Crystallography News

British Crystallographic Association

Issue No. 148 March 2019
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Successful BCA Group and Pan-African meetings

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We cannot solve our problems with the same thinking we used when we created them. *Albert Einstein*

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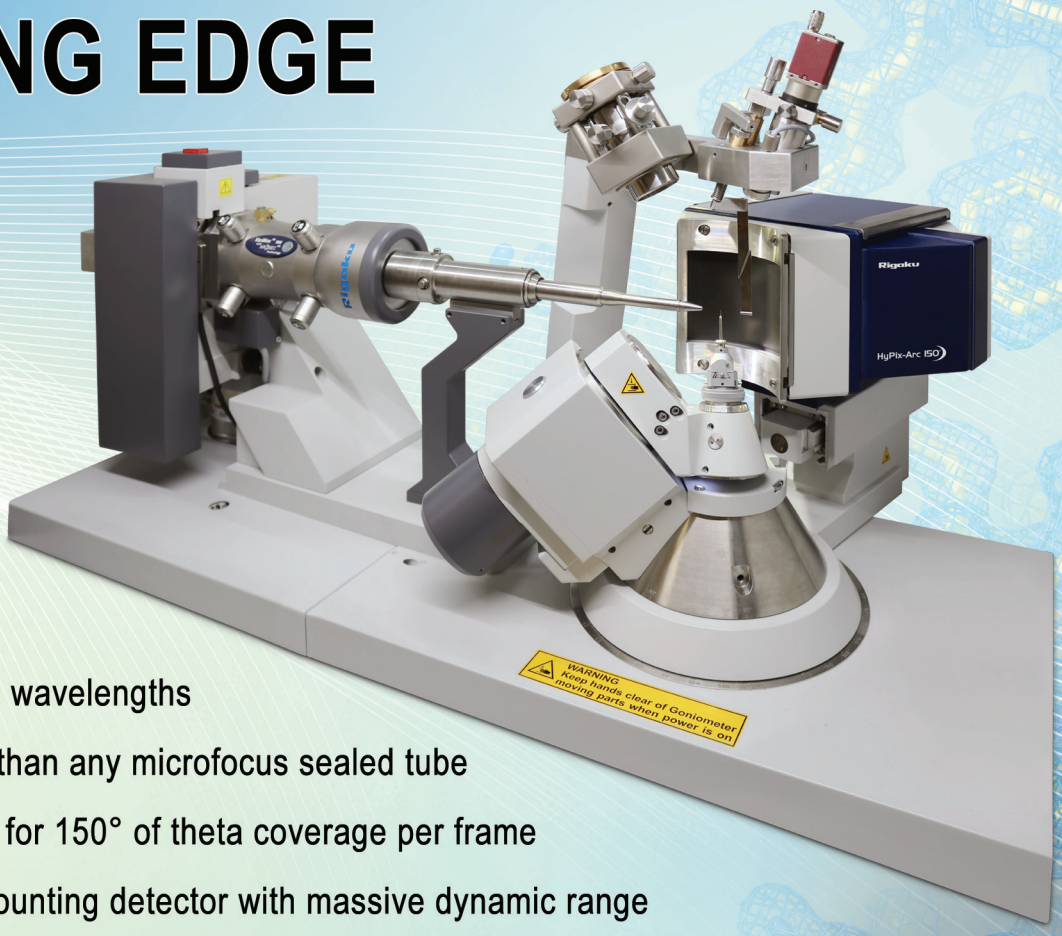

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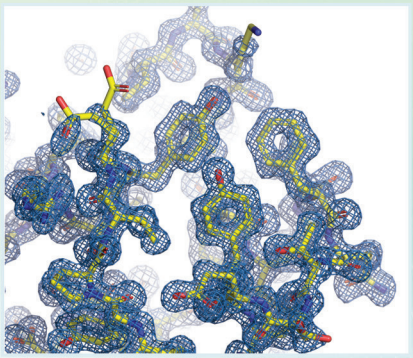
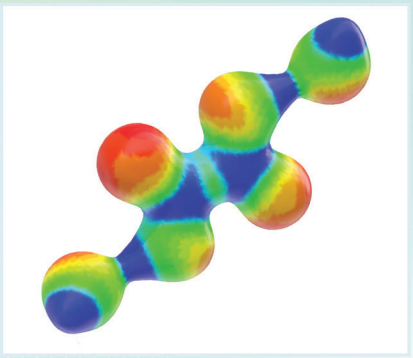


Density maps from a ten minute thaumatin dataset solved by S-SAD phasing



Electron density from a 0.37 Å quantum crystallography measurement of oxalic acid

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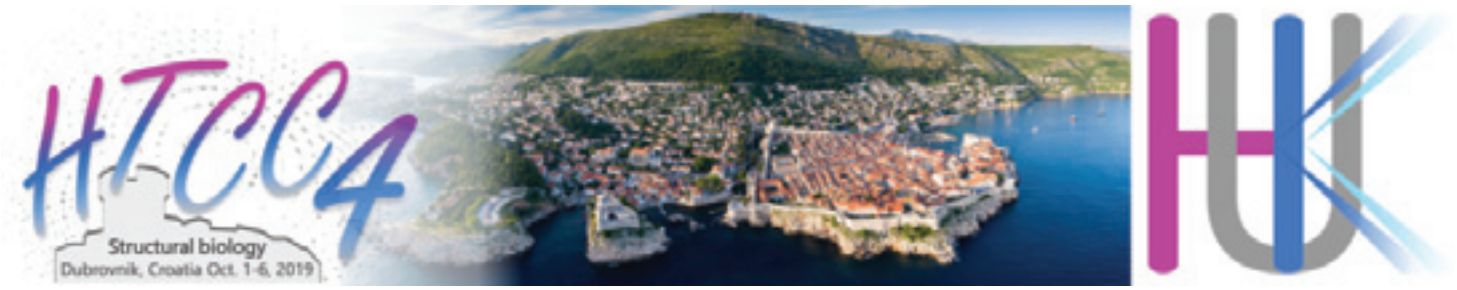
HOT TOPICS IN CONTEMPORARY CRYSTALLOGRAPHY 4 – Structural Biology

Mlini, Dubrovnik, Croatia, Oct. 1 – 6, 2019

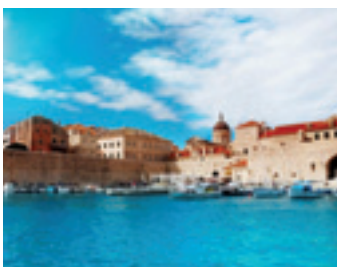


HTCC workshops – What is it all about?

The HTCC workshops tackle most fascinating achievements in both experimental methods and theoretical approaches, which lately put forward structural research to the front lines of natural sciences. We bring together leading experts in chosen domains as lecturers, and utterly ambitious scientists in crystallography or related fields as "students", who may come from both academia and industry, are keen to acquire new knowledge on the cutting edge methods in structural sciences and explore options to apply them to their ongoing research, or simply desire to find a glimmer of inspiration for their future projects based on the latest developments in structural research.

HTCC4 – Structural biology

HTCC4 will entirely be dedicated to structural biology. Over four intense working days, we shall cover techniques which go beyond classical crystallography, yet which complement it so smoothly: XFEL – X-ray free electron laser (HT1), cryo electron microscopy (HT2), NMR in macromolecular structural research (HT3) and biomolecular in-silico simulations (HT4). The lecturers and tutors shall explain fundamentals of these methodologies, give examples on their practical applications, tutor the practical and interactive sessions, and moderate round table discussions on how to apply these methods to your own research. The examples of particular systems studied with the presented methods shall emphasize intertwist between the four chosen hot topics in contemporary research. The complementarity of each of the hot topics with classical crystallography shall be discussed.

Contents

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Please ensure that items for inclusion in the June 2019 issue are sent to the Editor to arrive before 25 April 2019.

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

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

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This month's cover:

Scenes from the BSG, CCG, PCG, IG (clockwise, externally) and Pan-African meetings

From the President

IN October I went to an interesting reunion lunch at University College London. It was the 50th anniversary of the arrival in 1968 of about seventy fresh-faced new undergraduates, of which I was one, to register for a chemistry degree. About a third of us turned up to reminisce. The chemistry course was destined to be the root of my lifelong love of crystallography. The new Chemistry building was not quite finished when we arrived, so we had some lectures in the old building, now known as the Lonsdale Building, in honour of Kathleen Lonsdale. She was one of the first two women elected to the Royal Society in 1945, along with Marjorie Stephenson, and a major force in crystallography and social activism, while finding time to bring up three children. She joined Bragg's research group at UCL and, amongst other achievements, showed that the benzene ring is flat and hexagonal. The undergraduate practical that infatuated me with crystallography allowed us to determine the structure of hexamethylenetetramine, another of Lonsdale's crystal structures. The head of department when I was a student was the inorganic chemist Ronald Nyholm, who defined education as "a process in which a person receives a training for a *full life* in a rapidly changing modern society, carried out in such a manner as will ensure the maximum development of the individual personality". Times have changed, and it is a shame that universities have increasingly been encouraged to operate as businesses rather than educational institutions. Ron's signature phrase for us was "education through chemistry not education for chemistry" and he made a real effort to achieve this. One of my fellow students recalled that he had once been told "the best training for life is a PhD in X-ray crystallography", so there you have it.

All this reminded me of my 1st year organic chemistry lectures, and being taught the basics of nucleophilic substitution reactions, generally divided into S_N1 and S_N2. I apologise to readers who have not done an organic chemistry module, but many will have and it is not too hard to understand. Imagine a tetrahedral carbon atom bonded to four different substituents, it will be chiral, i.e. there will be two enantiomers that are related by mirror symmetry. There are two broad classes of reaction that allow one substituent to be replaced by another. In an S_N2 reaction, a new substituent approaches one side of the tetrahedron and forms a bond with the central carbon, the structure passing through a pentacoordinate transition state (triangular bipyramidal), with the new substituent in one axial position. The bond from the central carbon to the opposite axial substituent is weakened and breaks. The resulting tetrahedral structure will necessarily have the inverted configuration at the carbon (imagine an umbrella turned inside-out in a wind). If the starting material is enantiomerically pure, then the product will be too, so this is a way to retain asymmetric carbon centres. In an S_N1 reaction, on the other hand, the substituent to be replaced is lost first, leading to a trigonal, planar carbon with three substituents and carrying a positive charge, a carbocation. This is not chiral, and a new substituent can attack from either face to form a new tetrahedral structure. Generally, this will lead to a 50/50 mixture of tetrahedral products, a racemate, which is no longer enantiomerically pure. This is a key difference in reaction outcomes, which is of especial interest in medicinal and natural product chemistry where molecules need the correct chiral centres. Clearly you would expect S_N2 reactions to be the most useful for these applications, with chiral centres retained, albeit always inverted with respect to the starting material. Why am I telling you all this? My memories of learning the S_N1 and S_N2 reactions were also roused by a paper by Wendlandt, Vangal and Jacobsen in *Nature* in 2018. They report a catalyst allowing an S_N1 reaction to produce one enantiomeric product over the other. The catalyst is, necessarily, enantiomeric. Moreover, even a racemic mixture of the starting material will produce one enantiomeric product, the reverse of what we usually understand by SN1 reactions. An S_N2 reaction would need to be fed a single enantiomer reagent to produce and enantiomerically pure product, and then only the one related to the product by inversion. In the new S_N1 reaction, the enantiomer is controlled by the catalyst, not the starting material. This is an important step forward for asymmetric synthesis.

Members will have been saddened to learn of the death of **Aaron Klug** on 20th November 2018. Aaron was an Honorary Member of the BCA and a towering figure in structural studies. His major scientific achievements are too numerous to list here, but he is probably best known for developing the mathematics and methodology for three-dimensional reconstruction of biological assemblies, particularly viruses, from multiple views taken in the electron microscope. He suggested at the time that the techniques could be developed for three-dimensional medical X-rays, but this was apparently treated with scepticism by the physics community at the time. His suggestion was vindicated later by the invention of the CAT scanner, which we now take for granted as a routine method in hospitals around the world. He also worked on crystal structures of viruses, applying symmetry averaging to improve the maps as well as nucleic acids and their protein complexes. Perhaps less well known was his publication in *Acta Crystallographica* in 1958 of a comprehensive derivation of the mathematics underlying the joint probability distributions of structure factors and the phase problem, which went beyond the derivations routinely used in direct methods, and another on the theory of helical diffraction. His PhD thesis was on the kinetics of phase changes in solids. He won numerous awards and honours, including the Nobel Prize for Chemistry (1982), and was President of the Royal Society (1995-2000). Despite these heights of achievement, he remained mild-mannered and approachable. He will be sorely missed.

As I write this column, voting is well under way for the elections to 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 our futures. The results will be known by the time you read this. I look forward to seeing you all at the BCA 2019 Spring Meeting in Nottingham.

Simon Phillips

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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

ANYONE who has lingering doubts about attending the forthcoming BCA Spring Meeting should be convinced to attend by reading the fully fledged programme that appears in this issue. Because the dates (15-18 April) are relatively late, you still have a few days to take advantage of the Early Bird Registration discount, which closes on Monday, 11 March.

Our Groups recently held their focused autumn or winter meetings, which attracted strong interest. The themes were "Structures of Macromolecular Complexes" for the BSG, "Chemical Crystallography @ Central Facilities" for the CCG, "Holistic Approaches to Structural Characterisation" for the IG joined by the YCG, and a joint meeting with ISIS Crystallography and Diamond Crystallography Groups for the PCG. I am grateful to the authors of the write-ups that appear in this issue, and these reporters have also provided the pictures.

The second Pan-African Conference on Crystallography has just taken place in Ghana and benefited from help given by the BCA among others. With his report and pictures **Simon Coles** gives us a flavour of the enthusiasm it engendered. Simon wrote this article on the flight home. From the clarity of Simon's prose I conclude that it was a smooth flight without too many distractions of champagne and exciting inflight movies.

This summer offers a wealth of opportunities for interesting conference-going. First of all, our own Industrial Group will offer another in its series of well-regarded and well-attended X-ray fluorescence meetings on 12 June 2019 at Sheffield Hallam University. At the time I write this, the website recommends that participants wishing to contribute a talk should contact a committee member. Watch for an associated XRD meeting.

Our colleagues in the British Association of Crystal Growth will hold their annual meeting in the Rooms on Regent's Park, Central London, from 9-11 July 2019. This year's meeting is special because it is the 50th anniversary. Topics will include the latest developments in the areas of Crystallisation Fundamentals, Crystal Growth, Polymorphism, Multicomponent Materials, Modelling and new sessions on Interesting Crystal Properties and Alternative Routes to Crystalline Materials. More information can be found at **https://www.bacg.co.uk**

May I remind the travellers among you that the ACA meeting will take place in Covington, Kentucky, from 20-24 July (deadlines 31 March for abstract submission and 31 May for early registration), and the European Crystallographic Meeting will be in Vienna, Austria, from 18-23 August (deadlines 29 April for abstract submission and 15 April for early registration). As for advice about the best climbing equipment to get you over Trump's Wall, or the correct colour of paperwork to get you into post-Brexit Europe, I defer to experts with the relevant specialist knowledge.

Gordon Research Conferences and Gordon Research Seminars that are relevant to crystallography usually appear in the Calendar of Events on the IUCr website; but at the time of writing, this year's listings appear very sparse. I suggest that you check **www.grc.org** for yourself if you might wish to attend one of these enjoyable meetings.

In many years I have felt a pang of regret as I reported the award of Ludo Frevel Scholarships by our much appreciated supporters at the ICDD to a range of worthy graduate students in varous countries but not the UK. Happily, one of the recipients of this year's award is **Alexander Baker** from Cardiff University, for his research entitled *"Determining Mechanisms of Adenovirus Pathogenicity for the Development of Translational Virotherapies"*. We tend to think of the ICDD mainly in association with powder diffraction, but the wide range of topics supported this year, starting with Alexander's work on viruses, shows the breadth of research that can be supported by Ludo Frevel Scholarships. The prerequisite is the involvement of crystallography. Given the $2500 value of this year's scholarships, it is well worth preparing an application. The deadline for the next round of applications will be 17 October.

Some of you may remember that in 2012 I wrote an article (*Crystallography Reviews* **18**, 191-206) about **June Sutor**, her correct conclusion that C-H…O hydrogen bonds exist, and the harsh way it was rejected by some eminent crystallographers. Using this review as one of his sources, **Andy Extance** is writing an article for the wider chemical community about June Sutor that will soon appear in *Chemistry World*. In a recent issue I greatly enjoyed Andy's explanation of the Maillard reaction and why a roast turkey goes brown.

With sadness I reflect on the death of my colleague and friend **Joel Bernstein** on January 2 of this year. Some of his biographical data seem close to mine: he was born in Cleveland, Ohio in 1941 and received Ivy League postgraduate education. In Joel's case this was at Yale University, and the topic was solid-state spectroscopy. Postdoctoral work with **Ken Trueblood** at UCLA converted him into a "proper" X-ray crystallographer. Then he joined the highly innovative research group of **Gerhardt Schmidt** at the Weizmann Institute of Science in Israel, working on organic solid-state chemistry. During his career, his studies of polymorphism, hydrogen bonding and graph sets provided the insight necessary for the design and preparation of crystalline drugs, particularly pharmaceutical co-crystals. He was a Visiting Professor or visiting scientist at numerous institutions where important developments took place in understanding the systematics of crystal structures. These included the University of Minnesota, the Cambridge Crystallographic Data Centre and the University of Western Australia, Perth. Joel's research was an inspiration to all of us working in the field of pharmaceutical crystallography. I recall the fascinating and witty IG Plenary lecture that he gave at the 2014 BCA Spring Meeting (see page 8 of the June 2014 issue of *Crystallography News*). The fact that he held professorships at Ben-Gurion University of the Negev and at New York University Abu Dhabi demonstrates his unprejudiced and open-minded nature, in keeping with the internationalist traditions of crystallography.

Carl Schwalbe

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.

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

Puzzle Corner

THROUGH the inexorable increase of entropy, the letters have become scrambled in the names of the cities where recent and prospective meetings have been held or will be held. Help Maxwell's Demon to unscramble them.

Nhotmating .....

Elfbats .....

Nnaive .....

Donnol .....

Convoting .....

Murdah .....

Abonding .....

Answers to December Puzzle Corner

THE 2019 European Crystallographic Meeting will take place in a city much loved for its New Year's Day concert. By tradition the musicians give a greeting to the audience near the end of the concert. Use your knowledge of the elements and their symbols, admixed with a little group theory and linguistics, to construct it here.

Pr To an inorganic chemist, a rare-earth metal. To an organic chemist, C_3H_7-

O This makes what's above turn professional.

Si Together with what's just above, this makes sand.

T Schoenflies symbol for a tetrahedral group.

…

N An amine wouldn't be the same without this.

Eu Named for a continent that has this city near its centre.

Ja An enthusiastic "yes" in German.

H The first one of its kind (and the lightest).

R To an organic chemist, like the very first clue but completely general.

BCA Spring Meeting
15th – 18th April 2019, University of Nottingham

PLANNING is well underway for the 2019 BCA spring meeting to be held in Nottingham so please put the dates in your diaries! Details and titles for sessions are given below to give you time to think ahead to the registration deadline.

Monday 15th April 2019:
YCG meeting

YCG Research
*(Chairs: **Elliott Carrington** and **Rachel Wilkinson**)*

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.

Plenary:
Professor John McGeehan (University of Portsmouth)

Flash presentations:
*(Chairs: **Charlie Mcmonagle** and **Stephen Dodsworth**)*

Tuesday 16th April 2019:
YCG meeting

YCG/CCG:
Galvanising science through outreach and social media
*(Chairs: **Elliot Carrington** and **Rachael Wilkinson**)*

This session looks at all the excellent ways both outreach and social media can have an impact on science. How can we access a wider community? How can we inspire the next generation?

Plenary:
Dr Tim Easun (Cardiff University)

Keynote:
Dr Christine Beavers (Diamond Light Source)

Lonsdale lecture:
Professor George Sheldrick (University of Göttingen)
"SHELXT – dual space structure determination using the phases to determine the space group"

Tuesday 16th April – Thursday 18th April:
Main meeting

CCG plenary:
Carl Henrik Görbitz
*(Chair: **Iain Oswald**)*
"Slippery when hot: temperature-induced sliding phase transitions in amino acid crystals"

BSG:
Novel data collection strategies
*(Chair: **Ramona Duman**)*

Getting 'ideal crystals' for macromolecules has been the limiting factor for determining crystal structures. With the advent of novel diffraction techniques for micro/nano crystals, data collection strategies have accordingly evolved. This session will focus on novel data collection strategies such as 'Mesh and collect', line diffraction, *in situ* data collection, data collection of nano-crystals using micro/nanofocus instrument.

Keynote:
Dr Florent Cipriani (EMBL Grenoble)

CCG:
I didn't know Mercury could do that!
*(Chair: **Anuradha Pallipurath**)*

In this session we showcase the many applications of the CCDC tool Mercury. How users in the community are delving deeper into visualising their systems to gain better insights into its chemistry.

Keynote:
Dr Helen Blade (AstraZeneca)

Special lecture:
Dr Elna Pidcock (CCDC)

PCG:
Local structure probes
*(Chair: **Helen Playford**)*

An understanding of local structure and disorder in crystalline materials is increasingly recognized as the key to understanding their functional properties. Negative thermal expansion, dielectric response, thermoelectric properties, ionic conductivity, the list goes on. In all cases, a clear picture of the local atomic arrangements is essential for understanding these physical phenomena and developing new materials for practical applications. This session invites contributions from a variety of

fields, including total scattering/PDF analysis, X-ray absorption spectroscopy, NMR, and other techniques which aim to view structures from a local perspective.

Keynote:
Dr Karen Johnston (Durham)

"Probing ion mobility mechanisms in solid electrolytes using solid-state NMR spectroscopy"

BSG:

Complementary Structural Biology techniques
(Chair: James Garnett)

The session will focus on complementary structural biology techniques such as SAXS, NMR, Neutron diffraction, X-ray spectrometry that aid biological structure determination. Keynote: Dr Dmitri Svergun (EMBL)

CCG:

Neat structures
(Chair: Lucy Saunders)

This session celebrates structure and is a chance to share yours with the community; think those with interesting structural features, properties or behaviour.

Keynote:
Michaele Hardie (University of Leeds)

PCG/IG:

Structures of alloys and glass
(Chairs: Tony Bell and Lewis Owen)

PCG plenary:
Professor Igor Levin (N.I.S.T.)
(Chair: Anthony Phillips)

"Data fusion for determining atomic order on the nanoscale via the reverse Monte Carlo method"

Wednesday 17th April 2019:

IG plenary:

Professor Kevin Roberts (University of Leeds)
(Chair: Helen Blade)

"The Crystallisation Structural Pathway of Para amino Benzoic acid: From Solvated Molecule through Solute Clustering and Nucleation to the Growth of Facetted Crystals"

BSG:

Novel Crystallisation strategies
(Chair: Claire Naylor)

This session will focus on various crystallisation techniques for diffraction experiments using novel nucleants, novel buffer systems, membrane protein crystallisation techniques, crystallisation for serial crystallography etc.

Keynote:
Dr Apirat Chaikaud (Buchamann Institute)

PCG:

Energy materials
(Chairs: Tony West and Paz Vaqueiro)

Ensuring a sustainable energy supply is a pressing global issue. Advances in materials for energy applications are urgently needed to increase renewable-energy usage, and address current concerns about declining fossil fuel reserves and climate change arising from CO2 emissions. Diffraction plays a key role in understanding the structure-property relationships of materials for energy applications, including *in operando* studies. This session will examine recent developments in this field and contributions, oral or poster, are invited from across the diverse range of energy materials including batteries, fuel cells, solar and energy harvesting.

Keynote:
Dr Eddie Cussen (University of Strathclyde)

IG:

Characterisation of surfaces
(Chair: Mat Bryant)

When manufacturing a crystalline product in industry, understanding the chemistry and structure present at the surfaces of crystals is every bit as important as understanding the bulk. In this session we will explore cutting edge techniques to characterise and study the surfaces of crystals.

Keynote:
Dr Linda Seton (Liverpool John Moores University)

Early career prize lectures

BSG:

Computational structural biology
(Chair: Shozeb Haider)

This session will focus on the synergy between simulation and crystallography to biological structure analysis and inform future functional studies. The session will include molecular dynamics, QM/MM simulations, fragment screening, molecular docking etc.

Keynote:
Dr Gianni de Fabritiis (GRIB Barcelona)

CCG:

Chemistry of voids
(Chair: Hamish Yeung)

Voids in crystal structures, whether discovered by chance or incorporated by design, result in a range of interesting properties. In this session we celebrate the exciting chemistry that occurs in the spaces between the molecules, and the possibilities that lie beyond. Think storage, rearrangement, reactions, flexibility and more...!

Keynote:
Professor Andy Weller (University of Oxford)

"Solid–State OrganoMetallic (SMOM) Chemistry and Catalysis using Single–Crystal to Single-Crystal Solid/Gas Reactivity"

IG:

Prediction and modelling of surfaces
(Chair: Helen Blade)

Keynote:
Professor Mike Anderson (University of Manchester)

BCA prize lecture:

Professor Clare Grey (University of Cambridge)

BCA AGM and conference dinner followed by ceilidh.

Thursday 18th April 2019:

BSG Plenary:

Professor Liz Carpenter (University of Oxford)

BSG:

Multi-techniques for solving large macro molecular structures

(Chair: Christos Savva)

This session will focus on Cryo-EM and crystallography as structural techniques and how both complement each other in determining large macromolecular structures.

Keynote:
Professor Carolyn Moores (Birkbeck College / ISMB)

CCG:

Crystallography in chemical research

(Chair: Helena Shepherd)

This session is aimed at the wider community of chemists, doing all sorts of weird and wonderful things in their labs. We aim to open up a broader discussion in this session looking at how crystallography contributed to completing a research puzzle.

Keynote:
Professor Lee Brammer (University of Sheffield)

PCG:

Magnetic structures

(Chair: John Claridge)

Research work on magnetoelectrics, multiferroics, magnetocalorics, skyrmions, or any kind of functional magnetic material is welcome. Characterisation of all forms of magnetic structures, and their correlation with their physical properties. Special focus will be given to the most recent approaches.

Keynote:
Dr Sian Dutton (University of Cambridge)

BSG (joint with RaMP):

EU Network for Rationalising Membrane Protein Crystallisation

(Chair: Arwen Pearson)

This session will discuss some of the new approaches being developed by the EU network RaMP to rationalise membrane protein crystallisation thereby improving the crystallisation hits and facilitating structure determination of otherwise difficult membrane protein targets.

Keynote:
Professor Adrian Goldman (University of Leeds)

PCG/YCG:

In-situ methods

(Chairs: Hamish Yeung and Tom Wood)

Increasingly *in-situ* methods are being used to probe materials under non-ambient conditions. This session will highlight recent progress in both fundamental structural insight as well as that pertinent to real-world applications from biological systems through to solid state technology.

Keynote:
Dr Steve Hull (ISIS neutron and muon source)

PCG:

Topologically interesting materials

(Chair: Alex Gibbs)

Topological materials host a surprising range of unusual physical phenomena and are believed to provide a pathway to further intriguing electronic phases. Well known examples are topological insulators such as Bi_2Se_3 and topological Dirac semimetals. Their topological nature is ultimately facilitated and controlled by specific crystal and/or magnetic symmetries in combination with effects such as spin-orbit coupling. A key focus of the current intense study of these materials is the exploration of new physics driven by combining topology with magnetism and electron-electron interactions. They provide a large playground for fundamental research whilst also providing potential for transformative future technologies. This session will focus on the prediction, discovery and study of such topologically interesting materials (e.g. topological insulators and Dirac and Weyl semimetals) with a wide range of tools including e.g. crystal and magnetic structure analysis, electronic structure calculations and physical property measurements.

Keynote:
Professor Maia Garcia Vergniory (Donostia International Physics Center and University of the Basque Country, Bilbao, Spain)

Title TBC

AGM 2019

THE 2019 Annual General Meeting of the British Crystallographic Association will be held in the Exchange Building, Jubilee Campus of the University of Nottingham at 18:00 on Wednesday 17th April, 2019.

Draft Agenda

1) Approval of Agenda
2) Apologies for Absence
3) Minutes of last AGM
4) President's Report
5) Secretary's Report
6) Hg3 Report
7) Report of the Treasurer to include Presentation of the Accounts for 2018 and the Examining Accountant's Report
8) Acceptance of the Accounts
9) Appointment of Examining Accountant for 2019
10) Elections to Council
11) Honorary Members
12) Membership, annual subscriptions and subventions
13) Equality, Diversity and Inclusivity report
14) AOB

BSG / CCG / IG / PCG-SCMP Group Meetings 2018

Biological Structures Group (BSG) Meeting 2018

THE 2018 winter meeting of the Biological Structures Group was held at Imperial College, London on 17th December. The local organisers, Prof Thomas Meier, Prof Bernadette Byrne and Dr James Murray, must be thanked for assembling such a fascinating and excellent programme of speakers. The theme of the meeting was "Structures of Macromolecular Complexes" with an emphasis on integral membrane proteins.

Speakers and Organisers (left to right): ***Radu Aricescu***, ***James Murray***, ***Doryen Bubeck***, ***Bernadette Byrne***, ***Chris Tate***, ***Adrian Goldman***, ***Kostas Beis***, ***Bonnie Wallace***, ***Frank von Delft***, ***Xiaodong Zhang***, ***Naomi Chayen***, ***Thomas Meier***

The first session, chaired by Prof **Thomas Meier**, began with a lecture by Prof **Chris Tate** (Cambridge) on the structural basis for allosteric modulation of G-protein coupled receptors (GPCRs) by G-proteins. Prof Tate explained how the structures of the active states of a number of GPCRs have been solved by X-ray and EM analysis. These studies have generated much interest in how they explain the underlying pharmacology of these molecules, which play pivotal roles in the nervous-, cardiovascular- and immune-systems. The cytosolic G-protein component increases the affinity of the GPCR for its activating ligand and dissociates upon activation to trigger specific responses within the cell. Prof Tate explained how the first structure of the β2-adrenergic receptor in complex with a heterotrimeric G-protein was solved in 2011. He went on to explain the approaches his group have taken in order to further these structural studies, including the engineering of a range of mini G-proteins which are better suited to structural studies. He described the analysis of a complex of the adenosine A_{2A} receptor with a mini G-protein in three conformational states: inactive, intermediate and active. Binding of the agonist molecule causes a big conformational change due to the rotation of three helices and the resulting active state is stabilised by binding of the G-protein to one of these helices. Prof Tate then described the structure of the β1 adrenergic receptor bound to a nanobody which binds in the same place as the G-protein. He described how the active state of the receptor has a smaller binding pocket (and hence higher affinity) due to nanobody binding – these effects are being studied by molecular dynamics which have demonstrated the existence of an allosteric pipeline of interactions linking the G-protein binding site with the receptor binding site. Prof Tate went on to describe the range of G-protein families in the human genome and outlined further studies of the A2A receptor coupled to Gs by both EM and X-ray diffraction. Finally, he outlined on-going structural studies of the 5HT (serotonin) receptor coupled to a heterotrimeric G-protein.

Next, Dr **Konstantinos Beis** (Imperial) gave a presentation entitled: Structural understanding of the histamine H1 receptor (H1R). Dr Beis began by explaining the roles of histamine as a biogenic amine released from mast cells during inflammation. H1R regulates the severe allergic response and antagonists (better known as antihistamines) have been developed to treat various forms of allergy. Whereas the first generation of antihistamines had lots of side effects, such as drowsiness, the second generation have an additional carboxyl group which increases both the specificity of these molecules and the lifetime of the complex with the receptor. The structure of an H1R molecule with the first generation antihistamine doxepin bound was solved by So Iwata some years ago. Dr Beis explained that his group had set about trying to crystallise the H1 receptor with second generation antihistamines bound to it. To this end, crystals were obtained in lipidic cubic phase (LCP) and this led to the 3 Å structure of the receptor with acrivastine bound to it. The carboxyl group of the drug, which improves specificity, was shown to displace a phosphate anion from the protein and form a salt-bridge with a lysine residue, accompanied by some local movement of a helix. Mutagenesis studies of the binding site demonstrated that aromatic residues make the strongest contribution to specificity. The structure of a complex with olopatidine was solved at 3.8 Å resolution and subsequently shown to be similar to one determined by the Iwata group using FELS at 2.5 Å. In this structure two tyrosine residues were found to bind the drug carboxyl group by hydrogen bonds. Dr Beis then described molecular dynamics studies to investigate the basis of the long lifetime of the complexes with second generation antihistamines. These suggested that a second exit pathway involving aromatic interactions with a tyrosine residue was responsible for the slow off-rate and accordingly mutagenesis of this residue was found to reduce the lifetime of the complex a lot.

The final speaker of this session was Prof **Frank von Delft** (Oxford/Diamond) who gave a lecture entitled: Changing the compound discovery game with XChem fragment screening at Diamond. Prof von Delft began with an introduction to Diamond Light Source and the principles of structure-based

drug design including the roles of computational- and medicinal-chemistry. He continued with a comparison of traditional assay-based screening with the newer structure- or fragment-based approaches, the latter having the advantage of sensitivity, i.e. compounds which might not be effective in an assay may still bind to the protein in the crystal and can act as 'seeds' for the design process. Prof von Delft outlined the stages of a typical fragment-based screen with something like 30 min being required for adding the compounds to the crystallisation droplets, a few hours to allow them to soak into the crystals, 1.5 days for crystal harvesting and a similar amount of time for automated data collection, the full list of hits being revealed a few hours later. Technical developments pivotal to the success of this process were covered. These include the acoustic injection of the screen compounds to precisely defined points in the crystallisation droplets to minimise any damage to the crystals, a robotic crystal tray-shifter for harvesting the soaked crystals, high capacity beamline robots, automated data collection and careful map averaging for detection of low-occupancy ligands. These technologies have allowed the discovery of more than 2000 hits for 80 different protein targets in the last 3 years, during which 100,000 crystals have been screened. Prof von Delft then used the example of the breast cancer target, nudix hydrolase, as an example of a typical fragment screen which ultimately gave 50 hits and revealed a new 'druggable' subsite in the enzyme. He concluded with a mention of the new Rosalind Franklin Institute at DLS which is currently under construction. Part of its remit will be the development of methods for taking hit structures to lead compounds as efficiently as possible – a subject with Prof von Delft discussed at some length while concluding his talk.

Lunch provided an opportunity for attendees to meet with the meeting exhibitors and sponsors. Bruker, Generon, Douglas Instruments, F1000, ThermoFisher, Molecular Dimensions and Constant Systems are sincerely thanked for their generous financial support of the meeting.

The first afternoon session was chaired by Dr **James Murray** (Imperial) and began with a lecture by Prof **Bonnie Wallace** (ISMB/Birkbeck) entitled: The NavMs sodium channel: conformational states, drug binding and mutations associated with human diseases. Prof Wallace introduced the field of voltage-gated Na channels and their key role in the rising phase of the action potential. Some prokaryotes are found to possess sodium channels and these are highly similar to the human channels. In the disease context, these proteins are involved in arrhythmia, epilepsy and pain, amongst other conditions, and they are targeted by a range of natural toxins. The prokaryotic channels mimic just the voltage sensor- and pore-domains of the eukaryotic channels which have additional transmembrane domains. Prof Wallace reported on studies of the *Magnetococcus spirilum* NavMs which tetramerises via the pore domain to form an oligomer of approximately the same size as the eukaryotic channel. The structure of the drug lamotrigine bound to MavMs has been determined at 2.4 Å showing how the Na ions come into contact with polar side chains in the selectivity filter of the pore domain. The ions then have to pass through a hydrophobic pocket, where channel-blocking drugs bind, before leaving via the exit gate. The open state of the protein is stabilised by a network of hydrogen bonds involving Trp 77, a residue that is known to be mutated in two diseases. The transmembrane region of the protein possesses holes in its sides which are important to allow hydrophobic, membrane-soluble drugs to gain access to the channel. Prof Wallace explained how the open state of the protein has a smaller hole than the closed state and how this difference is potentially 'druggable'. Prof Wallace then described a range of ongoing EM studies of this system.

The next speaker was Prof **Naomi Chayen** (Imperial) who gave a presentation entitled: Enhancing the success of protein crystallisation. Prof Chayen covered a range of problems that are frequently encountered in protein crystallisation before moving on to the familiar phase diagram and how the different types of crystallisation behave in this context. Prof Chayen emphasised that it is important to create an environment that limits the number of crystallisation nuclei which are present and described how simply filtering solutions can achieve this. She then moved on to describe the importance of seeding and then introduced a range of non-protein nucleants which can help greatly. These include porous materials such beads of calcium-phosphate-silicate glass with cavities comparable in size to the protein being crystallised. Prof Chayen then described a new type nucleant known as molecularly imprinted materials, or MIPs for short. The nucleant is made of polyacrylamide gel that sets in the presence of proteins which cover a range of molecular weights. The proteins are removed and the resulting beads therefore possess protein-binding holes which act as the nucleation sites for subsequent crystallisation experiments. The use of MIPs was found to improve crystallisation of several proteins. Prof Chayen then described how liquid MIPs have been developed for use in automated crystallisations and concluded by stating that the materials described in her talk are perhaps not a 'magic bullet' for crystallisation but rather a selection of user-friendly techniques.

Next up, Prof **Adrian Goldman** (Leeds) gave a presentation entitled: Progress towards novel inhibitors of protozoan parasites. Prof Goldman describes numerous structure-function studies of the integral membrane protein pyrophosphatase (PPase) which couples pyrophosphate (PPi) hydrolysis to proton or sodium ion pumping. The enzyme from the malaria parasite, toxoplasma and trypanosomes has been studied and found to have a molecular weight in the range 70 – 85 kDa. The pyrophosphatase active site is on the cytoplasmic side of the membrane and has an acid-protease like character in which two enzyme carboxyl groups activate a water molecule to hydrolyse PPi. Prof Goldman described how a number of novel inhibitors were discovered by virtual screening, several having micro-Molar affinity. Structural studies of these compounds bound to the enzyme revealed that some were uncompetitive inhibitors. One compound bound at the dimer interface and led to a revised model of ion transport.

After much-needed coffee, the scientific programme recommenced with a session chaired by Prof **Bernadette Byrne** (Imperial). The first speaker in this session was Prof **Xiaodong Zhang** (Imperial) who gave a presentation entitled: Mechanism of transcription initiation and DNA opening. Prof Zhang began by emphasising how these processes impact on transcription and translation, which are central to the dogma of modern molecular biology. Prof Zhang explained that her main interest in this field is discovering the mechanism of DNA opening and template strand delivery. Opening of the DNA molecule is pivotal to replication, transcription and homologous recombination. Prof Zhang explained how the X-ray structures of yeast and human RNA polymerase in its closed form bound to DNA had been solved by other groups in prior work. Prof Zhang described the subunit structure of the prokaryotic enzyme and how it associates with the promoter region of DNA and, coupled with the binding of a σ factor upstream, it is able to bend the DNA molecule, forming an open complex ready for transcription. An activator ATPase is also involved in

this process. Prof Zhang described how they expressed selenomethionine labelled σ_{54} and used the resulting anomalous data to show where the sigma factor bound to the polymerase. Part of the σ_{54} molecule occupies the DNA-binding path, thus inhibiting the polymerase, and another part blocks the RNA exit channel. Prof Zhang explained how the conformational transition from the closed to the open state is mediated by the activator protein which relieves the inhibition imposed by the sigma factor. DNA opening involves the formation of a 'bubble' in the DNA starting at position -12 and large changes in the sigma factor. Prof Zhang summarised the process as being one of DNA binding to the polymerase followed by closure of a clamp region in the enzyme which causes the DNA duplex to unwind.

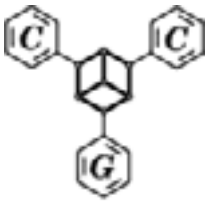
Next up, Dr **Doryen Bubeck** (Imperial) gave a presentation entitled: CryoEM reveals how the membrane attack complex (MAC) ruptures lipid bilayers. Dr Bubeck began by explaining the role of the complement system in innate immunity and how the protein CD59 protects innocent host cells from attack. Following activation of the complement cascade, the protein C9 forms a β-sheet pore in the plasma membrane which results in osmotic lysis of the target cell. Once fully assembled, the MAC has a molecular weight of around 1.8 mega-Daltons. The C8 protein also has a membrane penetrating region and is similar to a number of bacterial toxins. To study the MAC, the X-ray structures of individual complement factors have been fitted to lower resolution EM reconstructions of the entire complex. Dr Bubeck explained how her group had set about forming MACs on liposomes and, following solubilisation, had studied their structures using the new eBIC cryo-EM facility at Diamond. The assembly was found to have a split-washer structure with long β-hairpins forming the transmembrane pore. The transmembrane hairpins are formed by α-helix to β-sheet transitions within part of the C9 protein. Intriguingly, glycans are attached to the hydrophobic β-sheet pore all around its diameter, although removal of these sugar regions with PNGase does not affect the lytic activity of the complex. After sophisticated image analysis, her group achieved a resolution close to 4.5 Å for the MAC structure. It was shown that the complex adopts open and closed forms with the β-barrel being fully closed in the latter conformation. Dr Bubeck explained how charge-complementarity of the complement proteins causes their ordered assembly into the MAC – a process being studied by flicker spectroscopy. Dr Bubeck concluded by giving a comparison with bacterial β-pore forming proteins, such as pneumolysin, since these are found to have homology with the MAC pore-forming domain.

Last but not least, Prof **Radu Aricescu** (MRC LMB Cambridge) gave an interesting presentation entitled: Human $GABA_A$ receptor structures and signalling mechanisms. The receptor molecule is a pentamer made of three distinct protein components and acts as a ligand-gated chloride channel. It is the principal mediator of rapid inhibitory synaptic transmission in the brain and mutations are known to cause epilepsy, insomnia and anxiety. Prof Aricescu explained that there are 19 $GABA_AR$ genes in the human genome and the crystal structure of a (non-physiological) pentamer of β_3 subunits was first determined by his group, demonstrating a large α-helical transmembrane domain. The physiological heteromeric form of the receptor was solved by cryo-EM and demonstrated the existance of glycans in the pore or vestibule of the protein. In the face of some competition, the structure of the receptor was determined in the presence of nanobodies at 3.1 Å resolution. The receptor is well known in the pharmacology field as the target for benzodiazepines, barbiturates and anaesthetics, as well as insecticides. The structure of picrotoxin (a plant convulsant) bound to the protein was determined demonstrating that, as a channel blocker, this molecule binds directly in the pore of the receptor. The complex with GABA itself was then determined by cryo-EM showing that it binds mainly by interactions with aromatic amino acids, accompanied by closing of the C-loop of the protein. A complex with the antagonist bicuculline was solved at 3.7 Å resolution demonstrating that it bound by making similar interactions to GABA. The binding of benzodiazepines was also studied demonstrating that this class of drug binds in the anaesthetic pocket (site 2) thus stabilising the heteromer at its weakest interface. Complexes with flumazenil and bretazenil were also determined. Prof Aricescu concluded by saying that the pentameric receptor has only two GABA binding sites and binding of this neurotransmitter causes the main pore of the receptor to open.

This ended an exceptionally interesting day which all attendees very much appreciated. The organisers, who must be congratulated for arranging such an excellent meeting, invited the audience to thank all of the speakers, some of whom had accommodated a number of last minute changes to the programme. The meeting was concluded with a vote of thanks for the organisers from Dr **Mike Hough** (Essex), vice chair of the Biological Structures Group, and was followed by an excellent speakers' dinner at the nearby Ognisko restaurant till late into the night.

Jon Cooper

Chemical Crystallography Group (CCG) Meeting 2018



THE CCG ran a one-day Autumn Meeting in the School of Pharmacy at Queen's University Belfast in 2018. Investigating 'Chemical Crystallography @ Central Facilities', the meeting offered a wide variety of scientific talks about and around central facilities in the UK and Europe. Offering a poster session for the breaks and travel bursaries, the CCG actively encouraged participation of early-career researchers, whilst interaction was fuelled with coffee and scones. Four poster prizes were awarded to outstanding contributions, and discussions continued during the after-session in a near-by pub. Overall, this meeting was a success thanks to very engaging speakers, a good number of posters, superb discussions by all participants.

The meeting ran four sessions during the day starting off with the invited plenary delivered by Dr **Radoslaw Kaminski** from

Dr Katharina Edkins opening the meeting as local organiser

Warsaw University. This contribution was kindly sponsored by the BCA IG. Dr Kaminski took us into the field of time-resolved X-ray Laue diffraction to study metal-metal interactions. This was followed by the second talk of the day by Dr **Silvia Capelli** from the ISIS neutron and muon facility giving the audience a quick virtual tour of the facility, introducing the benefits of neutrons and showing what can be done at ISIS towards chemical crystallography.

After the sponsored first coffee break, Dr **Christine Beavers** from the Diamond light source gave us her take of science done and possible at synchrotron facilities beginning with a concise history of these central facilities. Following this, two PhD students talked about their research: Firstly, **Lois Wayment** from the University of Bath reported her results using *in situ* XRD analysis of continuous crystallisation, a topic highly important for industry. This was followed by the talk from **Laila Al-Madhagi** from the Schroeder group at Leeds University. She talked about the structural evolution of imidazole during cooling crystallisation. Of particular interest was her use of X-ray pair distribution functions to solve this problem.

After the lunch break and poster session the scientific programme was continued by a skype talk by Dr **Marie-Hélène Lemeé-Cailleau** from the Institut Laue-Langevin in Grenoble, France. She presented the instruments open for users at the European central facility and gave examples of research ranging from the inorganic to the biochemical fields. In the following talk, Dr **Helena Shepherd** presented her research on spin-crossover materials by using extreme conditions at central facilities.

The last session of the day was started off by Dr **Tim Easun** from Cardiff University talking about his combination of experimental approaches using the central laser facility on solid luminescent materials. As final speaker of the day, Dr **Scott Woodly** from University College London talked about the central computing facility ARCHER and simulations that can be run on this cluster towards understanding solid materials.

Some speakers and session chairs: Front row from left to right: ***Dr Christine Beavers***, ***Dr Tim Easun***, ***Dr Helena Shepherd***, back row from left to right: ***Dr Radoslaw Kaminski***, ***Dr Lauren Hatcher***, ***Dr Scott Woodly***, ***Dr Mark Warren***

Katharina Edkins
Queen's University, Balfast

Joint BCA Industrial Group (BCA-IG) Meeting 2018

Student report on the Joint British Crystallographic Association Industrial Group and CCP-NC Autumn Meeting

Holistic Approaches to Structural Characterisation

THE BCA-IG conference on 'Holistic Approaches to Structural Characterisation' was held at the Marriott Hotel in Durham on the 13th and 14th November organised by Paul Hodgkinson from the University of Durham, Helen Blade from Astrazeneca, and Luca Russo from GlaxoSmithKline (GSK).

The first day of the conference began with an introduction by Paul, who then introduced Helen as the first chair for session one, 'Role of Nuclear Magnetic Resonance (NMR) crystallography'. The first speaker of session one was **Jonathan Yates** from the University of Oxford's Materials department who answered the important question of 'What is NMR Crystallography?' describing nuclear spins as 'spies' that can provide important chemical information about their environments. He spoke about the high sensitivity of NMR spectroscopy and its growing popularity in the crystallography world. This was then linked to other analysis methods such as density functional theory (DFT) calculations and first principle analysis, which together with NMR can provide increased confidence in powder X-ray diffraction (XRD) structures, for which he provided examples. He also explained the AIRRS method for ranking crystal structures.

Neil Feeder, an industry expert working as an independent solid form consultant, gave a speech titled 'Why are Crystal Structures So Important and the Challenges We Face Getting Them?' He started by explaining the key factors to be considered to obtain a crystal structure including alternative elucidation methods. He then spoke about the importance of considering polymorphism of chemical structures, especially in pharmaceuticals, providing an anecdote about a drug that had been previously taken off the market due to unaccounted-for polymorphism.

The second session titled 'Structural Characterisation –

Complementary Techniques' was chaired by **Andrew Goodwin** of Oxford University's 'order, disorder, flexibility, function' group. This session included talks on methods of spectroscopy that used a variety of electromagnetic wavelengths. The first speaker was **Kenneth Harris** from the University of Cardiff's physical chemistry of solids group who spoke about 'Structure Determination of Organic Materials from Powder X-ray Diffraction Data: opportunities for multi-technique synergy'. He highlighted the importance of the quality of data collection and advised that screening the sample to check if it is multi-phase is an optimal starting point. He also stated that checking for preferred orientation before embarking on structural analysis can save time as if there is indeed a preferred orientation the sample must be re-prepared repeatedly until it disappears; normally this is done with an amorphous material.

Axel Zeitler from the University of Cambridge's Chemical Engineering and Biotechnology department was the second speaker of the session whose presentation was titled 'Terahertz Spectroscopy as a Complementary Technique for Structural Characterisation'. This technique is a high frequency version of dielectric spectroscopy, Axel stated, and went on to explain that it examines weaker forces in larger masses, such as hydrogen bonds in the whole molecule in a sample. The peaks in a spectrum are not assigned intuitively; therefore this technique is used in conjunction with DFT calculations, and in fact will provide validity of the calculations.

The final speaker of the morning, and of session two, was **Andy Brown** from the Engineering department of Leeds University, presenting on 'Analytical Electron Microscopy: prospects for atomic lattice imaging of organic crystals'. This method uses lower magnification meaning lower dosage applied to the sample; the spectrum can then pick up the defects and see where the probe has damaged the crystal. This is a sparse imaging technique with the probe at around 4 Ångstroms thus allowing it to outrun the damage, and it can be used to image organic compounds.

Following lunch in the hotel's restaurant, Market Kitchen, the conference attendees reconvened for session three, 'Early Career Session and Discussion', which was chaired by Luca. The first presentation was titled 'AIRSS: exploring disorder in hydrous Earth minerals and the basis of a new code for predicting experimentally accessible materials' given by **David McKay** from the University of St Andrews. This involved examining predicted and experimental ^{1}H double quantum magic angle spinning (DQMAS) NMR experiments for minerals from the Earth's mantle. David used AIRSS to generate random unit cells that were scaled to target volumes, which in combination with solid-state NMR has provided analysis of Earth minerals. The final talk of session three, and day one, was given by **Emily Corlett** from the University of Warwick titled 'A combined XRD, NMR and DFT Approach for the Characterisation of Multi-Component Crystals'. Emily presented examples of using the main complementary NMR crystallography techniques outlined in the conference to look at crystalline structures of multi-component systems containing fumarates. There was a discussion session at the end where some of the delegates shared the obstacles being encountered in their current research in hope to assist and encourage ideas in one another.

Conference attendees enjoying a three-course dinnerat the Radisson Blu Hotel.

Day one ended with an annual general meeting for industry members followed by a three-course dinner for all conference attendees at the Radisson Blu Hotel.

Day two of the BCA-IG conference began with **Kenneth Harris** giving an introduction and then chairing session four, 'Understanding Local Disorder – Amorphous/Hydrates/Solvates'. **Paul Hodgkinson** presented the first talk of the day titled 'NMR Crystallography of Disorder in Molecular Organics'. He spoke about observing dynamics via the relationship of T_1 as a function of temperature and that if the changes in a variable temperature experiment are reversible it indicates dynamics. He also mentioned the issues introduced from using solvates and the fact that the term amorphous is not uniform; a sample can be X-ray amorphous but not necessarily when using NMR spectroscopy. He concluded by saying that the use of computational chemistry with NMR helps to characterise why something is disordered thus allowing control and favourable adjustments.

The second talk of session four was presented by **Andrew Goodwin** on 'Nano Crystallography: pair distribution function (PDF), Bayes, ferrihydrite'. He began by explaining the use and implementation of PDFs, highlighting the main issue – the uniqueness problem; the PDF can be identical for molecules with the same number of atoms but very different three-dimensional structures, which can be problematic for amorphous substances. Bayes theorem then allows the likelihood of each model to be considered. He showed these techniques applied to ferrihydrite, a source of iron on Earth and Mars, which so far has been difficult to understand structurally.

Session three's final talk was given by **Tran Pham** from GSK titled 'Solid-State NMR and Computational Chemistry for Practical Pharmaceutical Problem Solving' that helped to truly bring crystallography into scenarios applied in industry. He began by emphasising the importance of fully understanding crystal structures for a pharmaceutical company and how the experimental data from both solution and solid-state NMR spectroscopy is compared with calculated structures. This is then combined with geometry optimisation using the CASTEP programme.

The fifth and final session of the two-day conference, 'Structure Property Relationship/Computational', was chaired by **Steven Brown** from the University of Warwick's solid-state NMR group. The first speaker introduced by Steven was **Aurora Cruz-Cabeza** from the University of Manchester's School of Chemical Engineering and Analytical Sciences whose talk was titled 'Conformational Aspects of Molecular Crystals'. She began by highlighting the importance of molecular conformation, especially in the pharmaceutical industry where it is imperative to know whether the drug will bind with the receptor. She mentioned how the MOGUL programme identifies unusual torsion angles by comparing the observed value with the

distribution of the population in the database. The main interest for her research was the impact of molecular shapes on crystal packing and examining how many conformations are needed to pack. She also spoke about unusual adjustment and conformational polymorphism, and how it impacts the properties of the substance, such as colour, stability, and solubility, again important considerations within industry.

The final presentation of the session, day, and entire BCA-IG conference, was given by **Cheryl Doherty** of Pfizer whose talk was titled 'Managing Risk during Drug Product Design by Understanding the Relationship between Structure and Property'. This research was done using X-ray tomography attempting to understand conversion between crystal forms during drug processing and ensuring drug survival for extended periods of time in storage. The focus of this talk emphasised the importance of knowing any possible dangers from leaving the drug for hours, days, or longer in case of delays that can occur during mass production. She concluded by acknowledging that increased accessibility to single-crystal XRD and computational resources have allowed better research and that she expects this to continue to get better with increased drug production.

Steven gave final thanks to the organisers before the attendees dispersed returning back to their various departments across the U.K.

A big thank-you to Luca, Paul, and Helen (pictured above) for organising such an informative and interesting conference, and to all of the speakers whose thought-provoking talks made the two days fly by.

Report prepared by Kiran Jandu, Zainab Rehman, Anjali Menakath, Sarah Mann, and Jacqueline Tognetti of the Solid State NMR group at the University of Warwick, pictured above with supervisor Steven Brown.

Reflections on the meeting by
Jake Musselle-Sexton (Newcastle University)

The BCA-IG Meeting in Durham was a wonderful opportunity to learn about many new techniques and facets of work beyond standard structure determination and to meet several researchers I may not have met at any of the other BCA crystallography meetings.
It was enjoyable to learn about the techniques used and the level of detail that SS-NMR could provide when analysing crystal structures and the various defects that were discussed. The technique, which was new to me, was well explained in opening talks by **Jonathan Yates** (Oxford) and **Neil Feeder** (Solid Form Consultant) which allowed novices of the field like myself to catch up on how and why this technique is used. I personally found it exciting during **Cheryl Doherty**'s (Pfizer) talk to see how crystallography and polymorphism affect the pharmaceutical industry and more importantly how they adapted their work to overcome the issues associated with this, as I used to work within a pharmaceutical company. These meetings help too with PhD researchers to look to the future and the impact of the work they could be doing when finishing their studies.

During breaks it was great to talk to the friendly representatives from Bruker about both X-ray diffraction and NMR. I am thankful to the organisers for inviting me to come to the meeting which I would have otherwise been unable to attend.

Physical Crystallography Group (PGG-SCMP) Meeting 2018

THE 2018 Winter Meeting of the Physical Crystallography Group was held on 5 and 6 November. Having outgrown our previous venue, the Cosener's House, we moved for the first time to the luxurious Milton Hill House, still not too far away from the Rutherford Appleton Laboratory. We were pleased to be joined once again by the ISIS Crystallography User Group and, for the first time this year, the Diamond Crystallography User Group, for a meeting that showcased an extraordinary variety of crystallographic and neighbouring techniques applied to a range of interesting and important materials.

Phoebe Allan (Birmingham) began the meeting in style, describing her work using pair distribution function analysis to probe anode materials for sodium-ion batteries. Other energy materials were represented by the work of **Maria Diez-Lopez** (ISIS) and **Julia Payne** (St Andrew's), while among other functionality **Tong Zhu** (Oxford) introduced electric polarisation and **Richard Dixey** (Kent) the magnetocaloric effect.

In the second session, **Emily Reynolds** (Oxford) gave the first of several talks that would emphasise the importance of disorder even in crystalline materials, discussing the behaviour of asymmetrical linkers in coordination framework materials. This was followed by two talks on electrical functionality –

Physical Crystallography Group pictured at Milton Hill House

Josie Auckett (Durham) on ionic conductors and **Rebecca Clulow** (St Andrews) on a ferroelectric calcium complex. **Harry Geddes** (Oxford) returned to the theme of disorder from a different angle in his work characterising the content of pharmaceutical materials, while **Thomas Simm** (Swansea) introduced an engineering perspective, analysing microstructural changes under plastic deformation.

The first day of the conference concluded with the prize lecture from **Lewis Owen** (Cambridge), the winner of this year's Malvern Panalytical Thesis Prize, which was presented by **Andrew Walton** and **Paul O'Meara**. Lewis' work using total scattering to analyse the local structure of alloys had been described by the prize judges as "highly accomplished" and leading to "valuable insights", and his impressive talk certainly bore this out.

Left to right: ***Lewis Owen*** (Cambridge), the winner of this year's Malvern Panalytical Thesis Prize, presented by ***Paul O'Meara***

The next morning, high-pressure techniques were represented by a comprehensive overview from **Christine Beavers** (Diamond), newly enticed across the Atlantic to lead beamline I15, and an entertaining explanation from **Dean Keeble** (Diamond) of why pair distribution function measurements under pressure are both tricky and worthwhile. Between **Mara Capone**'s (Edinburgh/ISIS) work on perovskites, **Hanna Boström**'s (Oxford) on Prussian blue analogues, and **Simon Parsons**' (Edinburgh) on molecular solids, we saw that pressure studies are relevant to almost any class of material.

This was followed by a session book-ended by **Edward Bilbe** (Johnson Matthey), discussing structure solution of an enigmatic series of platinum complexes from powder diffraction, and **Tom Bennett** (Cambridge) on metal-organic glasses. The diverse talks between ran the gamut from tomography of plant roots (**Thomas Clark**, Southampton/ISIS/Diamond) to titania nanoparticles (**Xiao Hua**, Oxford), via spin-ice analogues in cyanide frameworks (**Chloe Coates**, Oxford) and mechanochemical framework syntheses (**Jethro Beamish-Cook**, Reading).

The Winter Meeting wouldn't be complete without some magnetic scattering, and the final session of the meeting began with two interesting talks on different complex systems: **Roger Johnson** (Oxford) presented work on quadruple perovskites and **Anuradha Vibhakar** (Oxford) on diffuse scattering from a pyrochlore system. The meeting concluded with presentations from **Matthew Cliffe** (Nottingham) on the less well-known but fascinating metal-thiocyanate frameworks and **Fabio Orlandi** (ISIS) on the ferromagnetic shape-memory alloy Ni_2MnGa.

Thanks to continued sponsorship from the Institute of Physics and the ISIS Crystallography Users Group, we were able to present the biggest ever Winter Meeting at no charge to attendees. We are delighted to thank Malvern Panalytical for their continued sponsorship of the thesis prize, and **Helen Playford**, **Steve Hull**, and the **ISIS User Office team** for organising the meeting.

This year's meeting will be held on 4 and 5 November 2019, once again in Milton Hill House – *save the date!*

Anthony Phillips
Queen Mary University of London

The second Pan-African Conference (PCCr2)

THE second Pan-African Conference on Crystallography (PCCr2) promised to be a unique event. One reason for this was that it was to be coupled (for the first time) with the second African Light Source conference (AfLS2). This made for an interesting blend of structural science with the politics of establishing a synchrotron on the continent – which in itself meant that two different communities that share a common interest came together. This presented the scientific organising committee with a challenge that was both exciting and testing at the same time!

The conference delegation

Any event held in Africa is assured to be a unique experience – and this meeting was no exception! The conference was held in Accra, the capital of Ghana. I am no stranger to this country and so was confident that this nation of very welcoming, relaxed and happy people would make wonderful hosts. Ghana, a former British colony that was the first to gain its independence in 1957, is a very laid back and safe African nation – and this certainly helps when hosting a multinational conference. Accordingly, the delegation was very diverse indeed – most African nations were represented and they were joined by colleagues from numerous European countries, the USA, Brazil, Japan and Australia to name but a few. It was especially encouraging to see not only ethnic diversity, but also a reasonable gender balance – particularly from the strong representation of the student community. A particular feature of this conference was the fact that so many nations and organisations come together to support it – alongside student bursary support from the BCA, UK contributions also came from CCDC, Diamond, Wellcome and the RSC and without such funds most African students simply wouldn't be able to attend. Furthermore, given the goals of AfLS2, organisations such as IUCr, UNESCO, The International Science Council, The Royal Society and The African Academy of Science also attended and made strong contributions.

The meeting was held at a well-equipped conference centre at the University of Ghana, Legon. We commenced with a day of pre-conference workshops on protein crystallography, including a remote session on beamline I04 at Diamond by **Ralf Flaig** and introductory sessions on powder diffraction that led into the Open Lab hosted all week by Bruker who brought along a benchtop instrument to collect data for conference participants.

The meeting was opened by Ghana's Minister for Science who was formally representing the President himself – an indication of how seriously this conference was being taken by politicians. And then there was of course some drumming and traditional dancing! **Tom Blundell** gave a typically reflective and inspirational plenary lecture to begin the conference proceedings and fittingly next to him on stage was a model of Vitamin B12 donated to the University of Ghana by **Dorothy Hodgkin** (a long-time supporter of African science, she accepted her Nobel Prize while working in Ghana!). Parallel sessions then covered PCCr2 and AfLS2 topics respectively throughout the week, as well as CCDC conducting a day-long workshop. A city tour, with a particular highlight being a local craft market where haggling skills were somewhat tested, preceded the banquet. The food provided by our hosts was excellent and this was of course followed by more drumming and dancing.

Dorothy Hodgkin's model of Vitamin B12 given as a gift to the University of Ghana

The meeting lasted 5 days in total and covered most topics in crystallography. It was also highly successful in moving along the agenda for the construction of an African synchrotron – it seems clear that this will now happen and alongside political pledges, a roadmap to a feasibility design study was defined. The AfLS2 sessions also had a traditional twist to them involving the exchange of sticks – at Ashanti tribal gatherings a symbolic 'speaking stick' was given by the chief to a speaker at

Richard Catlow receiving the speaking stick from ***Felix Dapare Dakora***, President of the African Academy of Science

Traditional dancing at the conference banquet

community meetings and this act was also conducted between session chairs and their speakers! Finally, the close of the conference was marked by the establishment of a committee charged with bringing the African Crystallographic Association and the next Pan-African conference into being by 2021 – they certainly have their work cut out for them, but are clearly up for the challenge!

Simon Coles
University of Southampton

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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.

2-6 March 2019
Biophysical Society Annual Meeting, Baltimore, MD, USA.
https://www.biophysics.org/2019meeting#/

7-8 March 2019
Microscopy characterisation of organic-inorganic interfaces – 2019, Berlin, Germany.
https://mcoii-2019.mpikg.mpg.de/

11-22 March 2019
50th IFF Spring School: "Scattering! Soft, Functional and Quantum Materials", Jülich, Germany.
http://www.fz-juelich.de/pgi/EN/Leistungen/SchoolsAndCourses/SpringSchool/

17-20 March 2019
2019 West Coast Structural Biology Workshop, Asilomar, CA, USA.
https://wcsbw.chemistry.ucsc.edu/registration/

17-22 March 2019
School and Conference on Analysis of Diffraction Data in Real Space, Grenoble, France.
https://workshops.ill.fr/event/133/

25-28 March 2019
27th Annual Meeting of the German Crystallographic Society (DGK), Leipzig, Germany.
https://www.dgk-conference.de/

6-14 April 2019
17th BCA/CCG Intensive Teaching School in X-ray Structure Analysis, Durham.
https://community.dur.ac.uk/durham.x-ray-school/general.htm

9-12 April 2019
21st International Conference on Microscopy of Semiconducting Materials (MSM-XXI), Cambridge.
http://msmxxi.iopconfs.org/Home

15-18 April 2019
BCA Spring Meeting, Nottingham.
https://www.crystallography.org.uk/spring-meeting-2019/

15-18 April 2019
ISSC-22. Interdisciplinary Surface Conference, Swansea.
http://issc-22.iopconfs.org/home

22-26 April 2019
2019 MRS Spring Meeting & Exhibit, Phoenix, AZ, USA.
https://www.mrs.org/spring2019

29 April – 1 May 2019
CCP-EM Spring Symposium, Nottingham.
http://www.cvent.com/d/xbqsqk

5-10 May 2019
RapiData2019, Menlo Park, CA, USA.
http://smb.slac.stanford.edu/news/rapidata/rapidata-2019/

19-21 May 2019
2nd Annual Industrial Biostructures America, San Diego, CA, USA.
https://industrialbiostructuresamerica.org/

19-24 May 2019
Biological and Soft Matter Sample Preparation for High Resolution Imaging by High Vacuum Techniques. 89th IUVSTA workshop, Zakopane, Poland.
http://www.npl.co.uk/89th-iuvsta-workshop/

20-21 May 2019
Ubiquitin & Friends symposium, Vienna, Austria.
https://ubiquitin.at/

20-22 May 2019
CNIO Frontiers Meeting. Structural and molecular biology of the DNA damage response, Madrid, Spain.
https://www.cnio.es/en/eventos/structural-and-molecular-biology-of-the-dna-damage-response-2/

21-23 May 2019
ESRF workshop on sample preparation for Cryo-EM, Grenoble, France.
http://www.esrf.eu/events/conferences/

31 May – 9 June 2019
Cryo 3D Electron Microscopy, Erice, Italy.
https://crystalerice.org/2019/

31 May – 9 June 2019
Magnetic Crystallography, Erice, Italy.
https://crystalerice.org/2019/

2-6 June 2019
14th International Symposium on Macrocyclic and Supramolecular Chemistry, Lecce, Italy.
https://ismsc2019.eu/

2-8 June 2019
4th International Summer School of Crystallography, Hamburg, Germany.
https://conferences.cfel.de/issc19/

3-7 June 2019
Summer School on Mathematical Crystallography, Nancy, France.
http://www.crystallography.fr/mathcryst/nancy2019.php

4-7 June 2019
MLZ Conference 2019: Neutrons for Information and Quantum Technologies, Lenggries, Munich, Germany.
https://indico.frm2.tum.de/event/157/

9-14 June 2019
33rd Annual ResMed Course: The Residential School on Medicinal Chemistry and Biology in Drug Discovery, Madison, NJ, USA.
http://www.drew.edu/science-research/about-us/resmed/

12 June 2019
BCA-IG XRF Meeting, Sheffield.
https://sites.google.com/site/bcaxrf/

16-27 June 2019
The Zurich School of Crystallography 2019: Bring Your Own Crystals, Zurich, Switzerland.
http://www.chem.uzh.ch/linden/zsc/

17-19 June 2019
4th International Conference on Resonant Elastic X-ray Scattering (REXS 2019), Long Island, NY, USA.
https://www.bnl.gov/rexs2019/

17-24 June 2019
12th annual CCP4/APS school in macromolecular crystallography "From data collection to structure refinement and beyond", Argonne (near Chicago), USA.
https://www.ccp4.ac.uk/schools/APS-2019/application.php

23-28 June 2019
11th International Conference on Inelastic X-ray Scattering (IXS2019), Stony Brook, NY, USA.
https://www.bnl.gov/ixs2019/

1-5 July 2019
10th Workshop _ Combined Analysis in XRD by using MAUD software, Caen, France.
http://www.ecole.ensicaen.fr/~chateign/formation/agendas/2019agenda.pdf

1-5 July 2019
European Conference on Neutron Scattering, St Petersburg, Russia.
http://www.ecns2019.com/

1-5 July 2019
Mechanisms and Non-Linear Problems of Nucleation and Growth of Crystals and Thin Films, St Petersburg, Russia.
http://www.mgctf.ru/

1-5 July 2019
Intergranular and Interphase Boundaries in Materials, Paris, France.
http://iib2019.org/

4-5 July 2019
Macromolecules in Action, Grenoble, France.
http://www.esrf.eu/psbsymposium

8-11 July 2019
UCANS8: International Meeting of the Union for Compact Accelerator-Driven Neutron Sources, Paris, France.
https://ucans8.sciencesconf.org/

8-12 July 2019
DMI 2019. V International Workshop Dzyaloshinskii-Moriya Interaction and Exotic Spin Structures, Petrozvodsk, Russia.
https://oiks.pnpi.spb.ru/events/DMI-2019

9-11 July 2019
50th Annual Meeting of the British Association of Crystal Growth, Central London.
https://www.bacg.co.uk/bacg-50th-annual-conference/

20-24 July 2019
American Crystallographic Association Annual Meeting, Covington, KY, USA.
http://www.amercrystalassn.org/content/pages/main-annual-meetings

21-27 July 2019
The 17th International Summer School on Crystal Growth (ISSCG-17), Keystone, CO, USA.
http://www.crystalgrowth.org/ICCGE-19_-_ISSCG-17_Flyer_7-20-16.pdf

28 July – 2 August 2019
19th International Conference on Crystal Growth and Epitaxy (ICCGE-19) and 19th Biennial Workshop on Organometallic Vapor Phase Epitaxy (OMVPE-19), Keystone, CO, USA.
https://www.iccge19.org/

4-8 August 2019
Microscopy & Microanalysis (M&M 2019), Portland, OR, USA.
https://www.microscopy.org/MandM/2019/

18-23 August 2019
32nd European Crystallographic Meeting, Vienna, Austria.
https://ecm2019.org/home/

1-4 September 2019
17th ECSSC European Conference on Solid State Chemistry, Lille, France.
https://ecssc17.com/

2-6 September 2019
1st International Conference on Non-Covalent Interactions, Lisbon, Portugal.
http://icni2019.eventos.chemistry.pt/#page-top

16-18 September 2019
International Conference on Materials Science and Engineering, Melbourne, Australia.
https://www.materialsconferenceaustralia.com/

23-26 September 2019
J-PARC Symposium 2019, Tsukuba, Japan.
http://j-parc.jp/symposium/j-parc2019/

24-25 September 2019
International SAXS Symposium 2019: SAXS excites, Graz, Austria.
https://www.anton-paar.com/tu-graz/saxs-excites

1-6 October 2019
Hot Topics in Contemporary Crystallography 4 Structural Biology, Mlini, Dubrovnik, Croatia.
http://htcc4.org/

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