cajoled people into writing, often also taking this task on himself. Carl also chased and coordinated and pulled everything together – four times a year. He did an immense and admirable job. In taking this role on for just three issues, I quickly realised its not sustainable to have just one person to field all the necessary tasks. However, as well as being a quality publication, this magazine is important for members as it provides a sense of belonging and we have a great community that really does come together. There are members that do step forward – each time it comes to the crunch and just when I begin to dread filling up the empty pages in front of me, all sorts of publishable material starts coming out of the woodwork! With a bit of organisation, we can begin to formalise a network of people that feeds up through the groups of the BCA and can enable anyone to readily contribute.

Everyone has it in them – we don't need all articles to be lengthy pieces, we don't need all articles to be intellectual pieces, some people make witty authors, while others are rather more matter of fact. What matters is that people put pen to paper, or take pictures – not just when at conference as a formal report, but also more in your everyday professional life! Crystallography News can equally accommodate short, pithy pieces that aren't the standard reports or advertisements – so please bear this in mind and if anything strikes you as interesting or worth sharing then please get creative and get in touch…

I embrace technology. One thing that I have been sceptical about though is flipping a magazine to go fully electronic – especially one with such a tradition and established, close-knit audience. Crystallography News, along with other similar professional society magazines, has always felt for me like the type of thing you reached out for to flick through when having a cup of tea. Well, technology has moved on and while I do find myself reaching out for something to flick through when taking a bit of time out, it now seems equally natural to do that with electronic materials and devices. Software, graphics and hardware have all moved on massively in the last few years – as has our culture and acceptance of the electronic medium. The only newspaper I read these days is the very occasional free one I pick up outside the tube if I am in London for a meeting. So, we have recently seen the IUCr Newsletter (*https://www.iucr.org/news/newsletter*) and with this winter issue our sister organisation the ACA's magazine, RefleXions (*http://bit.ly/ACA2020winter*), go fully electronic and thus freeing themselves from some of the shackles of paper. I feel the results are excellent and actually outstrip the traditional format – I urge you all to take a look if you haven't already.

We have just come to the end of the International Year of the Periodic Table (in a 'Freudian slip' in my last column I referred to this as the International Year of Crystallography – oops, lost a few years somewhere!). I engaged quite a lot with #IYPT2019 and thoroughly enjoyed it, particularly culminating in Chemistry Week (#ChemWeek2019) pushed by the RSC. At my university we joined several others in a very successful campaign across the country, which has made me reflect quite a lot.

The theme of the campaign was the sustainability of the elements in the periodic table – and targeting a particular audience, used the mobile phone as an example. Did you know that our mobiles contain about 30 different elements? Six of these elements are very scarce: Y, Ga, As, In, Ta and Ag – and I expect you can all name several other applications where these elements are extremely important. We will run out of these valuable elements in less than 100 years (much worse in some cases – and there are other elements not named here that will also run out in the same timeframe) if we carry on as we are? Did you realise that there are over 40 million unused mobile phones in the UK? We clearly need to understand and educate about this – and start to change our habits now…

On a related point – we are still looking for volunteers to help us fill up our periodic table of crystal structures, see: *https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/*. It's a really good way to get your name associated with a 'novel publication', you will be acknowledged on the CCDC website and they have recently launched a competition for the best entry *https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/element-in-progress/*). We expect to make some teaching activities associated with it, so your contribution will definitely live on well beyond the end of the year and if you have any thoughts as to what some of these activities could be, please do get in touch with me.

This issue tends to cover a period of the year when the nights are long and days short – also there is a concerted teaching period for those in academia, so I was a little worried about content. However, the group autumn and winter meetings do offer some distraction and in this issue we have a number of meeting reports that illustrate this! We also include a preview of the upcoming Spring Meeting and some interesting articles about CCDC activities. I hope you enjoy reading this issue and look forward to seeing many of you in Leeds. Editing this magazine has been a genuinely insightful process that has challenged me in new ways – and been a pleasure…

Simon Coles

BCA Corporate Membership

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

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

From 2019, corporate membership will be **£800.00** for one year.

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

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

Puzzle Corner

This month's Puzzle Corner is a classic format – a word search! It was set by **Finn Coles** (an 8-year old BCA member 'by proxy'). There are 15 crystallography-related words hidden in the matrix below for you to find…

A	G	E	M	O	K	I	E	R	N
D	Z	B	R	F	A	R	C	O	U
B	E	P	E	E	P	H	I	T	C
M	L	O	S	T	P	T	T	C	L
A	E	D	I	R	A	E	T	E	E
L	C	H	D	L	N	G	A	T	O
I	T	N	U	L	S	R	L	E	T
H	R	D	E	B	Z	A	C	D	I
C	O	C	R	Y	S	T	A	L	D
M	N	L	A	R	E	N	I	M	E

Hint: The house copy of 'Fundamentals of Crystallography' (Giacovazzo et al, IUCr, 1992), was used for inspiration – however we do not necessarily recommend trawling that reference to solve this puzzle!

Answers to December Puzzle Corner

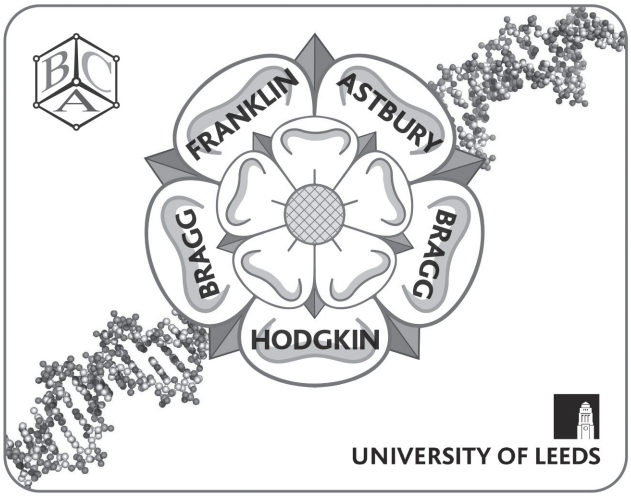
Here are three well known buildings whose shapes represent somewhat unusual polyhedra. Identify the buildings, the point group of their (idealised) symmetry and say whether they could represent a crystal form.

a – is the great pyramid of Giza, a tetragonal pyramid, point group 4mm, which could be a crystal form.

b – is the Pentagon in Washington, a pentagonal prism, point group 5/mm, not a possible crystal form

c – is the new World Trade Centre in New York, a square antiprism, point group mm, also not a possible crystal form.

BCA Spring Meeting 2020
6th – 9th April 2020, University of Leeds



Crystallography News BCA 2020 Spring meeting

6th-9th April 2020, University of Leeds

The 2020 BCA spring meeting will be held in Leeds this year and is almost upon us! So please check out the schedule and register to attend at *http://www.bcaspringmeetings.org.uk/58973* if you havnt done so already! Some details and titles for sessions are given below as a taster.

YCG Meeting Monday 6th April-Tuesday 7th April

Monday 6th April 2020: YCG meeting

YCG Plenary: 13:00

Dr Ehmke Pohl

Virus-X – from bio-prospecting to new structures and functions

YCG Research

(*Chairs: Natalie Tatum* and *Tom Roseveare*)

The YCG satellite meeting is an opportunity for all early career researchers in the field of crystallography to present their work in a supportive and friendly environment, which will be run by fellow early career scientists. There will be three sessions of talks on Monday, Session 1 chaired by Natalie Tatum/Tom Roseveare; Session 2 chaired by Elliot Carrington/Charlie McMonagle and Session 3 by Aly Abedeldaim/Tom Roseveare, along with posters and flash presentations.

Parkin lecture: 17.00

(*Chair: Charlie McMonagle*)

The Parkin lecture acknowledges the late Dr Andrew Parkin and his commitment to science and teaching. This prize lecture is awarded (announced early 2020) to a member of the YCG community who has demonstrated a passion for crystallography and communicating their research interests to a wider community. This talk, in the past, has covered a wide range of research topics and typically provides an interesting perspective on communicating science to a wider audience. Speaker to be announced in early 2020.

Tuesday 7th April: YCG meeting

YCG Plenary: 08.45

Dr Cheryl Doherty (GSK)

Exploring digital design for pharmaceutical solid forms

(*Chairs: Elliot Carrington/Charlie McMonagle*)

YCG/IG: A Career in Crystallography: Exploring the Interface of Academia and Industry

(*Chairs: Natalie Johnson and Rachael Wilkinson*)

Crystallography can lead to a wide range of exciting and varied careers. The start of this session will feature research talks exploring both academic and industrial research endeavours. This session will also offers a unique question and answer forum to discuss careers in crystallography via a selected panel of crystallographers who have taken different career paths. This session has been designed to provide greater information about the variety of careers available for young crystallographers, with attendees able to ask any and all questions they have about the careers to the panellists.

Tuesday 7th April 2020: Main meeting

BCA Main Meeting commences

Lonsdale lecture: 11:30

Dr Lucy Clark (Liverpool)

Quantum Magnetism and Crystallographic Complexity in Mineral Materials

(*Chair: Natalie Tatum*)

BSG Plenary: Rosalind Franklin Centenary Lecture 13.00-14.10

Professor Gabriel Waksman FRS (UCL/Birkbeck)

Mechanism of effector targeting by the Legionella type IV secretion system

(*Chair: tbc*)

14:20-15:50 parallel sessions

BSG: Structure-based drug design

(*Chair: Jane Endicott)*

Protein structures can assist drug development at all stages of the discovery pipeline, from choosing targets, through identifying hit matter, to supporting iterative medicinal chemistry to enhance potency, pharmacokinetics and pharmacodynamics. Historically, structure-based drug design has addressed well characterised active sites by identifying potential molecular interactions to inform subsequent chemical synthesis. Application of this approach has already contributed to the development of many potent and selective drugs. However, molecular targets with clear disease linkage can be extremely difficult to find, and for this reason more is being asked of structures in drug discovery campaigns. Examples of these new contributions include characterising and capturing biologically relevant protein conformations to help in the targeting of allosteric sites, and identifying novel classes of target that depend on protein-protein and protein-DNA/RNA/lipid interactions. The keynote lecture will review key advances in the field over the last decade and future possible directions while reflecting on what a drug discovery campaign looks like from the structural biologist's point of view.

Keynote:
Dr. Pamela Williams (Astex Pharmaceuticals)

Structure-based drug discovery: how did we get here and where are we going?

CCG: Advances in Software for Crystallography

(*Chair: Lucy Saunders)*

This session aims to reveal the latest and exciting developments happening in crystallographic software. We encourage abstracts from those in the community working on software for chemical crystallography research. We want to know about the latest tools on offer. This could be in the areas of data processing, structure refinement, property calculation or structure investigation to name a few.

Keynote:
Mairi Haddow (Heriot-Watt)

Can a solution for disordered molecules be automated?

BH Williams (Diamond Light Source)

Difficult data done quickly — dealing with the trickier cases of data reduction from single-crystal diffraction

E Schmidt (University of Oxford*)*

Possibilities for RMC modelling for single crystal diffuse scattering in molecular materials

PCG: Biominerals & Biomaterials

(*Chair: Julia Parker)*

From the exquisite morphologies of coccoliths and the incredible hierarchical architecture of bone, to the engineering of implants and joint replacements, the structure of biominerals and biomaterials plays an integral role in determining their properties and function. This session will examine the importance of structure in both natural systems and biomedical devices, explore how their composition and assembly controls physical properties and look at how this can be exploited in the development of novel bioinspired materials.

Keynote:
Melinda Duer (Cambridge)

The Bare Bones of Biomineralization: new insights into bone mineral composition, structure and formation

16:35-18:05 Parallel sessions

BSG: Time-resolved crystallography

(*Chair: Briony Yorke)*

Time-resolved crystallography allows the observation of molecular mechanism in real time, providing unique insight into the dynamics that link structure and function. The use of X-ray free electron lasers has pushed the boundaries of time-resolved crystallography, allowing structural changes to be determined with femtosecond time-resolution. The development of serial crystallographic techniques has also initiated a resurgence in synchrotron time-resolved experiments. This session will focus on the exciting developments being made at free-electron laser and synchrotron sources and the science that has been made possible by these developments. Contributions describing these and other structural time-resolved methods are welcomed.

Keynote:
Prof. Jasper van Thor (Imperial)

Optical control of protein structural dynamics by ultrafast X-ray crystallography

CCG: Electron crystallography

(*Chair: Simon Parsons)*

Electron diffraction is one of the mostly rapidly developing and exciting areas of crystallography. The publication of a number of recent papers describing its application in chemical crystallography has led to a great deal of comment and anticipation in the chemical community. The technique enables crystal structures to be obtained from samples with dimensions of the order of the few microns, or even 100s of nanometres. The strength of the interaction between electrons and matter that enables such small crystals to be studied carries with it the problem of multiple scattering, meaning that the kinematical model which has been so successful for X-ray and neutron diffraction no longer applies, and dynamical effects need to be taken into account. This session will give an overview of the most recent advances in the field and progress towards making electron diffraction a more widely used technique in the chemical crystallography community.

Keynote:
Lukas Palatinus (The Czech Academy of Sciences)

Structure refinement from 3D electron diffraction: where are the limits?

F Nudelman (University of Edinburgh*)*
Solid-state transformation and polymorphism in calcium carbonate crystallisation

A Stewart (University of Limerick)
Electron Diffraction: where does scattering stop and diffraction begin?

D Johnstone (University of Cambridge)
Multidimensional electron diffraction of organic solid"

PCG: Entropy & Structure

(*Chair: Anthony Phillips)*

In recent years, entropy has become an explicit target of materials design and synthesis: configurational and magnetic entropy can stabilise materials' structures or form the basis of their functionality. Understanding such disorder requires a variety of experimental and computational techniques drawn from the conventional crystallographic arsenal and beyond. In this session we welcome talks on all aspects of order and disorder: quantifying, designing, and exploiting entropy for materials ranging from high-entropy alloys to calorics.

Keynote:
Xavier Moya (Cambridge)

Giant caloric effects near structural phase transitions

PCG plenary: 18:15-19:00

Vaclav Petricek (Czech Academy of Sciences)

The role of crystal structure analysis in investigation of crystals with important physical properties

(*Chair: Anthony Phillips*)

Charles Morris on Campus Courtyard

Wednesday 8th April 2020

IG plenary: 08:45-09:30

Marcus Neumann (Avant Garde Materials Simulation)

Detecting and avoiding disappearing polymorph cases by crystal structure prediction

(*Chair: Helen Blade)*

10.15-11.45 parallel sessions

BSG: Enzymes

(*Chair: Wyatt Yue*)

Metabolic enzymes catalyse the biochemical reactions associated with survival and homeostasis in living organisms while the processes governing the behaviour of cells are mediated by tightly regulated cascades and complexes of cell signalling enzymes. Enzymes that perform various types of chemistry are therefore studied intensively in the fields of biochemistry and molecular cell biology. The essentiality of metabolic enzymes is underscored by various genetic and common disorders associated with their deficiency. Enzymes are also central to the field of biotechnology, where they are engineered to manufacture novel products or act upon novel substrates. This session will include examples of work in which structural biology methods are answering important questions relating to the activity and regulation of enzymes, with a view to understanding their functional, biotechnological and therapeutic applications.

Keynote:
Prof. Peter Moody (Leicester)

Using neutron crystallography to watch hydrogens in heme enzymes

PCG: <3D: Structure and Properties of Low-Dimensional Materials

(*Chair: Lucy Clark*)

There are many examples of crystalline solids whose structures feature quasi-one-dimensional chains or two-dimensional planes of atoms giving rise to low-dimensional interactions. This results in a diverse array of intriguing physical phenomena, from high-temperature superconductivity in, for example, layered iron arsenides to pronounced magnetocaloric effects in one-dimensional framework solids. Furthermore, since the isolation of graphene, there are has been an explosion of activity in the discovery and characterisation of different classes of two-dimensional crystals with remarkable properties that may underpin future advanced technologies. As such, this session is dedicated to showcasing recent developments of crystallography and complementary characterisation methods in the determination of the fascinating structure-property relationships in a variety of low-dimensional solids.

Keynote:
Maria Grazia Francesconi (Hull)

One-dimensional oxide and non-oxide materials

Mike Probert (Newcastle University) *The ENaCt Protocol – changing the face of small molecule crystallisation*

H Geddes (University of Oxford*) Structural characterisation of amorphous solid dispersions via Metropolis matrix factorisation of pair distribution function* data

H Moldovan (Cambridge Crystallographic Data Centre) *Probing the Interface Between Organic Crystals*

IG (joint with British Association for Crystal Growth): Pitfalls and challenges in industrial crystallisation

(*Chairs: Cheryl Doherty and Linda Seton)*

The control and prediction of crystallisation processes is a challenge but vital in many areas of industry. This session will cover practical and computational methods that aim to link understanding with the development of control strategies and predictive approaches. Talks from the perspectives of crystallisation, solid form and characterisation will be welcome.

Keynote:
Adam Keates (Syngenta)

Crystallisation in agrochemicals: The good, the bad and the ugly

Early career prize lectures 13:15-14:45

Winners to be announced prior to the conference.

15:30-17:00 parallel sessions

BSG: Computational biophysics

(*Chair: Matteo Degiacomi*)

To successfully carry out their task in an organism, biomolecules must interact with their designated substrates in a controlled manner. The function of a biomolecule thus emerges from its specific atomic structure and associated dynamics. Many computational techniques, as diverse as molecular dynamics simulations, homology modelling and protein-protein/ligand docking, can leverage crystallographic data to characterize molecular structure, dynamics and interactions. This session will focus on the application and development of such techniques.

Keynote:
Prof. Franca Fraternali (Kings College London)

Protein-protein interactions in health and disease: the importance of 3D structure

IG joint with CCG: Control and prediction of crystals

(Chairs: Helen Blade and Stuart Kennedy*)*

This session aims to cover a wide range of research used to control and predict crystals including both experimental and computational tools. We welcome talks on the control and prediction of solid forms, particle and mechanical properties by researchers from a wide range of fields of computational chemistry, informatics, solid state/crystallisation and materials science.

Keynote:
Sten Nilsson-Lill (AstraZeneca)

A Smörgåsbord of Predictive and Analysis Tools for Crystal Structures. Usage in pharmaceutical industry

PCG: >3D: Structure and Properties of Higher-Dimensional Materials

(*Chair: Phil Lightfoot*)

This session targets crystals and materials that go beyond a conventional description using three dimensional axes and indices. This includes aperiodic crystals, quasicrystals and incommensurately modulated crystals, structures, magnetic structures etc. Examples may include compounds exhibiting compositional, structural or spin disorder at the 3D level, but which is amenable to better description and rationalisation using 4D or higher dimensionality. We are interested in examples where the dimensionality may significantly affect materials' properties, as well as in the fundamental description and understanding of the higher-dimensional crystallography.

Keynote:
Fabio Orlandi (ISIS)

Superspace formalism and materials properties

Bragg Lecture: 17:10-18:00

Richard Henderson (University of Cambridge)
The continuing cryoEM revolution in Structural Biology.

(*Chairs: Simon Phillips and Paul Raithby*)

BCA AGM and conference dinner followed by ceilidh.

Thursday 9th April 2020

CCG plenary: 08:45-09:30

Franziksa Emmerling (BAM, Berlin)

Shaken not stirred: enhancing the flavor of mechanochemistry

(*Chair: Claire Murray*)

10:15-11:45 parallel sessions

BSG: Membrane proteins

(*Chair: Bonnie Wallace*)

Membrane proteins span a wide range of structural and functional types, ranging from multimeric complexes to monomeric or multimeric channels, receptors, and enzymes. They perform very important functions in cells and many are of interest for pharmaceutical development. However, they have proved to be challenging for structural studies due to their amphipathic nature, with both hydrophobic and hydrophilic domains, and the requirement for detergents, amphipols, nanodiscs, and other amphiphiles to solubilise, purify, and stabilise them. This session will include examples of work demonstrating how recent developments in sample preparation and in the complementary techniques of cryo-Electron Microscopy and X-ray crystallography are enabling structural studies of key membrane proteins.

Keynote:
Dr. Amandine Marechal (UCL)

Respiratory supercomplexes: what can we learn from yeast?

CCG: Chemistry in extreme conditions

(*Chair: Hamish Yeung*)

Crystallography has traditionally been a major technique with which to understand the structures and reactivity of molecules. This session focuses on how crystallography and other methods can reveal insight into phenomena that occur away from ambient conditions, such as very high or low temperatures, high pressure or electric fields. Think bonding, mechanics, distortions, phase transformations, changes in physical properties etc.—in and ex situ studies allowed!

Keynote:
Colin Pulham (Edinburgh)

Putting the Squeeze on Molecular Materials

PCG (joint with CCG): Structure Solutions from Powders

(*Chairs: Karen Johnston and Jeremy Cockroft*)

This joint session between the CCG and PCG explores structure solution from powders in a variety of organic, inorganic and mixed organic/inorganic systems. Despite considerable advances in the field, structure solution from powder diffraction is by no means routine and, increasingly, complementary methods are being used to aid structure determination. We are interested in recent examples where structure solution has been aided by complementary methods, including in situ and in operando techniques as well as total scattering methods. Examples where the combination of experimental and computational methods has resulted in successful structure solution are also of significant interest.

Keynote:
Kenneth Shankland (Reading)

Accelerating and enhancing the effectiveness of crystal structure determination from powder diffraction data

12.00-13.30 parallel sessions

BSG: Protein-protein interactions

(*Chair: Richard Bayliss*)

Cellular processes depend entirely upon interactions between proteins, either for the transient or regulated recognition of one molecule by another in interaction networks or the stable assembly of individual proteins into higher order complexes. Specific molecular recognition in protein-protein interaction networks is crucial in cell signalling while protein complexes function in cells as molecular scaffolds, hubs for cell signalling or as molecular machines carrying out concerted functions. This session will include examples of work in which structural biology methods have been used to determine the molecular basis of interaction between proteins and their assembly into multiprotein complexes.

Keynote:
Elton Zeqiraj (Leeds)

Structure and function of ubiquitin signalling complexes

PCG: Phase Transitions

(*Chair: Lewis Owen*)

Phase transitions are of critical importance to our understanding of a materials structure and its physical and chemical properties. This session will aim to explore a broad range of structural phase transitions; from crystalline solid state transformations to crystalline-amorphous transitions. Particular interest will be placed on novel characterisation including novel experimental set-ups and techniques (e.g. Bragg diffraction, PDF, NMR etc), data-processing methodologies, and structural parameterisation.

Keynote:
Joe Hriljac (Diamond Light Source)

Phase transitions in zeolites driven by pressure and ion exchange

CCG: Hot and cold structures

(*Chair: Charlie McMonagle*)

In this session we look at how temperature can affect materials in a huge number of interesting and useful ways. This could be structural effects, multiple phase behaviour, electronic, and/or magnetic transitions across the entire temperature range. Temperature can be key to phenomena such as superconductivity, phase transitions, spin-crossover, negative thermal expansion, and many others. Insights into new instrumentation or techniques for accessing these temperatures will also be considered along with combining variable temperature with other stimuli (pressure, light etc.). This session aims to highlight the important role of temperature across a wide range crystallography.

Keynote:
Sven Lidin (Lund)

Incommensurate intermetallics - The simple, The challenging and The confusing: Making sense of complexities in reciprocal space.

End of Conference

The Roger Stevens building, University of Leeds

CCDC: European UGM & Science Day 2020

THE European UGM & Science Day will be held across Downing College and CCDC in Cambridge UK, on the 2nd and 3rd June 2020.

The UGM on Tuesday 2nd June will include presentations and talks from CCDC experts and invited speakers, as well as software demonstrations and discussions around the latest product development and research from the CCDC and users. A networking reception with drinks and canapes will follow the presentations and discussions on day 1.

Our annual Science Day, held on Wednesday 3rd June, will offer the opportunity to discover more about research carried out by our PhD students via a range of scientific sessions and discussions. Both days will offer great opportunities to meet with peers and colleagues from across industry and academia and find out about the latest developments in the sector.

This event is free of charge, but places are limited and will be allocated on a first come first served basis. Visit our website at *https://www.ccdc.cam.ac.uk/News/Events/* and register your place. A detailed agenda will be available online soon.

20 Years of the CCDC Prize

THE CCDC Chemical Crystallography Prize for Younger Scientists (or 'CCDC Prize' for short) was created by the CCDC and the Chemical Crystallography Group (CCG) of the British Crystallographic Association (BCA) to both inspire and recognise excellence in crystallographic research coming from early career scientists in the UK. This prize is awarded every year based on original research in the field of chemical crystallography or the application of crystallographic information to structural chemistry, including advances in instrumental, experimental, theoretical or computational techniques within this field.

The winners of the CCDC prize over the last 20 years are a very impressive group, representing the best of early career scientists within the UK Chemical Crystallography community over the years. Most of the past winners have gone on to become research group leaders in the field inspiring the next generation of chemical crystallographers! The focused research areas of the various CCDC prize winners encompass a range of topics including metal-organic frameworks, photo-crystallography, high pressure studies, disorder, supramolecular chemistry, crystal engineering, hydrogen-bonding, crystal structure prediction, powder diffraction, neutron diffraction and non-linear optics. At the heart of all this research is molecular or metal-organic crystal structures and the knowledge that can be gained from those structures - exactly the knowledge that is at the heart of the CCDC's charitable mission.

I personally (**Dr Pete Wood**) have thoroughly enjoyed being connected with the CCDC Prize over the years, having attended many of the CCDC Prize award lectures in my early years in the UK crystallography community as a PhD student, then winning the 2011 edition of the award for my contributions to the understanding of intermolecular interactions in the solid state. Finally, I have had the privilege of designing the commemorative models for many years as well as presenting most of the CCDC prizes between 2013-2019.

More information about the CCDC Prize & nominations

The CCDC Prize is awarded annually and presented as part of the BCA Spring Meeting. Nominations for the award are considered by the CCG Committee and that group chooses the overall winner, with the CCDC providing the award itself in the form of a monetary contribution and a commemorative item. Nominations must be made to the Secretary of the BCA Chemical Crystallography Group. The CCG website *https://ccg.crystallography.org.uk/* provides full details of the CCDC prize and rules.

Peter Wood
Senior Product Manager at CCDC

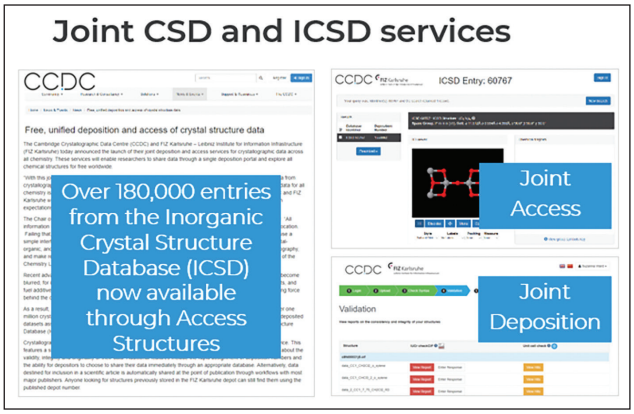
Sharing Structural Data – A Collaborative Journey

AT the CCDC over the last few years we have been working hard to expand our collaborations with other databases and resources to make structural data as accessible as possible. As many of you know, in 2017 this led us to collaborate with FIZ Karlsruhe to develop free joint deposition and access services covering organic, metal-organic and inorganic data which were launched in 2018. We thought that 18 months on we should reflect on the success of this collaboration and explore what the future may hold.

Photo of Jürgen Harter (CEO), Ian Bruno (Head of Strategic Partnerships), Matthew Lightfoot (Editorial Team Leader), Suzanna Ward (Head of Database) from the CCDC in front of the timeline of the ICSD at the ICSD headquarters in FIZ Karlsruhe

The CCDC and FIZ Karlsruhe have teams dedicated to the creation and distribution of the CSD and the ICSD, respectively. Our organisations have many similarities, we have similar missions, values, serve the same communities and provide high quality, trusted data and software. Both institutions are world-leading experts in structural data and their databases combined contain every published organic, metal-organic and inorganic crystal structure and are essential resources for the structural chemistry community. Datasets in both databases have to pass rigorous quality checks with both automated and manual curation being performed on every entry by scientific experts. These rich, high-quality data resources alongside advanced software provided by our two institutions are designed to help you to extract new insights from the data and discover novel scientific trends. The annual BCA meetings always provide us with an excellent opportunity to hear how you have been using the databases and it is always a pleasure to learn about the new structures being determined and the new insights you have gained from the wealth of structural data that is now available. Collectively the licensed databases are installed in over 1,300 institutions worldwide and the UK remains in the top 10 countries that are responsible for publishing small molecule crystallographic data.

At some of the conferences that we have attended over the last few years we have heard about advances in chemistry, such as research to design new batteries, gas storage systems, zeolites, catalysts, magnets, and fuel additives, and this has highlighted the challenges that some researchers have operating across two independent data sources. Thankfully our joint access and deposition services have provided a solid foundation to combat some of these challenges. In 2019 alongside the more traditional organic and metal-organic usage the joint deposition service was used by over 1,000 inorganic crystallographers to deposit data. The joint access service also saw more than 100,000 views and downloads of inorganic data in 2019 and usage has steadily increased since the service was released.



The joint services developed through the CCDC and FIZ Karlsruhe collaboration

These services already seek to promote the FAIR guiding principles and their release in 2018 has been well received. However, we feel the ability to harness the knowledge contained in both databases to generate new insights of relevance to the wider structural chemistry community could require this foundation to be expanded to more advanced solutions. Both institutions are dedicated to developing services of most benefit to the communities that we serve and so to this end we want to hear what your use cases would be for future joint advanced services. Please seek us out at the BCA in Leeds to talk about this with us. We are also hosting a joint workshop at the IUCr Congress in Prague this year so come along to learn more about how to use our two databases and to give your feedback on what our priorities should be in the future for our collaboration. You can find out more details about our joint workshop here:

https://iucr2020.auletris.com/workshops/

We hope that that this collaboration and other community initiatives that we are involved with are of value to researchers worldwide and we look forward to being driven towards new opportunities and collaborations based on your needs.

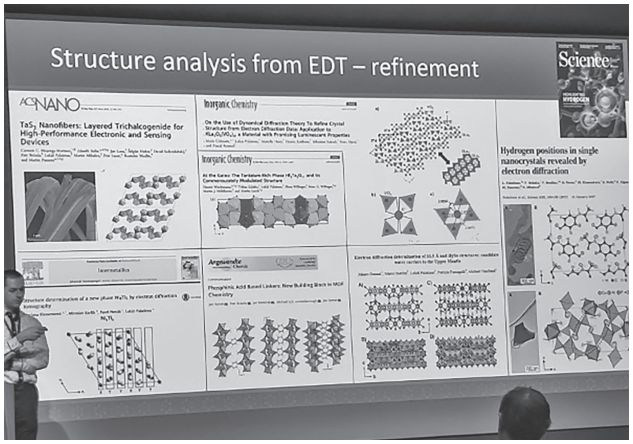
Suzanna Ward
Head of Database, The CCDC

Reports on the CCG/IG Autumn meeting 2019:

‘By Hook or by Crook – Structural Solutions from Challenging Crystals’

I arrived at the University of Southampton in the beginning of November to start a short but very intense period of research in the group of Prof. Simon Coles as part of the EU Erasmus scheme. The visit arose from a long-time and active collaboration between Southampton and my research group headed up by Prof. M. Carla Aragoni at the University of Cagliari, Italy. As my PhD project is based on the development of novel materials prepared by means of supramolecular interactions, X-ray diffraction analysis is absolutely essential. Thus, I was really excited when Simon proposed to me that I should attend the CCG/IG BCA Autumn Meeting at GSK in Stevenage – and that there was a bursary available to help pay for it!

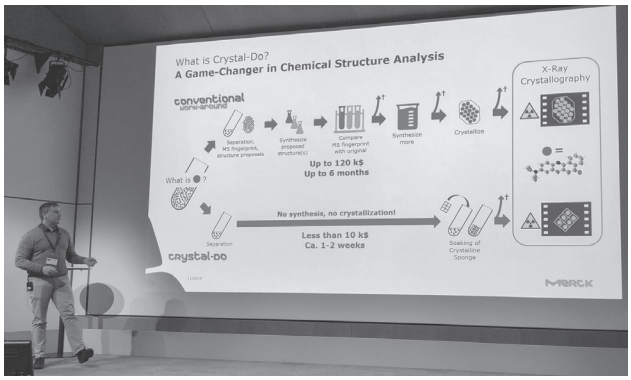
The meeting started at 10:30, just after a refreshing cup of coffee (an important thing for Italians!), with a brilliant talk by **Dr. Lukáš Palatinus** based on recent advances and limitations in structure analysis from electron diffraction data. He presented several examples, beautifully illustrated in the slide shown below, in which electron diffraction analysis can be applied to the structural elucidation of new materials for electronic and sensing devices, alloys and in-deep study of nanocrystals for the determination of hydrogen positions.



Lukáš Palatinus

The second speaker, **Dr. Clemens Kühn** from Merck, turned out to give a very inspiring and meaningful presentation on the Crystalline Sponge (CS) method. Introduced by Prof. Fujita in 2013, crystalline sponges are porous metal complexes suited for hosting guest molecules inside their framework, leading to the structure elucidation of typically non-cristalline organic molecules by conventional single crystal diffraction analysis.

The CS method is a perfect candidate for the absolute structure determination among chiral organic molecules and natural products employed as drugs nowadays. Although crystalline sponges are being widely used for the



Clemens Kühn

structure determination of natural extracts which are commonly in the liquid phase, there are basically infinite possibilities for crystalline sponges to be applied in still unexplored fields meaning that a prosperous future is coming for this new trend in structural analysis. The important contribution that the abovementioned project aims to provide was also clarified by the interesting talk of **Dr. Katharina Edkins**, which highlighted the influence of water in drug design and production.

After a generous lunch break, the afternoon session of the meeting started with **Dr. Sihai Yang** giving his CCDC Younger Scientist CCG Prize lecture on porous materials and their application in green chemistry at the industrial level. The following speakers presented very intriguing topics ranging from, crystallization of biodiesel in extreme conditions, High-Pressure XRD and structural resolution from Powder XRD analysis.
I believe that such interesting meetings are a great opportunity for scientists to network and be able to see and understand a wide range of ‘real life’ applications of crystallography’. I am really thankful to the organising committee for giving me the opportunity to participate in this fantastic one-day meeting, which was dedicated to our common passion: research.

Enrico Podda (Universities of Cagliari & Southampton).

This year’s Chemical Crystallography Group Autumn meeting was jointly held with the Industrial Group hosted at GSKs site in Stevenage. I was particularly looking forward to the third session of the day; advanced XRPD applications, as solving crystal structures from powder data is still an area I need to comprehend.

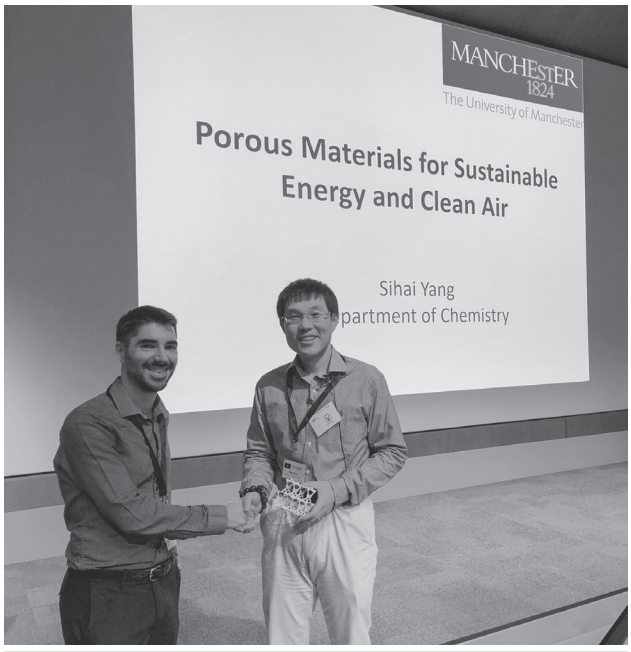
The plenary talk was given by **Dr Lukáš Palatinus**, based at the Czech Academy of Sciences. He discussed the

advances in structure analysis from electron diffraction data. As someone who is fairly new to the world of crystallography, I enjoyed learning about something other than the X-ray diffraction I am used to, which is why out of all of the excellent talks delivered at the meeting this one happened to be my favourite… Nothing to do with his fabulous shirt. Electron crystallography offers a larger interaction strength and can be used for crystals with dimensions spanning as little as a few nanometres. However, electron diffraction poses a greater amount of radiation damage due to the smaller probed sample but offers the opportunity to analyse samples six orders of magnitude smaller than X-ray.

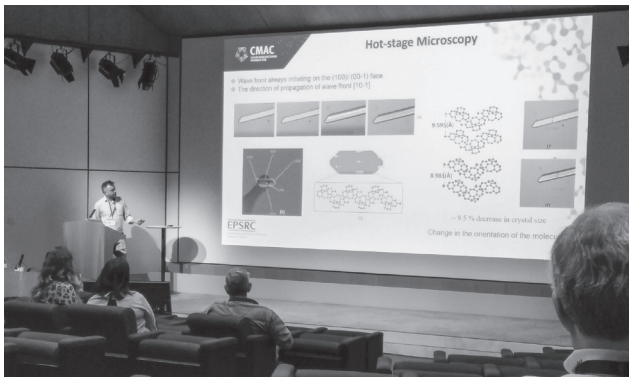
This was followed by talks given by **Clemens Kühn** from Merck's Innovation Centre and **Katharina Edkins** from Queen's University Belfast who discussed crystal-less crystallography and research into drug hydrates respectively.

Morning session speakers: Katharina Edkins, Clemens Kühn, Lukáš Palatinus with chair Luca Russo

Post lunch we were treated to the CCG Prize Lecture from **Dr Sihai Yang**, but before the talk Sihai was awarded with a 3D model of his aluminium-based metal organic framework by Pete Wood (CCDC). His cutting-edge research focussed on using porous material to capture carbon dioxide which could be used to produce sustainable clean air. **Xiaojiao Liu** discussed the crystallisation of biodiesel at extreme conditions, using methyl stearate as a model compound and using Diamond Anvil Cells to facilitate high pressures and ultimately polymorphic transitions.



Peter Wood (CCDC) presenting the CCDC prize to Sihai Yang



Vijay Srirambhatla

After a much-needed coffee break came the session I was most looking forward to. **Kenneth Shankland** (University of Reading) started off the proceedings with his talk on improved crystal structure determination from powder diffraction using information from the Cambridge Structural Database. Following on was **Mathilde Reinle-Schmitt** from Excelsus SLS. Her talk was titled "Beyond the limits of conventional techniques: subtle structural differences influencing solubility unveiled by synchrotron-XRPD". **Vijay Srirambhatla** (University of Strathclyde) finished off the day with his presentation on the curious twisted crystals of oxcarbazepine form III.

Final session speakers: Kenneth Shankland, Vijay Srirambhatla, chair Cheryl Doherty and Mathilde Reinle-Schmitt

Attending BCA conferences always motivates me to jump straight back into my research with the hope that one day I will be presenting my work to fellow crystallographers, and this meeting was no exception!

Eleanor Jones (University of Strathclyde)

The Autumn 2019 meeting for the chemical crystallography and industrial group this year was held at the GSK site in Stevenage. We really enjoyed the opportunity to spend time at GSKs global R&D hub.

The first talk of the day started with **Lukáš Palatinus**, who gave a fantastic talk surrounding electron diffraction and the recent advances in the field. It was highly insightful to see alternative methods of structural determination and the strategies Lukas and coworkers have used to overcome the dynamic scattering effects that have previously hindered the practicality of ED crystallography. The next talk was presented by **Clemens Kühn** who spoke about the use of metal organicframeworks as 'crystalline sponges'. The sponges have been used as the basis for the identification of unknown compounds that can be otherwise difficult to crystallise. We thought this was a very novel idea, allowing liquid solutions of unknown molecules to be absorbed into MOF pores before undergoing diffraction experiments on the whole ensemble to identify the small molecules trapped inside. **Katharina Edkins** was able to blend crystallography approaches with real world pharmaceuticals advances in her talk surrounding hydrates of drugs. Hydrates can cause potential issues with solubility and dosage of drugs and therefore need to be studied carefully.

Lunch was the perfect opportunity to socialise and network with fellow crystallographers, both in academia and industry. It also gave us the chance to ask any unanswered questions we had about talks in the first session.

We had the pleasure of listening to **Sihai Yang**, who was the CCG prize winner of 2019. He gave a riveting talk of his use of MOFs to selectively capture common green house gases such as NO2 and SO2. One of the most interesting points was the gases absorbed into the MOF pores can be recycled by washing with water and air to give products such as nitric acid. These porous materials could lead to highly exciting developments for green chemistry and helping tackle climate change in the future.

Xiaojiao Liu from the University of Edinburgh spoke of the various problems with Biodiesel and methyl stearate at low temperature and high pressure. Both of these conditions can be present in a modern diesel engine, the biodiesel forms small crystals and wax which clog up filters. Using diamond anvil cells to study the polymorphs which could be present under these conditions and provide solutions to improving biodiesels. In the world of powder diffraction **Kenneth Shankland** informed us of the improving ability to solve structures with increasingly large degrees of freedom with the help of the DASH software package and the CSD. The second talk of this session presented by **Mathidle Reinle-Schmitt**, discussed the case of problematic solubility for a reagent which by SC-XRD seemed identical. Using synchrotron XRPD proved that there was differences in the bulk material provided and therefore causing issues with solubility in manufacturing. The final talk of the day was given by **Vijay Srirambhatla** who told us about the work being undertaken at Strathclyde with an array of different crystal structures solved by XRPD including an unusual crystal that had a twisted confirmation seen via imaging techniques.

Overall It was a well organised and enjoyable day, all of the talks were highly engaging and covered a diverse range of crystallographic developments.

Jake Musselle-Sexton and **Lucy Hunter**
(Newcastle University)

CCP4 Study Weekend 2020 – report on page 16

CCP4 Study Weekend 2020

THE annual CCP4 Study Weekend (now usually mid-week!) was organised by Jon Agirre (York), Robbie Joosten (NCI, Amsterdam) and Alan Roseman (Manchester). It was preceded by the Diamond User Meeting. After an overview of MX facilities by Dave Hall (Diamond), updates were presented on various topics; software (DIALS now including scaling and merging), beamlines (VMXi, I24), best practices (data collection on Eiger detectors, automation on I03, preparing samples for VMXm) and future directions (serial experiments and the new Rosalind Franklin Institute). This was followed by a networking event (for those not attending the WG1/ speakers dinner), including food and a quiz, which was hugely enjoyed by everyone present.

For those not attending the WG1 meeting (open to all PI's), there was a "What's New in CCP4" session. This included four talks: a brief update on new programs by **Ville Uski** (CCP4, RAL), followed by three more in-depth talks – **David Waterman** (CCP4, RAL) on DIALS 2.0, Huw Jenkins (Newcastle) on "Improved validation and deposition in CCP4i2" and **Ronan Keegan** (CCP4, RAL) on CCP4 Cloud based services.

The main meeting kicked off with a session on model building. Introductory talks were given by **Helen Saibil** (Birkbeck) and **Eleanor Dodson** (York) on building into EM maps and high resolution X-Ray maps respectively. **Tom Terwilliger** (Phenix, Los Alamos) then gave a talk showing how density modification was statistically different between X-Ray and EM and why it didn't provide as great a benefit in EM, though it was still possible to do. **Isabel Usón** (ICREA, Barcelona) explained how SHELXE now uses side tracing to improve (especially) mainly beta structures where the automated built model may get interrupted in poorly defined loops. **Kevin Cowtan** (York) finished the session with a thought provoking look at how the software we use may be biasing the results we get and that we should all be using a combination of all possible software for the best result.

Lunchtime Bytes ran during lunch on both days allowing users to see presentations and demonstrations of the latest software by the developers and also ask direct questions of the programmers.

The second session started with **Garib Murshudov** (York) showing how the electron densities seen for X-Ray and EM are similar, but different. At high resolution, where the scattering from the nuclear charges becomes apparent, the maps can look very different around charged side chains. **Dorothee Liebschner** (LBNL, Berkeley) then showed the real-space refinement tools in PHENIX and showed how extra restraints were needed to keep the correct geometry in EM maps. She also introduced the Re-refine project (similar to PDBredo) for older EM structures and highlighted the lessons learned. **Ana Casañal** (LMB, Cambridge) introduced the next COOT upgrade (0.9), which features multi-threading, Geman-McClure restraints, morphing, improved chain extension and many more to enhance building into low resolution maps. **Tristan Croll** (Cambridge) showed the latest low resolution aids in the ISOLDE model building program including real time new maps and adaptive torsion restraints. The session was completed by **Hamish Todd** (Hauwei) who amusingly concluded that his CootVR project was probably not going to replace COOT anytime soon.

The last session of the day focused on 'other' bits of the model with **Mihaela Atanasova** (York) showing the SAILS and Privateer programs for building and validation of carbohydrate structures, which try to reduce errors in models. **Antonio Rosato** (Florence) then introduced the MetalPDB database and the MetalS^2 and MetalS^3 programs to find and compare similar metal sites. **Rob Nicholls** (MRC, Cambridge) showed the tools in COOT and ACEDRG to correctly create descriptions of covalent links in proteins (many of which are wrong in the PDB).The final talk was given by **Rachel Skyner** (Diamond) on WONKA and Fragalysis, which can be used to analyse fragments bound to proteins for drug discovery and help suggest new compounds to try.

The first session on the second day started with **Agnel-Praveen Joseph** (CCPEM, RAL) (standing in Maya Topf) speaking about model fitting and validation by the program TEMPy. **Vileriy Titarenko** (Manchester) then introduced a pipeline to use model masks generated from PDB files to fit into density features in EM maps. **Helen Ginn** (Diamond) then showed the latest iteration of her novel refinement program, Vagabond, which uses refinement in torsion space to significantly reduce the number of parameters required. The final talk of the session was from **Sarah Harris** (Leeds) on FFEA, a simulation tool to look at the structure and dynamics of super-macromolecular complexes at the mesoscale. Validation was the theme of the next session with **Wah Chiu** (Stanford) who introduced their new Q-score, which can be used on a residue basis as well as a global score to validate EM structures. **John Berrisford** (EBI, Cambridge) then showed how the PDB was using validation, standardisation and sanity checking to keep the PDB clean and gave some amusing examples of errors they have found. **Jiří Černý** (CAS, Prague) showed that nearly 30% of PDB entries with RNA/DNA have incorrectly built nucleotides. He introduced a web page (DNATCO) that can be used to analyse PDB files to check for correct geometry. **Rafiga Masmaliyeva** (LMB, Cambridge) completed the session by showing how B-factors could be used to judge the local and global correctness of models and concluded that most entries in the PDB conform to expected statistics.

The final session was started with more validation from **Anastassis Perrakis** (NCI, Amsterdam) with the new features in PDB-REDO that use homology to improve the automated rebuilding of, especially, missing loops and glycosylation. PDB-REDO improves around 80% of structures. The next two speakers, **Marc Baaden** (IBPC, Paris) and **David Sehnal** (CEITEC, Brno) showed how we can visualise complex macromolecules to highlight particular aspects well using their software UnityMol and Mol* respectively. The final talk was given by **Jeroen Claus** (Phospho) who showed how structures can be animated with easy-to-use available software to make movies of biological processes.

Mark Roe
(University of Sussex)

A bright future in Bénin

ON Sunday 24th November I was lucky enough to be on my way to Bénin for the second X-TechLab training session.

X-TechLab (*https://www.xtechlab.co/en/*) is a project designed **by Thierry d'Almeida** and **Marielle Agbahoungbata**, whose mission is to provide the local and regional scientific communities with expertise in X-ray techniques to help solve specific critical socioeconomic issues. The project includes an X-ray diffraction and X-ray tomography lab, designed to support researchers from Benin and West, Central and East African countries. Alongside the establishment of two labs a significant part of the project is dedicated to training and education with two schools a year planned, and I was invited to teach at the second training session held in Cotonou.

Michele Zema (Executive Outreach Officer - IUCr) and I arrived in Cotonou for the second week of the school in November and were warmly welcomed into the country by Thierry and Marielle. After a restful sleep we joined fellow attendees on the short bus journey to the school. Along the way we passed the huge port gates of Cotonou and also the site of Sèmè City, where the X-TechLab is being relocated to in 2021.

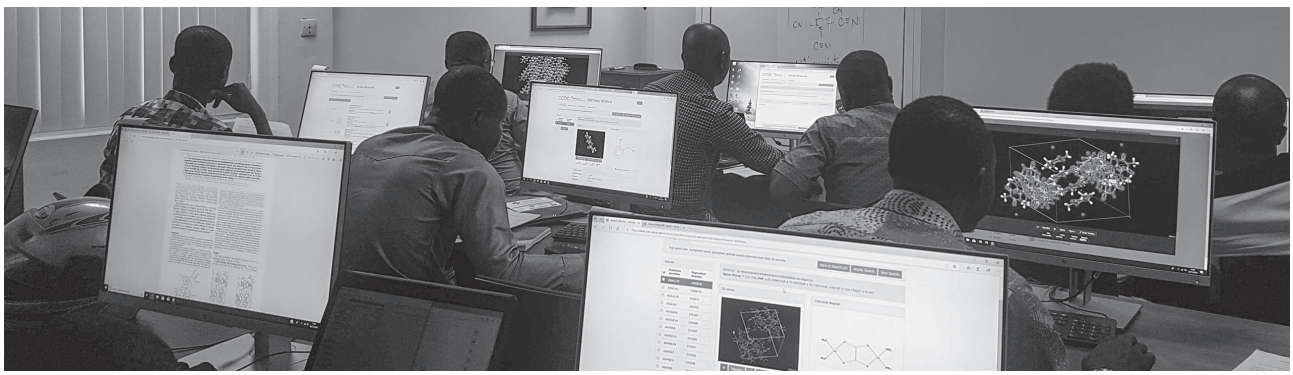
The training session had two different streams on X-ray diffraction and X-ray tomography, with the diffraction class attracting about 20 students from Benin and neighbouring countries. Over the next couple of days Michele spent the mornings explaining symmetry and the basics of diffraction while I spent the afternoons teaching students about the Cambridge Structural Database (CSD). The students were taken on a wonderful adventure on the first morning learning about symmetry through a series of photos displaying different symmetry elements. With a single crystal diffractometer due to be installed, the first afternoon saw all the students deposit example data to the CCDC. Subsequent afternoons saw the class searching the CSD using ConQuest and WebCSD, analysing structures using Mercury and Mogul, and learning how to create publication ready, high-resolution images. It was a delight helping the students through the hands-on tutorials and seeing their excitement exploring structures in the CSD. The school was right next to the Lagune de Cotonou with views out to the Gulf of Guinea and so coffee breaks enabled us to briefly (it was over 30 degrees outside!) venture out onto the balcony to watch the local fishermen. Lunches always involved a tasty buffet of fish, chicken, rice, plantains and of course spicy chilli sauce at the restaurant over the road while watching eagles soar over the river.

The scene looking out from the hotel

The first training course in May had been in French but thankfully for me (my French is unfortunately very limited!) the second course was all in English. This should help the students communicate their science more easily in the future but two weeks learning new scientific concepts not in their first language can't have been easy. Despite this they did a great job following the lectures every day and working through the tutorials. Their enthusiasm was perhaps at its peak during a quiz about the CSD, demonstrating just how much they had learnt during the last couple of days.

All in all, it was an inspiring but tiring week. Being able to help engage a new generation of scientists in Benin was definitely a privilege I won't forget. I am sure there will be challenges along the way, but I know that the project is in good hands with Thierry and Marielle driving the initiative forward. I am looking forward to seeing new structures being published in the CSD through this project and I hope it can also help develop the next generation of experts that will be the users of the future Pan African Synchrotron that is currently being discussed. As a charitable organisation the CCDC are certainly committed to helping initiatives like this succeed both through the support of training events and through the FAIRE programme (*https://www.ccdc.cam.ac.uk/Community/FAIRE/*) that provides free access to the CSD and associated software in developing countries. I want to finish by saying a huge thanks to the organisers, particularly Thierry and Marielle, and to the attendees for their warm welcome, their enthusiasm and for making the days I spent in Benin enjoyable. Alongside the memories of the school I think Bénin will be the only place I have been picked up on the tarmac on arrival and gone to a nightclub for a drink on departure after checking into the flight home!

Suzanna Ward
Head of Database, The CCDC



Training session participants learning how to use the CSD

AsCA 2019

THE 16th Conference of the Asian Crystallographic Association (AsCA) was held at University Town, National University of Singapore (NUS) on 17-20 December 2019, with additional workshops in the days leading up to the conference.

Alongside workshops on Olex-2, TOPAS and CCP4, the CCDC held a workshop on the Cambridge Structural Database (CSD) on the morning of the 17th December. This workshop guided over 30 participants through the CSD, demonstrating how small molecule structural data could be used in research and teaching. It was held in a fantastic computing room at the NUS Kent Ridge Campus with computers pre-installed with CSD software available to all the attendees. The morning whizzed past and the journey through the CSD involved deposition, Mercury visualisation, and training on Crystal Engineering applications through the use of Mogul Geometry Check, Full Interaction Maps, and polymorph assessment using Hydrogen Bond Propensity tools.

Upon completion of the workshops everyone headed to the NUS ready for the opening talk and plenary lecture on "Microbial Invasion and Host Defense" by **Myunghee Kim**. That afternoon then saw three parallel keynote lectures and flash presentations in Macromolecular Crystallography, Chemical Crystallography and Materials and Applications. Each of the flash presenters lined up ready to speak and had just three minutes to describe their posters and in many cases the research of their entire PhD. I have to say it went surprisingly smoothly with both students and chairs doing an excellent job despite the time pressures. After the session the exhibition opened and the students presented their posters. It was a slow start at the CCDC stand as we were competing against some delicious food and drinks, but it did start to get busier and true to tradition we began our leaderboard competition.

On Wednesday the day began with three parallel sessions on Disease-Related Protein Structures, MOFs/CPs in Sustainable Energy and Hybrid Methods in Crystallography Including SAXS/SANS. Later sessions included some interesting talks on the advances of cryoEM as well as luminescence/chromaticity-based sensing, and another micro-symposium focused on MOFs. Fittingly the last talk of the day was a plenary by **Susumu Kitagawa** on "Dynamic Structures and Properties of Porous Coordination Polymers / Metal-Organic Frameworks". Prof. Kitagawa described some unique porous properties of PCPs, which respond to specific guests, dissimilar to conventional porous materials and explained how this new class of materials provides the possibility of creating a platform for porous functions.

Wednesday night also saw the celebration of one million structures in the CSD. The CCDC hosted an evening to say thank you to the community for contributing over one million structures, and to award a prize to the author of the millionth structure to **Yao Wang**. During the evening there were three short talks about the CSD from **Suzanna Ward**, Head of Database (CCDC), **Genji Kurisu** from PDBj and Osaka University and **Jurgen Harter** the CEO of the CCDC. Yao Wang from Shandong University in China was then awarded a 3D model of the millionth structure. After receiving the award he gave a wonderful talk about the importance of using the CSD in his research.

Thursday saw nine more microsymposia covering topics ranging from Solid-state Reactions and Dynamics, Aperiodic, Amorphous and Disordered Materials, and Materials and Applications. A particular highlight of the MOF session was **Marc Little**'s presentation on tuning the properties of porous organic cage co-crystals for gas separations. He described how the cavity sizes of porous organic cages can be fine-tuned using a unique, four step, site-selective, protocol: crystallisation protection => single-crystal to single-crystal

Overlooking the Gardens by the Bay from the Marina Bay Sands Hotel

Jurgen Harter presenting the millionth structure award to Yao Wang

solid-state reaction => solution based deprotection => cavity size optimization reaction. Another interesting talk in that session was by **Vijay Kumar** about research into synthetic graphene and 2D layered materials using organic quinones. The next microsymposium on Materials and Applications saw a number of fascinating talks including one by **Samantha Chong** about integrating powder diffraction into organic materials discovery, **Michel Bosman** talking about spectroscopy and atomic-resolution structural analysis with aberration-corrected STEM and **Shago Kawaguchi** describing a real-time resolution powder diffraction measurement system under gas pressure. Before we all headed off to the conference dinner there were three interesting keynotes. **Alison Edwards** talked about "The experimental underpinning of the structure-function paradigm" She gave a number of examples of high-profile mistakes in chemistry and detailed some of the pressures researchers face to publish. Her messages were loud and clear, and she stressed the importance of ensuring crystallography doesn't become pigeon-holed as just a service pursuit, highlighting the importance of educating chemists and crystallographers more and the part major facilities can play in that. **Chilla Malla Reddy**'s keynote lecture described adaptive flexible crystals that not only pose challenges in establishing the role of various types of intermolecular interactions involved in solid-state dynamics but also provide a unique opportunity to design new functional crystals with unseen combinations of properties using crystal engineering principles.

The conference dinner was a chance for the delegates to relax and network with other attendees as well as learn more about our discipline and Singapore's culture. The evening started with a traditional Singaporean Lion dance with two colourful lions weaving their way through the tables before completing their dance on stage. After the delights of the lions was a wonderful talk by **Gautam Desiraju** about a selection of crystallographers that changed the way we work today. The crystallographers included **Kathleen Lonsdale** who he described as knowing what the right questions to ask were; **JM Robertson**, the first person to solve the structures of two polymorphs; **Isabella Karle** for her work on direct methods; **Olga Kennard** for founding the CSD; and **Phillip Coppens**, a pioneer in the field of X-ray charge density analysis and quantum crystallography, as well as in the field of photocrystallography.

Friday ensured the conference finished on a high with some illuminating lectures on co-crystal design, microelectron diffraction and Covalent Organic Frameworks. The sessions saw **Hidehiro Uekusa** talk about how to solve poor solubility and stability in pharmaceuticals through the modification of the crystal composition and the incorporation of a co-crystal. We also heard about how carbamazepine co-crystallises with natural polyphenols from **Jonghwi Lee** and an analysis of chloride...pi(chelate) ring interactions by **Edward Tiekink**.

Friday finished with the awards and closing ceremonies. It was heartwarming to see so many young scientists win prizes for their posters and flash presentations and I think everyone would agree it was a fantastic way to end a successful meeting. The last day also saw the CCDC award its very own champion and fittingly **J.J. Vittal** the Chair, Local Organizing Committee, was crowned the winner of the CCDC leaderboard! I am sure like me everyone that was able to join AsCA16 is now looking forward to AsCA17 in Malaysia in 2021.

Suzanna Ward
Head of Database, The CCDC

CSD workshop participants

Exotic Forms of Ice Workshop (13-14 October 2019)

A two-day workshop on ice? Surely you must be joking! Its very simple structure has been known for nearly a century from W.H. Barnes's 1929 single crystal X-ray measurements. What more is there to learn about it?

A great deal, it turns out. Indeed the oxygen framework structure of the hexagonal ice Ih in your freezer may be a simple ABAB stacking of puckered hexagonal rings of hydrogen bonded H_2O molecules. But why and how are the hydrogens on that framework disordered (it's actually an 'orientational glass'). And why is it so difficult to order the hydrogen positions as we lower the temperature? And why has it proved so difficult to produce an ordered ABCABC stacked cubic structure – attempts to do so resulting in random stackings such as ABACBACB…? And noting that the normal ice Ih structure is a very open one – with a density only about half that of a close-packed structure – how many ways can you arrange the water molecules to form other, denser structures as the pressure is increased and still retain full four-coordinated hydrogen bonding? And what about the apparently non-crystalline or glassy structures that can be formed by either rapid cooling of the liquid or by pressurising ice Ih at low temperature? Are there really two (or perhaps more?) distinct non-crystalline structures, and how might these relate to the structure of the supercooled liquid?

A complex system indeed, and one on which a recent workshop was organised in Chattanooga by **Chris Tulk, Luke Daemen** and **Alexander Kolesnikov** from the Spallation Neutron Source at Oak Ridge National Laboratory (ORNL). The workshop aimed to identify what the outstanding questions concerning ice in its many phases and environments are, and how they might be approached by the research community.

The icy environments discussed ranged from the interstellar to the interfacial – and under laser-induced shock! The workshop kicked off in interstellar space and the solar system, with **Murthy Gudipati** (Jet Propulsion Lab., Pasadena) reviewing our knowledge of both crystalline and amorphous ices 'out there'. Future challenges he set out included answering questions on the nature of cometary ice and of ice in the outer solar system. He also underlined our basic lack of understanding of the physical properties of ice containing salts and other trapped molecules at the pressures and temperatures as might be found on, for example, Europa, Ganymede, Enceladus, Titan and Pluto.

Although most of the workshop addressed structural issues, several talks did indeed address physical properties. Dielectric properties of crystalline and amorphous ices over wide temperature and frequency ranges were reported by **Ivan Popov** (ORNL), who demonstrated how sample preparation could significantly affect the results. The effects of externally-applied electric fields were discussed by **Niall English** (University College Dublin), showing among other things how such fields can shift phase boundaries. **Dominic Fortes** (ISIS) sought to understand the anomalous volume isotope effect (VIE) in ice Ih – the molar volume of D_2O is larger than

The Chattanooga steam train

that of H_2O whereas the normal situation would be the other way round. Using high resolution neutron diffraction, he found that the VIE in high pressure ices II and VI were normal, while for ice III and its hydrogen ordered form ice IX, the effect is normal along the ***a***-axis and anomalous along the ***c***-axis. As ices III and IX exhibit negative area expansion in the ***a-b*** plane below about 40K, he interestingly suggested that there may be a relationship between anomalous isotope effects and negative expansivity.

The nature of ice at interfaces was discussed by several speakers. **Larry Anovitz** (ORNL) showed how ultra-confinement in, for example the 5.1Å tunnels in beryl, could facilitate proton tunnelling. The possible relevance of this work to the potential role of proton tunnelling in biological systems was raised in discussion, and hopefully links can subsequently be made with others associated with ORNL who are active in studying the role of water in biological processes. The influence of a single surface on the structure and dynamics of water was explored by **Hsui-Wen Wang** (also ORNL) with respect to SnO_2 nanoparticles. He produced evidence of very strong hydrogen bonding of water molecules to the surface, and commented again on the potential relevance to biological processes, as well as to heterogeneous catalysis and environmental remediation. **Tianshu Li** (George Washington University), using results from computer simulations, addressed the influence of an interface on the stacking disorder of ice crystals grown in confinement or at surfaces.

The three themes of pressure, hydrogen ordering and amorphous ices characterised most of the rest of the workshop.

On the pressure front, there has been much speculation over several decades about the structure of the 'ultimate' phase of ice: what is its structure under extremely high pressures where the molecules must approach some kind of close packing? In that state, as hydrogen-bonded molecules are pushed very close together, what happens to the hydrogens? Do they become delocalised, leaving us with what is essentially an ionic solid? **Malcolm Guthrie** (European Spallation Source, Lund) took us through what we know so far experimentally, with initial results at 62GPa

showing significant distortion of the water molecule. Data at even higher pressures have been taken, but problems with thermal parameters and diffuse scattering are making data interpretation challenging. X-ray diffraction results obtained by **Marius Millot** (Lawrence Livermore National Lab.) at the even higher pressures (up to 400GPa) produced by laser-driven shock waves showed convincing evidence of superionic ice, with a transition from a bcc to an fcc structure above about 270GPa and 2000K. That these conditions are consistent with those one-third of the way down below the surfaces of Uranus and Neptune stimulated a discussion on water in the Earth's mantle being possibly superionic. However, that suggestion was dismissed by **John Loveday** (Edinburgh), who presented gas-storage relevant results on mixtures of ice with simple molecules such as CH_4 and NH_3, argued that the pressure was too low for mantle water to be superionic. Icy systems such as gas hydrates are also important in a number of energy applications, and **Carolyn Koh** (Colorado School of Mines) presented results on the influence of promoter guest molecules, chemical additives and synthesis methods on the production of stable and metastable clathrate hydrate phases.

Hydrogen ordering in ices has been a bone of contention for many years. The consensus opinion is that, as the temperature on, for example, ice Ih is reduced, the molecular motions required to facilitate hydrogen (or molecular orientational) ordering become frozen in at a temperature around 120K. However, early work on ice Ih has shown that doping with small amounts of a base (e.g. KOH) can overcome this thermal blockage. In trying to order high pressure ices such as V, VI and XII, however, such base doping is ineffective – but ***acid*** doping can work! **Christoph Salzmann** (University College London), who was the first to discover the acid doping approach, took us on a short (?) stroll through the ice phase diagram, discussing both these doping issues and pressure-induced amorphisation.

This latter issue has also been a matter of intense discussion since Ted Whalley's Canadian group produced in 1985 an apparently amorphous ice by pressurising ice Ih at 77K and 1GPa. This amorphous structure (named high density amorphous ice HDA) is structurally different from the low density amorphous ice (LDA) produced by rapid cooling of the liquid, and there have been robust discussions as to whether the pressure-induced amorphisation is a melting process or is rather the consequence of mechanical instability of the crystal structure leading to a collapse of the crystalline lattice. **Dennis Klug** (National Research Council of Canada) – who used to work with Ted Whalley – set the scene with a historical survey of HDA and LDA. He addressed the possible relationship of the structure of LDA to that of the supercooled liquid (is there structural continuity between them?), and also the extremely controversial idea of a second critical point in the water phase diagram. **Thomas Loerting** (Innsbruck) reviewed his recent results on the formation and relaxation dynamics of HDA with the aim of coming to a fuller understanding of its thermodynamic nature. He argued that unrelaxed HDA contained remnant microcrystalline regions, and also used the results of mechanical penetration measurements to argue that he had obtained the high and low density liquids that the second critical point scenario requires. The discussion of these results was intense, with one participant arguing that as you have to have movement of atoms in order to call something a liquid, the putative liquids obtained here must still be regarded as glasses. This argument will no doubt continue to run and run…

Another argument that before the workshop I thought had been recently resolved also looks like running a little longer. This goes back to the pressure-induced amorphisation of ice Ih to HDA mentioned above, and also links in with the kinetics of water motions at low temperatures. First, **Chris Tulk** (ORNL) showed that this pressure amorphisation no longer occurs if the ice Ih is compressed at a slower rate and discontinuously – thereby allowing 'breaks' for the system to recover in stages. Under these conditions, no amorphous form is produced: what is obtained are the phases as expected from the phase diagram – a welcome simplification! **John Tse's** (Saskatchewan) results led to the similar conclusion that the ice structures obtained on pressurisation are indeed sensitive to the compression/decompression rate and the temperature – the interconversion of the various ice forms are controlled by the kinetics, so in working with ices, you go too fast at your peril (as I and Werner Kuhs did in our early work on ices VII and VIII, and so missed out on interesting things we might have seen had we been in less of a hurry…). John also argued that in his results on the direct conversion of HDA to LDA, the 'phase boundary' does not extrapolate to the proposed second critical point. As expected when the second critical point issue is raised, the ensuing discussion was exhilarating, with other results brought up to argue against its existence.

As in all good workshops, lots of time was given to a final discussion session led by **Chris Tulk** (ORNL). Things he thought we should talk about – and called for further work – included trying to understand what the precise ordering/disordering mechanism was that froze at about 120K and could be released by doping. Resolving the differences in results between different workers on the pressure amorphisation issue was important, though there seems to be general agreement that the pressure-induced amorphisation of ice Ih to HDA was mechanical collapse of the lattice. The structural continuity or otherwise between LDA and supercooled water needed further work, while the relevance or otherwise of amorphous ice (and a range of other experimental) to the second critical point/two liquids scenario looks like continuing, despite a paper published two months prior to the workshop by **Alan Soper** (ISIS) that presents powerful thermodynamic arguments against this idea.

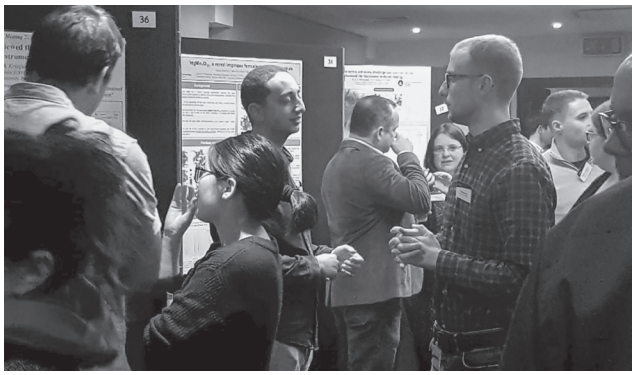
The ice on the ski run may have a simple structure, but the workshop underlined that many controversies and poorly understood issues remain. As I said in my contribution to the workshop, which showed old – and still unexplained – results on possible yet-to-be-discovered phases and on the detailed hydrogen-bonded network structure of amorphous ices, there is much unfinished icy business that developments in X-ray and neutron sources, instrumentation and sample environment can help us complete. Though having wandered around the unpredictable and capricious ice fields for a research lifetime, perhaps complete is the wrong word...

John Finney (UCL)

The Physical Crystallography Group Winter Meeting, 2019

PCG Winter Meeting attendees

THE "Winter Crystallography Meeting", an amalgamation of the winter meeting of the PCG, the ISIS Crystallography User Group meeting and the Diamond Crystallography Group, was held at Milton Hill House near Didcot on the 4th-5th November 2019. The 120 attendees enjoyed a packed schedule of talks that covered a wide range of crystallography and crystallography-adjacent subjects.



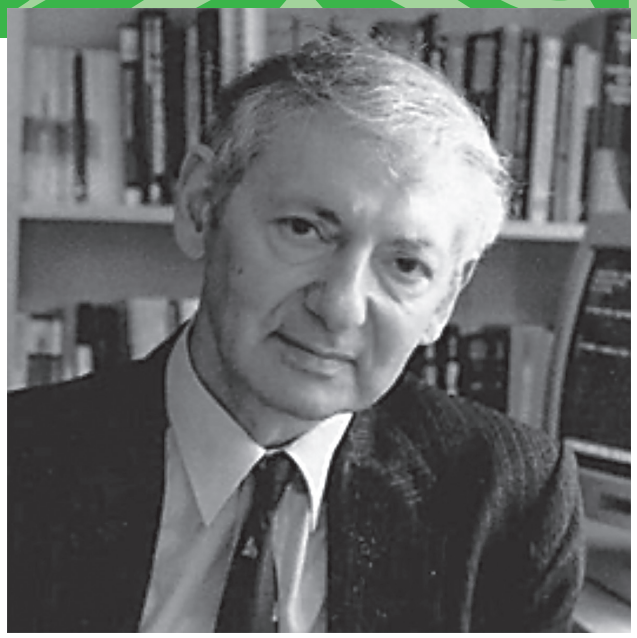
The poster session had a record number of submissions and the attendees enjoyed a colourful and exciting display covering an enormous variety of structural science. Poster prizes were awarded to **Emily Reynolds** and **Philip Welch** (both Oxford) and a new prize established in memory of Prof. Sten Eriksson (who sadly passed away in December 2018) was awarded to **Anna Herlihy** (Warwick).

A full meeting report has been written up for the IUCr Newsletter and can be viewed at *https://www.iucr.org/news/newsletter/volume-27/number-4/pcg-scmp-winter-crystallography-meeting*. So that you can reserve time in your diaries, we can let you know now that the 2020 meeting will be held on 2nd-3rd November (at a venue to be confirmed).

Paul O'Meara from Malvern PANalytical awarded the annual Malvern PANalytical Thesis Prize to **Noah Waterfield-Price** for his work on "Domains and functionality in multiferroic BiFeO3 films" that was carried out at the University of Oxford.

Obituary for Professor Michael Woolfson FRS

PROFESSOR Michael Woolfson, who died on 23rd December 2019, was a seminal member of the British Crystallographic community. He contributed to the theory and practice of X-ray crystallography for over 60 years. He made major contributions towards a general solution of the phase problem for determining crystal structures and provided tools to use the theory of "direct methods" to enable structures to be deduced directly from the diffraction data.



Michael Woolfson FRS
(Photography courtesy of the Royal Society)

Michael was primarily a physicist and mathematician, but he was always excited by applications of his elegant theoretical work. Early on he realised that the full power of the direct methods phasing would require computing resources, and set out, first to educate himself in how to do this, and then to recruit others to contribute. Peter Main joined his group in 1967 and was a GOOD THING! Software developed in his laboratory, such as Peter's program MULTAN, were responsible for about half of the structures determined around the world during the 1970s and 80s. As well as developing the theory, they thought carefully about practical issues such as how best to obtain normalised structure amplitudes (E values), what figures of merit would best indicate success, and how to display the results in a way meaningful to users, usually chemists who are anxious to visualise their structure.

Michael obtained his first academic appointment in 1955 at UMIST, and was appointed to the University of York as the founder Professor of Theoretical Physics in 1965. He was an enthusiastic and excellent teacher at all levels. From 1970 to 1980 he directed six Direct Methods schools across Europe, attended by many young scientists who subsequently became leading crystallographic theoreticians, and also published in several volumes of the Computational Crystallography series where papers given at IUCr International Summer Schools were included. It is interesting to look back at these; many complex ideas are described, (often in extremely complex ways!), but Michael's contributions are models of clarity.

He contributed greatly to many IUCr publications, both as an author and editor. He was a Co-editor of Acta Cryst. from 1977 to 1980, and Book-Review Editor for the Journal of Applied Crystallography from 1968 to 1975. He served on the IUCr Executive Committee in 1981-1984 as the first Convener of the IUCr Finance Committee during a particularly difficult period.

By the 1980s he was extending his interests to protein crystallography. Synchrotrons were extending the available resolution for protein data sets, and there were techniques for estimating initial phase sets from heavy atom positions or anomalous measurements, so methods combining these experiments and the underlying theory of direct methods were being developed. He had a long collaboration in this area with scientists from the Institute of Physics, Chinese Academy of Sciences, Beijing.

After his retirement in 1994 Michael continued to teach, and to carry on with research. One particularly powerful idea he pursued is coded into the program, ACORN, (named for the proverb – Mighty oaks from little acorns.) This uses the fact that if there is near atomic resolution data available, and this data set is enhanced to 1A simply by adding E values with the expected mean intensity for that resolution range (viz, 1), then density modification of a map phased only from a correctly placed small fragment, such as a few heavy atoms, the sulphur sites, or a helix, can quickly generate an extremely accurate set of phases for all reflections. It is still widely used to improve initial phase estimates for large molecules.

Michael was one of the founding fathers of the British Crystallographic Association (BCA). This had a somewhat complicated gestation. In British universities, departments of Chemistry and Physics were independent, (often fiercely so), and each group had an appropriate society; the Chemical Society, and the Institute of Physics. Each society included crystallographers, but there was no simple mechanism for local joint meetings of the two groups. By the end of the 70s after convoluted negotiations it was agreed to form a BCA, but it was still not clear how it would be financed. Finally at the inaugural meeting at Durham in 1982 David Blow suggested inviting crystallographers to become "Founder Members" on payment of a life membership fee of £100. Michael was one of these founder members – you can see his signature in the figure at the end of this issue.

Michael was awarded many well-deserved honours: he was elected as a fellow of the Royal Society in 1984, received the Royal Society Hughes Medal in 1986, the Patterson Award from the American Crystallographic Association in 1990, the Gregori Aminoff Prize from the Royal Swedish Academy of Sciences in 1992, the Dorothy Hodgkin Prize by the BCA 1997 and the Ewald Prize from the IUCr in 2002.

He will be especially remembered for his innovative science, for the enthusiasm he brought to the subject, for the quality of his teaching, and for his interest in and kindness to his many colleagues and students.

Eleanor Dodson (University of York)

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, news@crystallography.org.uk . Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

2nd Mar 2020 - 3rd Apr 2020
HERCULES European School: Neutrons & Synchrotron for Science, Grenoble, France.
http://hercules-school.eu/

16th Mar 2020 - 20th Mar 2020
Understanding Biology through Structure, Santa Fe, NM, United States.
https://cvent.me/4kq9P

22nd Mar 2020 - 24th Mar 2020
From 3D Light to 3D Electron Microscopy, London, United Kingdom.
https://www.zeiss.com/microscopy/int/cmp/ind/20/corrmic-workshop-2020/from-3d-light-to-3d-electron-microscopy.html?vaURL=www.zeiss.com/corrmic-symposium

23rd Mar 2020 - 27th Mar 2020
4th International Symposium on Halogen Bonding (ISXB4), Stellenbosch, South Africa.
https://isxb42020.net/

23rd Mar 2020 - 25th Mar 2020
S2C2 Workshop. Cryo-EM Specimen Preparation and Data Collection, Menlo Park, United States.
https://cryoem.slac.stanford.edu/s2c2/training/s2c2-workshops/next-workshop

25th Mar 2020 - 27th Mar 2020
11th International Workshop on Radiation Damage to Biological Samples, PSI, Villigen, Switzerland.
https://indico.psi.ch/e/rd11

26th Mar 2020 - 29th Mar 2020
3rd LACA School on Small Molecule Crystallography, Mexico City, Mexico.
https://www.iquimica.unam.mx/LACA/

29th Mar 2020 - 2nd Apr 2020
Powder Diffraction and Rietveld Refinement School 2020, Durham, United Kingdom.
https://community.dur.ac.uk/john.evans//webpages/pdrr_school.htm

31st Mar 2020 - 8th Apr 2020
CCP4 Crystallographic School in South Africa: Data Collection to Structure Refinement and Beyond (CCP4 2020), Cape Town, South Africa.
https://www.iucr.org/calendar/events/types/schools/ccp4-crystallographic-school-in-south-africa-data-collection-to-structure-refinement-and-beyond-ccp4-2020

6th Apr 2020 - 9th Apr 2020
British Crystallographic Association Spring Meeting, University of Leeds, UK.
https://crystallography.org.uk/spring-meetings/#next-meeting

13th Apr 2020 – 17th Apr 2020
Materials Research Society 2020 Spring Meeting and Exhibition, Phoenix, United States.
http://www.mrs.org/spring2020/

20th Apr 2020 - 21st Apr 2020
Magnetism 2020, Sheffield, United Kingdom.
http://magnetism2020.iopconfs.org/Home

20th Apr 2020 - 1st May 2020
School on Advanced Light Sources: Principles, Methods and Multidisciplinary Applications, Trieste, Italy.
http://indico.ictp.it/event/9080/

27th Apr 2020 - 29th Apr 2020
CCP-EM Spring Symposium, Nottingham, United Kingdom.
https://www.ccpem.ac.uk/symposium.php

27th Apr 2020 - 1st May 2020
ICDD Clinic - Practical X-ray Fluorescence, Newtown Square, United States.
http://www.icdd.com/xrf/

4th May 2020 - 8th May 2020
14th European Conference on Surface Crystallography and Dynamics (ECSCD-14), Grainau, Germany.
http://ecscd14.com/ecscd14/EN/Home/home_node.html

8th May 2020 - 12th May 2020
EMBO workshop on Molecular Neurobiology, Heraklion, Crete, Greece.
https://meetings.embo.org/event/20-molneuro

11th May 2020 - 22nd May 2020
Radiation Damage in Nuclear Systems: from Bohr to Young (ICTP2020), Trieste, Italy.
https://www-amdis.org/workshops/ictp-2020

24th May 2020 - 29th May 2020
7th International School of Crystallization: Pharmaceuticals, Foods, Agrochemicals, Minerals, New Materials (ISC2020), Granada, Spain.
https://iscgranada.org/

24th May 2020 - 26th May 2020
Topas Users Meeting, Šibenik, Croatia.
https://www.epdic17.org/satellite-meetings

25th May 2020 - 29th May 2020
Nanomaterials and advanced characterization, Strasbourg, France.
https://www.european-mrs.com/new-developments-modeling-and-analysis-radiation-damage-materials-ii-emrs

26th May 2020 - 30th May 2020
17th European Powder Diffraction Conference (EPDIC17), Šibenik, Croatia.
https://www.epdic17.org/

29th May 2020 - 6th Jun 2020
55th Course of the International School of Crystallography (Structural Drug Design), Erice, Italy.
http://www.crystalerice.org

31st May 2020 - 7th Jun 2020
2020 ACA Summer Course in Chemical Crystallography, Purdue University, United States.
https://acasummercourse.net/

1st Jun 2020 - 5th Jun 2020
ICDD Clinic - Fundamentals of X-ray Powder Diffraction, Newtown Square, United States.
http://www.icdd.com/xrd/

2nd Jun 2020 - 3rd Jun 2020
CCDC European UGM & Science Day 2020, Cambridge, UK.
https://www.ccdc.cam.ac.uk/News/Events/

7th Jun 2020 - 11th Jun 2020
Magnetic Small Angle Neutron Scattering – from Nanoscale Magnetism to Long-Range Magnetic Structures, Bad Honnef, Germany.
https://www.we-heraeus-stiftung.de/veranstaltungen/seminare/2020/magnetic-small-angle-neutron-scattering-from-nanoscale-magnetism-to-long-range-magnetic-structures/main/

8th Jun 2020 - 12th Jun 2020
ICDD Clinic - Advanced Methods in Powder Diffraction, Newtown Square, United States.
http://www.icdd.com/xrd/

8th Jun 2020 - 10th Jun 2020
UK Neutron and Muon Science & User Meeting, Warwick University, UK.
https://www.isis.stfc.ac.uk/Pages/NMSUM-2020-dates.aspx

13th Jun 2020 - 27th Jun 2020
22nd National School on Neutron and X-ray Scattering, Argonne & Oak Ridge National Laboratories, United States.
https://www.anl.gov/education/national-school-on-neutron-and-xray-scattering

14th Jun 2020 - 18th Jun 2020
8th International Workshop on Crystal Growth Technology (IWCGT-8), Berlin, Germany.
https://iwcgt-8.ikz-berlin.de/

15th Jun 2020 - 22nd Jun 2020
13th annual CCP4/APS crystallographic school: From data collection to structure refinement and beyond, Chicago, United States.
http://www.ccp4.ac.uk/schools/APS-2020/index.php

16th Jun 2020 - 24th Jun 2020
15th Bombannes Summer School: Scattering Methods Applied to Soft Condensed Matter, Gironde, France.
https://workshops.ill.fr/event/219/

16th Jun 2020 - 19th Jun 2020
Neutrons for Life Sciences, Lenggries, Germany.
https://indico.frm2.tum.de/event/197/

20th Jun 2020 - 21st Jun 2020
Crystal Engineering (GRS), Newry, United States.
https://www.grc.org/crystal-engineering-grs-conference/2020/

21st Jun 2020 - 26th Jun 2020
Three-Dimensional Electron Microscopy. Gordon Research Conference, Castelldefels, Spain.
https://www.grc.org/three-dimensional-electron-microscopy-conference/2020/

23rd Jun 2020 - 26th Jun 2020
16th International Conference on Surface X-ray and Neutron Scattering (SXNS16), Lund, Sweden.
https://www.sxns16.org/

30th Jun 2020 - 3rd Jul 2020
AFC 2020: Congress of the French Association of Crystallography, Grenoble, France.
https://afc2020.afc.asso.fr/

5th Jul 2020 - 11th Jul 2020
Sixth European Crystallography School (ECS6), Budapest, Hungary.
http://www.ecs6.chemcryst.hu

15th Jul 2020 - 17th Jul 2020
RIXS-REXS 2020: Workshop on Resonant Elastic and Inelastic X-ray Scattering 2020, Port Jefferson, United States.
https://www.bnl.gov/rixsrexs2020/

19th Jul 2020 - 24th Jul 2020
Gordon Conference on Research at High Pressure, Holderness, NH, United States.
https://www.grc.org/research-at-high-pressure-conference/2020/

26th Jul 2020 - 31st Jul 2020
Diffraction Methods in Structural Biology. Gordon Research Conference, Lewiston, United States.
https://www.grc.org/diffraction-methods-in-structural-biology-conference/2020/

31st Jul 2020 - 7th Aug 2020
ACA2020, San Diego, United States.
https://www.acameeting.com/

19th Aug 2020 - 22nd Aug 2020
Electron Crystallography School – 3D Electron Diffraction/MicroED Bridging Small Molecule and Macromolecular Crystallography, Tabor, Czech Republic.
https://www.xray.cz/iucr/workshops/tabor/default.htm

19th Aug 2020 - 21st Aug 2020
School on SAXS/SANS and BioSAXS/BioSANS data analysis, Prague, Czech Republic.
https://www.xray.cz/iucr/workshops/kh/default.htm

22nd Aug 2020 - 30th Aug 2020
Twenty-Fifth Congress and General Assembly of the International Union of Crystallography, Prague, Czech Republic.
http://www.iucr25.org/

30th Aug 2020 - 1st Sep 2020
Workshop on electron Pair Distribution Function (ePDF), Kutná Hora, Czech Republic.
https://www.uni-ulm.de/einrichtungen/hrem/epdf/

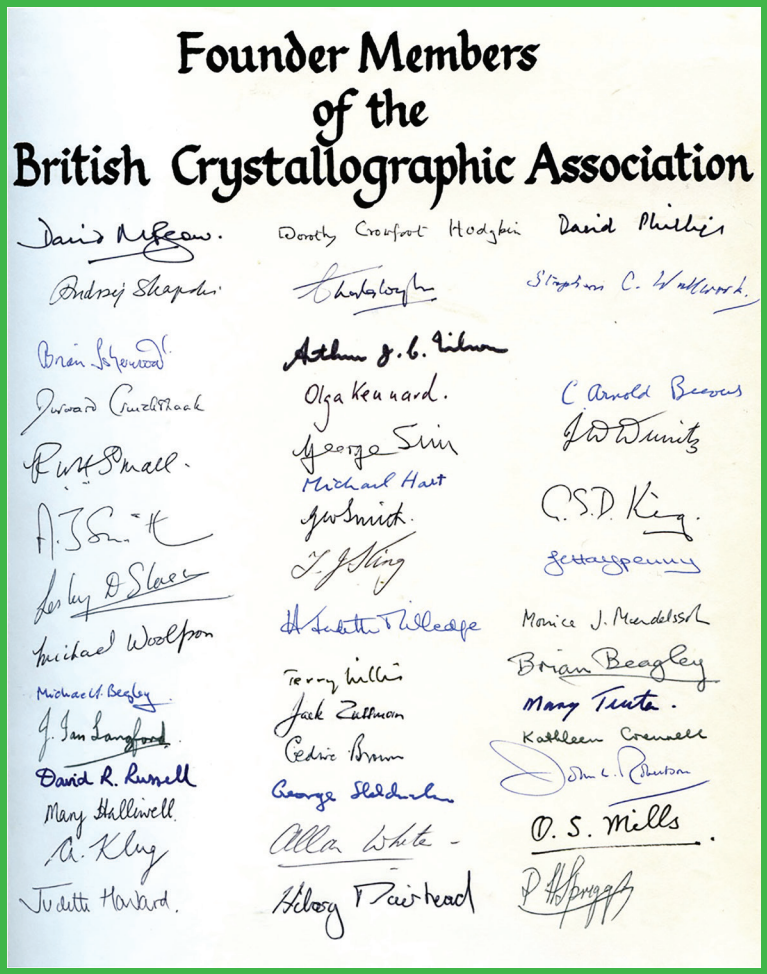
28th Sep 2020 - 2nd Oct 2020
ICDD Clinic - Rietveld Refinement & Indexing, Newtown Square, United States.
http://www.icdd.com/rietveld/

1st Oct 2020 - 2nd Oct 2020
Italian Crystal Growth - Crystal growth: from Theory to Application, Torino, Italy.
https://www.icg2020.net/

3rd Oct 2020 - 5th Oct 2020
10th International Conference of the Hellenic Crystallographic Association, Athens, Greece.
https://www.iucr.org/calendar/events/topics/general/10th-international-conference-of-the-hellenic-crystallographic-association

29th Mar 2021 - 4th Apr 2021
British Crystallographic Association Spring Meeting, University of Sheffield, UK.
https://crystallography.org.uk/spring-meetings/#next-meeting

24th Aug 2021 - 28th Aug 2021
Thirty Third European Crystallographic Meeting, Versailles, France.
https://www.ecm33.fr/



The list of signatures of the founder members of the BCA. Michael Woolfson's signature is amongst this list of legends, friends and memories – he will be sorely missed.

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