Crystallography News

British Crystallographic Association

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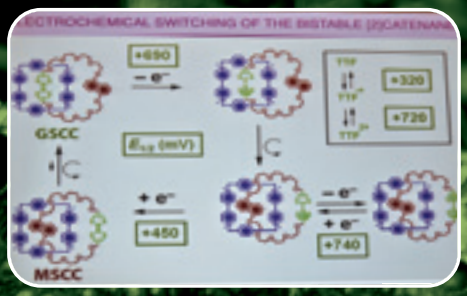

2017 ACA Meeting in New Orleans

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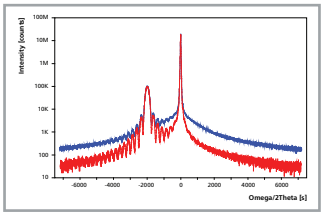

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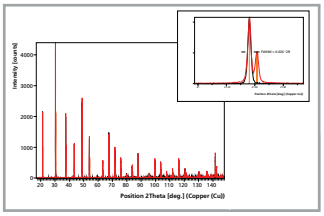

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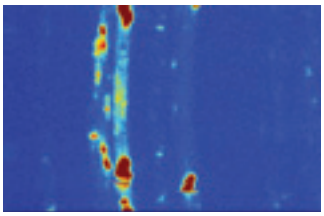

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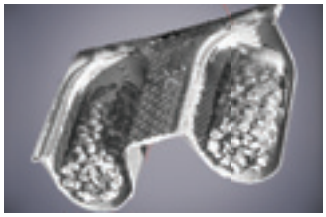

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Please ensure that items for inclusion in the December 2017 issue are sent to the Editor to arrive before 25 October 2017.

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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:

ACA, New Orleans and Louisiana scenes, photographed by Joan Schwalbe

From the President

SINCE my last column plans have moved forward for the 2018 Spring Meeting. This will be held on the campus of University of Warwick, which is well-equipped for staging the conference. Warwick was most recently visited by the BCA for the 2012 Spring Meeting, but was also the venue for the 2013 ECM. The 2018 Programme Committee, chaired by Leo Brady, met on June 1st at the conference venue and the programme is taking shape. An outline can be found elsewhere in this issue and will also be available via the BCA website, which will be updated as the programme develops. In 2018, the Dorothy Hodgkin Prize Lecture will be given by Prof. Eleanor Dodson (University of York) and the Lonsdale Lecture will be given by Prof. Bill Clegg (University of Newcastle).

We are also planning ahead for future Spring meetings, and have already approved a return to University of Nottingham in 2019. We are currently exploring venues for 2020, but are finding that fewer and fewer universities are making available their accommodation and meeting facilities for use during the traditional Easter break. We have also considered the possibility of moving away from a campus meeting, but so far such options have proven to be considerably more expensive. We would be keen to hear from BCA members regarding where you would like future meetings to be held.

I would like to re-iterate the process for nomination of candidates for positions on BCA Council as the nomination deadline will be fast approaching when this issue of *CN* appears. It is important to note that no changes have been made to the current mechanism for nomination of candidates by two BCA members. This nomination process will continue alongside that involving the Nominating Committee, also using the **Sept 30th nomination deadline**. In the interests of fairness to all candidates, the mechanism by which candidates have been nominated will not be identified prior to elections. The inaugural BCA Nominating Committee has been appointed. Its members are: **Elspeth Garman** (BSG), **Paul Raithby** (CCG), **Paul Fewster** (IG, **Phil Lightfoot** (PCG) and **Dave Keen** (BCA Past-President). Elspeth Garman has agreed to serve as chair of the committee. Nominations will be needed for the positions of President, Education & Outreach Officer and Ordinary Member. My term as President ends in April 2018. **Simon Coles** completes a 3-year term as Education & Outreach Officer, but is eligible to stand for re-election. Similarly, **Mark Senn** completes a 3-year term as Ordinary Member of Council, but is also eligible to stand for re-election. I would like to encourage all BCA members to send suggestions for nominations to the new Nominating Committee or considering standing for election or making nominations themselves.

The four BCA Officers held our summer teleconference meeting on July 14th and discussed a variety of future planning matters. The next full BCA Council Meeting will be held in Oxford on September 19th.

As I write this column, the IUCr Congress in Hyderabad is only a couple of weeks away. I expect there is likely to be a good attendance by UK crystallographers and have noted UK keynote speakers in previous column. I'm pleased that the BCA Arnold Beevers bursary fund will be able to support 5 students who are attending the Congress: **Amy Danson** (University of Reading), **Dannielle Kydd-Sinclair** (University of Reading), **Charlie McMonagle** (University of Edinburgh), **Rebecca Eno** (Durham University) and **Matthew Dunstan** (University of Cambridge). I hope that you enjoy the meeting and look forward to reading your reports about the meeting in *Crystallography News*. I will also be at the Congress, to speak in one of the microsymposia and as part of the UK delegation at the IUCr General Assembly meetings and the ECA Council meetings. I hope to see many of you in Hyderabad.

Lee Brammer

BCA Council 2017

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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

LED by Leo Brady, the Programme Chair, our 2018 Spring Meeting at Warwick University is taking shape. An outline is presented in this issue, and further details will appear on the website as they are finalised as well as in our December and March issues. Our 2017 Spring Meeting had a wide variety of excellent sessions on biological crystallography offering too much material to write up in a hurry. I am grateful to Mark Roe and our BSG for preparing the comprehensive and considered report that appears in this issue. The same combination of wide variety and high quality was also evident in our Young Crystallographers' satellite meeting. I am grateful to Sam Horrell for providing a write-up. In June our Industrial Group held their XRF meeting. Certain aspects appear to be traditional: the date (mid-June), the venue (Leicester) and the co-sponsors (our brothers and sisters in the Royal Society of Chemistry). However, their report shows that this field is making steady progress. Furthermore, for the Autumn Meeting 21-22 November they have joined forces with our Chemical Crystallography Group on the topic "Design of Crystalline Products". Held in the agreeable surroundings of Downing College, Cambridge, it will give valuable pointers to the future for a wide variety of crystallographers.

As the Cambridge Structural Database continues its ever-swifter gallop towards the million-structure mark, it has now reached the milestone of 900,000 structures. The new arrival has the refcode PATXEQ. For old-timers like me this is reminiscent of the program PATSEE (it could be misinterpreted as "execute PATSEE"). Published by Egert & Sheldrick in 1985 [*Acta Cryst.* A41, 262-268] PATSEE enhanced our ability to solve structures by locating a fragment of known geometry through the use of combined Patterson, packing and direct methods.

The well-attended American Crystallographic Association meeting in New Orleans was full of interest. To allow a bit of time for sightseeing, Joan and I arrived 3 days before it started. Most unusually for New Orleans in May, there was a strong wind blowing all the way from Canada. Before the usual muggy heat returned, we enjoyed blue skies and low humidity during a boat trip on the Mississippi and a swamp tour where we saw numerous alligators and some very bold feral pigs. A particularly noble alligator appears on our cover. The conference featured two personal "firsts" for me, starting with the very opening session. For the first time in my life I spilled ice water on a Nobel laureate's chair! There was a buzz of excitement as we awaited the Plenary Lecture by Sir **James Fraser Stoddart** on "How Crystallography Helped to Create the Mechanical Bond in Chemistry". Joan and I arrived well in advance so that we could get seats in the middle of the front row for the best possible camera angles. Having become somewhat dehydrated in the New Orleans heat, I equipped myself with a refreshing drink of ice water. A little later, Sir James sat down beside me. Because he was obviously deep in thought about his forthcoming lecture, I didn't disturb him. I steadily sipped ice water, finishing the water during the introduction of the speaker. Engrossed in note-taking, I perched the plastic beaker with its residual ice on my chair as I hastily scribbled on hotel stationery. About 5 minutes into Sir James's talk I reached for a fresh piece of stationery and knocked my beaker, which now contained a significant amount of meltwater, sideways onto his chair. As surreptitiously as is possible in an exposed front-row position I swept the ice cubes back into the beaker and blotted the chair with a pocketful of tissues. Fortunately the very interesting talk elicited an extensive question-and-answer session, giving time for any obvious patches of wetness to evaporate. As for my other "first": that was to give 3 talks at an ACA meeting.

It is my sad duty to include another obituary, this time for **Philip Coppens**, who did so much to advance the methodology of charge density determination and the science of photocrystallography. Far from selfishly hanging on to the technology for his own benefit, he generously shared it with other interested scientists. **Paul Raithby**, our own eminent photocrystallographer, has written the obituary.

In the June issue of *Chemistry World* I found the "Last Retort" article to be thought-provoking. With the title "Now you're talking my language" it was written by **Sally Bloodworth** (University of Southampton). From the point of view of an organic chemist she described the importance and the difficulty of communicating with scientists in other fields. Given the precision inherent in our discipline, understanding terminology is of especially great importance for crystallographers. Sally illustrated her point by defining the Greek letter symbol ρ (rho), mentioning its usage by physicists to mean charge density, among other things. We crystallographers likewise use ρ to mean electron density (see the residual electron density in an *Acta Cryst.* paper) but also the density as mass per unit volume calculated from the cell dimensions, Z and the mass of a formula unit (look at your SHELXL output). Or is it the density measured by a method such as flotation? I collaborate with colleagues in pharmaceutics, who have a concept called "true density". Measured for a powder by using a helium pycnometer, it should relate only to the solid, ignoring voids and crevices. If preparation of the powder, usually by grinding, has not disturbed the crystal structure, the true density should be the same as our density. However, if surface layers have been altered, it will differ. Our familiar R factor could be a "false friend" to chromatographers, who know it as the "retardation factor". They may wonder why we spend so much time messing around with TLC but never report the conditions, and why we are childishly happy when our sample barely moves off the starting point. Fortunately, Sally works at one of the UK's greatest centres of crystallography. I suggest that she should treat her crystallographic colleagues to some cups of posh coffee and prepare to delight in our terminology and notation.

Carl Schwalbe

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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.
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Puzzle Corner

THE venues for the European Crystallographic Meeting of 2016 and the American Crystallographic Association meetings of 2017, 2018 and 2019 all are sited on important bodies of water. By doing some alchemy involving chemical symbols, identify them.

Start with two inert gases, neither one quite the lightest. Add manganese, rhodium and thorium. Add a greater quantity of phosphorus, double this amount of oxygen and sulfur, and a lot more iodine. By some innovative particle physics break the two-letter symbols into individual letters. You now have all the letters you need to identify the waterways.

Answers to June Puzzle Corner

With Einstein he can form a condensate. **Satyendra Nath Bose**

He turned protein crystallographers into plotters. **Gopalasamudram Narayanan Ramachandran**

Research institute founded in Kolkata in 1876; sounds a bit horticultural but does basic research. **Indian Association for the Cultivation of Science**

If you're a star, beware if you exceed his limit. **Subrahmanyan Chandrasekhar**

He showed how the order of nucleotides controls protein synthesis. **Har Gobind Khorana**

The first letters of the last names spell "brick".

BCA Spring Meeting
Monday 26th – Thursday 29th March 2018

WE are pleased to announce that the 2018 BCA Spring Meeting will take place at the University of Warwick from 26th until the 29th March 2018. As in recent years, this year's meeting will be prefaced by the Young Crystallographers meeting which begins at 13:00 on Monday 26th March and runs through to lunchtime on Tuesday 27th March. The main meeting will start at 10.30 am on Tuesday 27th and closes at 13.30 on Thursday 29th March. A varied programme is currently being assembled and promises highly relevant, interesting and prescient talks in every session. The programme truly offers something for everyone. Coupled with a readily accessible venue for all, this meeting is a great opportunity to catch up with the latest crystallographic science, and of course with your fellow crystallographers.

We are very pleased to announce an eminent list of prize and plenary lecturers as follows:

Hodgkin Lecture:
Prof. **Eleanor Dodson** (University of York).

Lonsdale Lecture:
Prof. **Bill Clegg** (Newcastle University).

BSG Plenary:
Prof. **Ilme Schlichting** (MPI Heidelberg).

CCG Plenary:
Prof. **Jonathan Nitschke** (University of Cambridge).

IG Plenary:
Prof. **Susan Reutzel-Edens** (Eli Lilly).

PCG Plenary:
Prof. **Nicola Spaldin** (ETH Zurich).

The traditional early-career prize session will be held on the afternoon of Wednesday 28th March. Throughout the rest of the program there will often be three sessions running in parallel in addition to a range of workshops. Brief details of the planned sessions are below, along with some practical information concerning deadlines and abstract submission. Further details and updates will be available from the BCA Spring Meetings site: http://www.bcaspringmeetings.org.uk/

We very much look forward to seeing you at Warwick University in Coventry.

Leo Brady
Programme Committee Chair

Biological Structures Group (BSG)

BSG Session (1): Membrane and multi protein complexes
Chair: Alex Cameron (University of Warwick)
Keynote: TBC

BSG Session (2): Crystallisation of macromolecules
Chair: Naomi Chayen (Imperial College)
Keynote: **Terese Bergfors** (Uppsala University)

The past two decades have seen remarkable advances in the miniaturisation, automation and analysis of crystallization experiments. However, production of high quality crystals of proteins and other bio macromolecules persistently remains a major hurdle to structure determination. The focus of this session is on strategies, techniques and tools for obtaining useful crystals for x-ray crystallography.

BSG Session (3): Structural dynamics and time-resolved crystallography
Chair: Mike Hough (University of Essex)
Keynote: TBC

Macromolecular crystallography typically provides structures that are averaged over many molecules and over the time taken to measure the diffraction data. However, proteins are dynamic, sample many functionally-relevant conformations, and undergo time-dependent structural change, e.g. through an enzymatic cycle or signalling pathway. This session will focus on the exciting science made possible by developments in structural dynamics and time-resolved X-ray crystallography using synchrotron and free-electron laser sources. Contributions describing these and other structural time-resolved methods or computational simulations are welcomed.

BSG Session (4): New instrumentation
Chairs: Pierre Aller & Anna Warren (Diamond Light Source)
Keynote: **Tim Grüne** (Paul Scherrer Institute)

Crystallisation is often the bottleneck when it comes to obtaining a crystallographic structure, due to the difficulties in obtaining crystals of suitable size for diffraction experiments. To overcome issues of getting decent sized crystals or crystals in the first instance, new instrumentation and techniques are being developed to help the user community get the most out of their samples. New beamlines at synchrotrons are maturing to accommodate smaller and smaller crystals for either regular crystallography or serial crystallography. XFEL instruments, cryoEM and microED are becoming more popular as either an alternative to regular crystallography or to obtain complementary data. This session will focus on the scientific opportunities offered by the development of new instrumentation, and how these are aiding the crystallographic community.

BSG Session (5): Protein structure and human disease
*Chair: **Svetlana Antonyuk*** (University of Liverpool)

Keynote: TBC

Changes in protein structure are associated with many human diseases. Whether studying familial disease, viral invasion or drug resistance, proteins are at the centre of nearly all therapeutic strategies. The focus of this session is on recent discoveries in targeting proteins to alter neurodegeneration in ALS, Alzheimer's and Parkinson's diseases, to understand disease mechanisms, to prevent adverse drug reactions, and recover from viral and parasitic invasion or antibiotic resistant bacteria.

BSG Session (6): Ligand binding
*Chair: **Atlanta Cook*** (University of Edinburgh)

Keynote: **Richard Bayliss** (University of Leeds)

The binding of ligands (peptides, nucleic acids, small molecules) to proteins is essential for the formation of protein complexes, allostery, enzyme catalysis and signalling. In turn, the ability of proteins to bind other molecules very specifically is exploited in drug discovery. Structural studies of ligand bound complexes are essential to understanding the rules of recognition and specificity, which will be the focus of this session.

Chemical Crystallography Group (CCG)

CCG Session (1): Chemistry in action (time resolved crystallography)
*Chair: **Claire Murray*** (Diamond Light Source)

Keynote: TBC

The inherently active nature of chemical reactions means crystallography is perfectly placed to (quite literally) shed light on how molecules move, bonds break and structures stretch or shrink. This session will explore cutting edge experiments being explored in labs and at central facilities as well as advances in *in situ* insight.

CCG Session (2): MOFS: Molecular machines, rotaxanes
*Chair: **Stephen Moggach*** (University of Edinburgh)

Keynote: TBC

Following the Nobel Prize awarded to Feringa, Sauvage and Stoddart in 2016, this session will highlight recent advances in the area of molecular machines. These fascinating materials and their properties will be the cornerstone of the session, highlighting the role of crystallography in the analysis and development of this research area.

CCG Session (3): Surfaces and polymorph selection
*Chairs: **Iain Oswald*** (University of Strathclyde) & ***Cheryl Doherty*** (Pfizer)

Keynote: TBC

Surfaces play a significant role in phase transformations and isolation of new polymorphic forms of materials. Whether it is through nucleation of pharmaceuticals on heterogeneous surfaces, or through the use of seeds to isolate new polymorphic forms, surfaces and their interaction with the molecule of interest pose key questions that are fundamental for us to manipulate the solid state. This session will explore the advances in our understanding of the role of surfaces on the isolation of particular polymorphs.

CCG Session (4): Electron diffraction
*Chair: **Andrew Stewart*** (University of Limerick)

Keynote: TBC

This session will explore the application of electron diffraction techniques to solving a broad range of crystallographic problems for small molecule crystallographers. Electron diffraction is a very versatile tool, with multiple modes which can be utilised to explore the nano world. Electron diffraction tomography (EDT) mimics X-ray crystallography at the nanoscale for *ab initio* structure solution of unknown crystals. Nano beam diffraction (NBD) can be used to identify individually nano scale crystals, whereas convergent beam electron diffraction (CBED) enables the study of crystal defects and accurate determination of crystal symmetries. While scanning electron diffraction (SED) facilitates the study of polycrystalline materials, via mapping of grain orientations, identification of multiple phases in a specimen, as well as stress and strain measurements within crystalline materials.

CCG Session (5): Service crystallography forum
*Chair: **William Lewis*** (University of Nottingham)

Keynote: **Amber Thompson** (University of Oxford)

A large proportion of published crystal structures are collected by service crystallographers. This session will offer an opportunity to share and discuss common issues and best practices encountered in a modern crystallography laboratory.

Industrial Group (IG)

IG Session: Hydrates and solvates in pharmaceuticals
*Chair: **Helen Blade*** (AstraZeneca), ***Spoorthy Dharmayat*** (GSK)

Keynote: TBC

Crystalline solvates or hydrates are frequently encountered within the pharmaceutical field and the development of functional medicines requires the need for a thorough understanding of their structural aspects along with the mechanisms of their formation and desolvation. The aim of this session is to link the critical factors important in building an understanding of solvated systems to mitigate the problems encountered when developing a solvate or a material that readily solvates. Such an understanding can be used to devise control strategies during handling, processing and storage to ensure that the desired functionality of the medicine can be achieved and maintained.

Physical Crystallography Group (PCG)

PCG Session (1): Computational crystallography
Chair: John Claridge (University of Liverpool)
Keynote: TBC
Computational techniques are important in both materials discovery and the understanding of the origin of their physical properties, particularly when combined with crystallographic studies. This session is devoted to computational structure prediction and materials "design" as well as the combination of computational techniques with experimental studies.

PCG Session (2): Ferroics and multiferroics
Chair: Mark Senn (University of Oxford)
Keynote: **Phillipe Ghosez** (University of Liege)
Ferroics are a technologically important class of materials that include ferromagnets, ferroelectrics, and ferroelastics. This session is devoted to experimental and theoretical studies that explore the relationship between structure and ferroic properties. Abstracts for talks exploring the coupling between different ferroic orderings in multiferroic materials are particularly encouraged.

PCG Session (3): Perovskites
Chair: Mike Glazer (University of Oxford)
Keynote: **Patrick Woodward** (Ohio State University)
The study of perovskites has been of increasing interest in the last 30-40 years, since they show such a large range of useful physical properties. The number of publications has been growing exponentially (approximately 22400 in 2016!). The latest discoveries centre around the discovery that so-called hybrid perovskites show a highly efficient photovoltaic effect, thus making them candidates as inexpensive solar cells. This session is devoted to the structures and properties of perovskites and perovskite-related materials.

PCG Session (4): Functional materials
Chair: Helen Playford (Warwick/ISIS)
Keynote: TBC
Much of current research effort in materials science is targeted towards improving functional materials to meet the increasingly complex demands of modern society. However, this can only be done in a rational manner if the structural origins of desirable properties are understood. The focus of this session is on the use of state-of-the-art crystallography to determine structure/property relationships in functional materials, including catalysts, batteries, fuel cells, etc.

PCG Session (5): Neutron and synchrotron techniques
Chair: Anthony Phillips (QMUL)
Keynote: TBC
The range of experiments available at central facilities goes far beyond traditional diffraction measurements. This session will focus on techniques that take advantage of modern instruments and enhance or complement our understanding of crystallographic data. Such techniques might include magnetic X-ray scattering, anomalous scattering, small-angle scattering, total scattering, and X-ray and neutron spectroscopy.

PCG Session (6): Hot topics
Chair: Jan-Willem Bos (Heriot-Watt University)
Keynote: TBC
Session covering hot topics in physical crystallography not covered by the other session themes. This could for example focus on new developments in instrumentation and data analysis or studies of "hot" materials.

Young Crystallographers Group (YCG)

YCG Sessions 1-3 will showcase the work of the next generation of crystallographers from across the BSG, CCG, PCG and IG. We aim to provide new researchers (undergraduate to postdoctoral level) with the opportunity to present their work in a relaxed, friendly environment and to encourage discussion of their work.

YCG Session (1): YCG Presentations
Chair: Matthew Dunstan (University of Cambridge)
Plenary: **Serena Corr** (University of Glasgow)

YCG Session (2): YCG Presentations: Failing badly – of all the things that can go wrong in macromolecular crystallography
Chair: Sam Horrell (University of Hamburg)
Plenary: **Ivo Tews** (University of Southampton)

YCG Session (3): Flash poster presentations
Chair: Alex Cousen (University of Bath)

YCG Session (4): When crystals go wrong
Chair: Claire Hobday (University of Bath)
Plenary: TBC
Crystals can be unpredictable, both small molecule and macromolecular ones. This session hopes to cover a wide range of topics where crystals can make you want to pull your hair out such as incomensurate crystals, quasi crystals, severe twinning, inability to calculate the phase and, hopefully, how to deal with these problems if you are unfortunate enough to encounter them.

Parkin Lecture: TBC

Registration and Abstracts

Registration and abstract submission will open in October 2017. The deadline for early-bird registration is Friday 23rd February 2018, and the final registration deadline is Tuesday 20th March 2018. The deadline for abstract submission is Friday 19th January 2018.

Programme Committee

Chair: **Leo Brady** (University of Bristol)

BCA: **Lee Brammer** (University of Sheffield), **Richard Cooper** (University of Oxford)

BSG: **Mike Hough** (University of Essex), **Mark Roe** (University of Sussex)

CCG: **Iain Oswald** (Strathclyde University), **William Lewis** (University of Nottingham)

IG: **Helen Blade** (AstraZeneca), **Spoorthy Dharmayat** (GSK)

PCG: **John Claridge** (University of Liverpool), **Jan-Willem Bos** (Heriot-Watt University)

YCG: **Sam Horrell** (DESY), **Matt Dunstan** (University of Cambridge)

Organisers: **Joanne McBratney**, **Nicola Hardaker** (Hg3 Conferences)

BCA Spring Meeting 2017 Reports

BSG Sessions

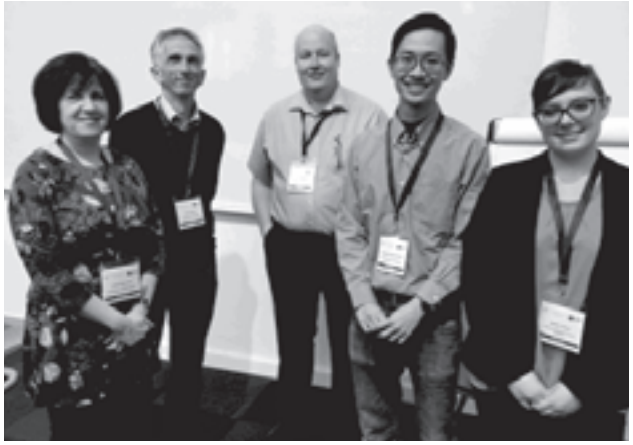
Session I: Anti-Microbial Targets

THE first session was chaired by Lydia Tabernero and was started off by Andrew Munro (Manchester) with the keynote on 'Targeting pathogen P450 enzymes using fragment screening methods'. He told us of the 20+ cytochrome P450 enzymes in the *Mycobacterium tuberculosis* genome and that this large number pointed to important roles for the enzyme. Andrew took us through the use of fragment screening to identify several low molecular weight hits with crystallography, which were then progressed on to more specific and better binding compounds.

The second talk was given by **John Rafferty** (Sheffield) titled 'Structural studies of the hemerythrin proteins in the human pathogen *Camplyobacter jejuni* using X-ray crystallography'. John showed the diffrences between hemerythrin, which has non-haem di-iron sites, and haemoglobin and haemocyanin and went on to show structures of the enzymes bound to O_2.

The third talk was by **Natalie Tatum** (Newcastle) on 'New leads for tuberculosis booster drugs by structure-based drug discovery'. After showing us the challenge of TB, Natalie showed us that EthR inhibitors boosted the efficacy of the antibiotic ethionamide. Using virtual screening and chemical knowledge, six million compounds were whittled down to just a representative 100, which then went on to biophysical screening. Co-crystal structures indicated both expected and novel binding modes and these will be used to create better compounds.

The last talk of the session was delivered by **Kangsa Amporndanai** (Liverpool) on 'One target for two parasitic diseases, the study of cytochrome bc1 for malaria and toxoplasmosis drug development'. Cytochrome bc1 is an essential enzyme for both *Plasmodia* and *T. gondii* and a number of lead compounds, shown to inhibit the redox site Q_0, have been shown to be effective against this target, but single mutations often result in resistance. This work showed new leads that bind at the Q_i site, offering novel medicines.



left to right: *Lydia Tabernero* (Chair), *John Rafferty*, *Andrew Munro*, *Kangsa Amporndanai*, *Natalie Tatum*.

Session II: Extracellular Matrix and Cell Adhesion

THE keynote lecture was given by David Hulmes (CNRS, Lyon) entitled "Structural mechanisms of intra- and extra-cellular assembly of fibrillar collagens". David explained how the ECM holds cells together and also has major roles in signaling before continuing on to the physical structure of collagen. We were shown how the pro-collagen forms the correct homo or hetero trimers in the collagen fibres. David finished his talk by looking at the proteases that remove the N-pro and C-pro domains.

left to right: *Matt Bowler*, *Alice Parnell*, *Mike Lockhart-Cairns*, *David Hulmes*, *Jordi Bella* (Chair).

The second talk was given by **Matt Bowler** (EMBL, Grenoble) on "Architecture of the *Deinococcus radiodurans* cell envelope". Matt showed how some bacteria have pseudo-crystalline layers on their surfaces (S-layers) which come in many forms. *D. radiodurans* has a hexagonally packed layer which can be separated from the bacteria and reassembled in vitro. EM analysis of one of the components showed that it was ~270Å, deep enough to penetrate to the inner membrane of the bacteria. It was hypothesized that this gave the coat extra mechanical strength, both laterally and vertically.

Mike Lockhart-Cairns (Manchester) gave the third talk entitled "Elongated structure of BMP regulator BMPER works in concert with twisted gastrulation in inhibiting BMP signaling". SAXS and EM were used to show that BMP (Bone Morphogenic Protein) and BMPER both have long elongated structures. BMPER regulates BMP signalling by binding to it and modulating it. Twisted gastrulation (tsg) also inhibits BMP signaling and appears to work in concert with BMPER.

The last talk of this session was given by **Alice Parnell** (Bristol) on "Tails of two adhesins: exploring the structure and

function of conserved adhesins from streptococci". Alice explained how targeting adhesins may provide new vaccines and antiadhesive agents. She showed crystal structures of domains of CshA (which binds to fibronectin) and BspA (expected to bind carbohydrates), which allowed explanation of their mechanism of action.

Session III: Multidisciplinary Protein Structural Analysis

SESSION III started with a keynote from Stephen Muench (Leeds) entitled "Combining Electron microscopy and X-Ray crystallography to guide structure based drug design". Stephen started by explaining how the new developments in EM technology have resulted in structures around 3Å and have allowed inhibitors to be located and refined. He presented two cases, Arabidopsis IGPO and malarial cytochrome bc1. Both are large and do not crystallise, however with the use of EM inhibitor binding could be seen clearly.

The next talk was from **Jordi Bella** (Manchester) on "Combining SAXS, hydrodynamic measurements and torsion-angle molecular dynamics for the structural analysis of macromolecular flexibility in solution". Jordi started by explaining the overall structure of multidomain proteins, like cadherin, as domains linked by flexible linkers. Standard X-Ray crystallography can get the structures of, at best, two linked domains, but larger constructs do not crystallise. With SAXS and hydrodynamic measurements as restraints on torsion-angle molecular dimensions, much larger structures could be interpreted.

The third talk on "Variable temperature serial crystallography on single crystals: making reaction mechanism movies" was presented by **Sam Horrell** (Essex). Sam was using serial crystallography to look at the turnover of NO_2 in Cu-dependent nitrite reductases, using the X-rays themselves to start the reaction. He also repeated the experiments at different (lower) temperatures, where the hydrogen transfer reactions were much slower and so could be studied more easily.

The last talk was given by **Bart van Beusekom** (NCI, Amsterdam) on "Improving low-resolution protein structure models with knowledge-based and homology-based hydrogen bond restraints". Bart showed how PDB-REDO were using high resolution structures to produce knowledge-based restraints. These were not improving low resolution structures as much as medium res structures, so they have also implemented homology-based hydrogen bond restraints. These give better geometry to low-resolution structures.

left to right: *Clair Baldock* (Chair), *Jordi Bella*, *Sam Horrell*, *Stephen Muench*, *Bart van Beusekom*.

Session IV: Advances and Challenges in Drug Discovery

THE keynote ion Session IV was given by Rod Hubbard (Vernalis/York) entitled "A life in pieces: fragments for drug discovery and chemical biology". Rod gave an excellent introduction to fragment screening, with examples of fragment growing and fragment merging to provide lead compounds and showed how these were also good for biology, by highlighting interesting sites.

left to right: *Rod Hubbard*, *Martin Noble* (Chair), *Frank von Delft*, *Jon Read*.

The second talk was given by **Jon Read** (Astrazeneca) on "MTH1: use of structure and biophysics to investigate target validity in a new paradigm for cancer therapy". Jon started his talk explaining the role that MTH1 (MutT Homology 1) was supposed to play in cancer, which was reported as preventing oxidized nucleotides from being incorporated into DNA. After making and characterizing three separate series of inhibitors to MTH1, which appeared to have no effect on cancer, they then showed that the response reported was probably due to off-target effects of the published tool compounds.

The last talk in the session was given by **Frank von Delft** (Diamond/Oxford) on "Crystal based fragment screening comes of age: up to 1000 crystals per week at Diamond's XChem facility". Frank showed how the I04-1 beamline at Diamond has been upgraded to allow very high automatic throughput of up to 1000 compound soaks a week, from crystal targeting and soaking through to data processing and analysis in their new Pandda software. He also talked about how to take these poised (ready for follow-up) fragment hits and move on to hit and lead compounds by simple and robust techniques.

Session V: Tackling Cancer: New Approaches to Therapy

THE keynote in this session was given by Jane Endicott (Newcastle) on "CDK structures reveal some unique and conserved features: lessons for drug design". Jane started by explaining how CDK's orchestrate and control the cell cycle and showed that they have a large number of substrates. To pick apart the different roles for each CDK requires an inhibitor specific to that CDK, however the various CDK's are very similar around the active site. It was found though, that when bound to their cyclins the active sites become very different with the position of the active site loop being very plastic, allowing potent and selective inhibitors to be designed.

left to right: *Mark Richards*, *Ed Hohenester* (Plenary Speaker), *Peter Canning*, *Jane Endicott*, *Aude Echalier* (Chair).

Mark Richards (Leeds) gave the second lecture on "Structural basis of N-Myc destabilization by Aurora-A kinase inhibitors". Mark explained the role of Aurora-A in stabilizing the oncogene Myc, a large part of which is intrinisically disordered. Inhibitors of Aurora-A cause conformations in the Aurora-A that are not compatible with Myc binding, thus increasing the amount of Myc that is degraded by the proteasome and sensitizing the cancer.

The third talk in this session was "Accidental and intentional inhibition of the Discoidin Domain Receptor" by **Peter Canning** (Oxford). Peter started by giving us an overview of collagen fibres and how they interact with Discoidin Domain receptors, which belong to the family of receptor tyrosine kinases. It was providentially found that the DDR's are inhibited by the common type-II kinase drugs, imatinib and ponatinib. The crystal structures of the DDR's with these inhibitors show clear avenues for developing them into specific DR inhibitors.

Session VI: Multiprotein Complexes

THE final BSG session was kicked off by Mark Banfield (John Innes Centre) on "Neutralising cereal killers: Engineering plant immune receptors to help feed the world". Mark told us about plant NLR proteins that can mediate disease resistance in plants. He then carried on to the specific case of PIK, a rice NLR, that detects and binds to the pathogenic rice blast effector AVR to neutralize it. A complication is that there are several alleles of both PIK and AVR and they have differing affinities for each other.

The next talk was given by **Lydia Tabernero** (Manchester) entitled "Structural basis for the regulation of endosomal pathways by the tumour suppressor HD-PTP". Lydia's talk centered on HD-PTP which is a master regulator for endosomal sorting. As HD-PTP is a large multi-domain protein, crystallography was used to study the domain interactions with ESCRT peptides and SAXS was used to study larger assemblies.

The third talk was "Lysine relay mechanism coordinates intermediate transfer in vitamin B6 biosynthesis" given by **Ivo Tews** (Southampton). Ivo told us about how they managed to trap and study the various intermediates in vitamin B6 synthesis by a combination of crystallography and on-line micro spectrophotometry. Of special interest is the I320 intermediate that is covalently bound by two lysine residues simultaneously.

The last talk of this session (and the conference) was given by **Claudine Bisson** (Sheffield) on "The mechanism of formaldehyde-sensing in the transcriptional regulator FmrR". FmrR is a transcriptional repressor that is specifically inactivated by formaldehyde, which in turn turns on genes that can remove the formaldehyde before it can harm the organism. The FmrR protein binds the formaldehyde by formation of a methylene bridge between Pro2 and Cys35, which has large effects on the structure of the protein, causing it to disassociate from its operon.

left to right: *Claudine Bisson*, *Mark Banfield*, *Ivo Tews*, *Lydia Tabernero*, *Steve Prince* (Chair).

Young Crystallographers' Satellite Meeting

THE first session of the 2017 Young Crystallographers' Satellite meeting was chaired by Claire Hobday from the University of Bath and began with the Chemical Crystallography Group plenary talk from Prof Stefan Kaskel from Technische Universität Dresden; who delivered an interesting lecture on in-situ crystallography of Metal-Organic Frameworks. Prof Kaskel showed us the power of using non-ambient crystallography to understand adsorption and the mechanical response of these porous materials. He also demonstrated many examples of using the isoreticular approach to create MOFs with a desired function.

Thomas Roseveare from the University of Sheffield was the first young crystallographer to take the stage, discussing the phase transitions in an extrinsically porous halogen-bonded network. These variable temperature diffraction studies reveal a number of interesting transitions upon desolvation.

Mohd Nadzri Bin-Mohd-Najib from the University of Durham spoke next describing his work on hydrate formation of sodium ditrizoate and their complexities.

Next up was **Nur Dayana Nisbar** from the Manchester Institute of Biotechnology who presented our first biological talk of the session explaining her work on fragment-based drug discovery.

Ruth Lunt from the University of Bath was next to take the stage delivering a talk on her work as part of CMAC,whereby she told us about the use of seeding for selectivity in multi-component crystallisation.

Wilhelm Hützler from Goethe-University Frankfurt am Main went on to talk about crystal engineering, and explained his research on the use of thiols as synthons.

Matt Reeves from the University of Edinburgh closed the first session of the meeting with an interesting talk explaining his work on using the CCDC's python API to validate oxidation states of metals in the CSD.

The second session of the meeting was chaired by **Sam Horrell** from the University of Essex and began with an education and outreach talk from Prof **Simon Coles** from the University of Southampton. Simon elaborated on the importance of outreach in science to educate and engage the public to better understand the importance of science in our society. He then discussed the BCA's commitment to providing new digital and physical resources that will allow small scale outreach events as opposed to previous large events once per year. The YCG looks forward to supporting and promoting this new outreach across the UK.

Dean Ottewell from Diamond Light Source followed the plenary lecture giving a talk on his work on the development of new tools in the DAWN workbench for analysis of powder diffraction data to improve peak fitting and indexing and streamline data analysis with a view to increase automation in powder analysis in the future.

Merina Corpinot from University College London was up next discussing the prediction of isostructural salts/cocrystals using experimental derived results on a series of test compounds. In particular the importance of considering electrostatic potentials was highlighted along with simple volume relationships.

This was followed by a talk from **Amirul Bin Abd Aziz** from the University of Sheffield who talked about his work characterising the structure function relationship between a variety of different deaminase toxins, pathogenic effectors that block function through deamination of conserved glutamine and asparagine residues.

Hayley R Green from the University of Oxford spoke next, discussing porous materials and how their host:guest chemistries are affected by their synthesis (mechanochemistry or solution crystallisations). The aim of the project is to tailor materials for desired applications, such as gas sorption.

The penultimate talk of the session was delivered by **Paolo Lucaioli** from the University of Lincoln on the viability of leucine-leucine dipeptides as therapeutic agents through the formation of multicomponent crystals by co-crystallisation.

Hanna Boström from the University of Oxford closed session two with an interesting talk about symmetry-breaking shifts in molecular perovskites, extending the traditional view of inorganic perovskite tilts to the additional degrees of freedom allowed by polyatomic linkers.

The YCG AGM saw a significant change in the committee with many new faces joining the ranks. We would like to welcome **Matthew Dunstan** and **Natalie Tatum** to the committee as Vice Chair and BSG representative, respectively, and **James Cumby**, **Lucy Mapp** and **Matt Reeves** as ordinary members. For a full account of the current YCG committee members and their research interests please visit the YCG website at www.ycg.crystallography.org.uk/the-committee/.

Day one of the YCG meeting ended with session three, the Flash Poster Presentations, where all YCG poster presenters are invited to sell their poster in thirty seconds. The session was chaired by **Natalie Johnson** from the University of Newcastle and **Alex Cousen** from the University of Oxford. The YCG flash poster presentation prize was awarded to Paolo Lucaioli from the University of Lincoln for his excellent salesmanship.

Session four was chaired by **Charlie McMonagle** from the University of Edinburgh and started with the Parkin lecture, awarded to **Briony Yorke** from the University of Hamburg. Briony gave a fascinating lecture that invited the audience to think about the presentation of crystallography in new ways, in particular how collaborating with artists can give entirely new approaches to presenting data. Briony began with a summary of innovative presentation of crystallography data from the visual, Dorothy Hodgkin's wallpaper, to the auditory, The Unit Cell (ASMbly LAB) and finally her own project on

data sonification. Briony converted diffraction images into sound with the pitch and tone represented by the position and intensity of reflections, allowing you to listen to your data. It turns out this sounds like an eery backing track from a scf-fi thriller. This soundscape gave a new perspective to data that are normally limited to the visual in a very intriguing way that Andy Parkin would surely have enjoyed.

As has become tradition at the YCG satellite meeting the final session is devoted to teaching. This year's theme was dubbed "How the other half live", and aimed to unite the fields of chemical, physical and biological crystallography and give YCG members a better idea of the work performed in the diverse groups represented by the YCG. The session was also chaired by **Charlie McMonagle** from the University of Edinburgh. The first speaker representing the physical section was Dr **Matthias Gutmann** from ISIS who gave an introduction into single crystal diffuse scattering and how ab initio calculations are allowing a first insight into the lattice dynamics that gives rise to this. Matthias showed some of the extraordinarily beautiful images collected at ISIS of diffuse scattering and how these closely compare to the calculated images.

The second talk of the session was given by Dr **Helen Playford**, representing the chemical section, who introduced total scattering and the pair distribution function (PDF) and how we can look between the *Debye-Scherrer rings* to look at not just the average but also the local structure. Helen went on to show how the PDF can give us a unique insight into short-range structural disorder that can be extremely important for increasingly complex functional materials.

The final talk of the session, representing the biological section, was delivered by Prof **Jane Endicott** from the University of Newcastle. Jane explained the ins and outs of crystallography as a tool for basic bioscience and drug design, particularly through structure function studies and fragment based drug design targeting cyclin-dependent protein kinases (CDKs), a prominent family of enzymes involved in the development of a wide array of cancers.

Danny Watkins from the University of Sheffield then went on to present work related to flexible metal-organic framework systems, discussing the structural transitions that occur during removal of guest molecules.

Phillip Maffetone from the University of Oxford followed this with an interesting talk on the use of Bayesian reverse Monte Carlo methods using a pair distribution function and prior chemical knowledge from Ramachandran distributions to solve protein structures without crystallisation and put macromolecular crystallographers out of a job. Congratulations to Phillip for being awarded the ICG-YCG prize for his talk.

This was followed by **Harry Geddes** also from the University of Oxford who presented his work in characterising amorphous pharmaceuticals using PDF methods; in particular applying non-negative matrix factorisation to extract information about individual components from a complex amorphous formulation.

Diane Barret completed the University of Oxford triple and finished off the final session of the YCG satellite meeting with an interesting talk on specific radiation damage in DNA crystals, a topic generally superseded by radiation damage in proteins. Diane demonstrated that protein/DNA complexes appear more resistant to specific radiation damage than protein alone in cryogenic and room temperature diffraction experiments.

XRF Meeting Report 14th June 2017

THE meeting took place at its usual venue, the Geology Department of the University of Leicester. 46 delegates attended. After the welcome and introduction, the meeting got under way with the Exhibitors' Forum. This is an opportunity for each of the exhibitors to present a quick-fire overview of their latest XRF-related developments. Each exhibitor was allowed 4 minutes: Nick Marsh acted as referee.

Front row: *Frédéric Davidts* (XRF Scientific), *Dave Speake* (SPEX Europe), *Jennifer Horner* (Spectro), *Ros Schwarz* (DOT round up), *Allan Finlay* (Specac Ltd), *Nick Marsh* (chair), *Tom Warwick* (Blue Scientific).

Back row: *Mike Brogan*, (PANalytical,) *Jan Roms*, (Thermo Fisher,) *Ralph Vokes*, (Shimadzu), *Chris Calam*, (Thermo Fisher Scientific), *Thierry Theato*, (Spectro), *Paul Vanden Branden*, (SciMed), *Adam Housley*, (Datech Scientific Ltd).

The rest of the morning session is reported by
Oli Williscroft (University of Hull and Intertek)

I found one of the most interesting talks of the day was given early on by **Ros Schwarz** on her DOT scheme results. Each meeting Ros has encouraged participants to partake in analysing her unknown samples that contained a few surprises with elements not typically seen at significant concentrations for most routine work. Ros's results showed that without carefully approaching unknown samples it is very easy to introduce significant errors to the results, with one of her samples containing a high concentration of bromine that enhanced the line of another element of interest leading to inaccurate results for both elements. Furthermore Ros spoke about the differences between XRF and ICP for trace elements and how below certain concentrations results from XRF become far less precise than those from ICP.

The second talk of the day was given by Dr **Tony Bell** from Sheffield Hallam University. Tony's talk focussed on the advantages of the two analytical techniques WD-XRF and XRD, and how they can be incredibly complementary when unknown samples are to be analysed in the lab. Data obtained from one technique can then be used to 'feed' the other technique allowing rapid analysis by reducing the number of possible compounds. In Tony's university lab where students' time on equipment is limited it allowed faster analysis of the students' ceramics giving information on the overall composition from XRF as well as the individual silicates from XRD.

Speakers at the morning session: *Thierry Théato* (SPECTRO) and *Frédéric Davidts* (XRF Scientific) and *Judith Bain* (Chair).

Kevin Talmage from Rigaku gave an interesting talk on the use of online XRF analysis for process control. Many companies seek ways to ensure that their production line stays within their control limits without the need for time consuming, slow, costly lab analysis. By installing XRF equipment directly on the production line, often in very challenging environments, Rigaku products allow the process to be continually monitored. One example of this was the control of sulphur content in an oil refinery process, and the challenges the Rigaku team had to overcome for the development of this process monitoring equipment.

Thierry Théato from SPECTRO Analytical Instruments delved into the realm of classical fundamental parameters (FP) and its usefulness for the analysis of small unknown samples. In many labs it is common to receive a large range of unknown samples for which a calibrated analysis isn't practical; in these cases many labs turn to the use of 'standard-less' analysis through the use of the FP model. Thierry showed that the measured intensity of samples below the critical depth can have a significant impact on the calculated concentration for organic and oxide samples. Furthermore we all know that for samples in a light matrix analysis can be difficult when the sample thickness is less than the critical depth. Thierry also demonstrated that modifications to the fundamental equations in their newest EDX equipment allowed far more accurate analysis of sulphur and other trace elements in used vegetable oil.

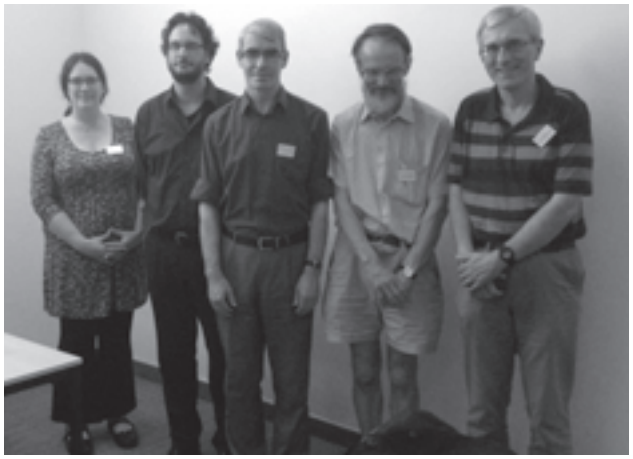
The first afternoon session is reported by
David Beveridge (HARMAN technology Ltd)

In the first afternoon session, Prof **Kenneth Harris** of Cardiff University spoke about validation in structure determination from powder XRD data, and how synergies between techniques could be exploited to this end. Structure

determination of organic materials directly from powder X-ray diffraction data is nowadays carried out extensively in both academia and industry. The most common approach is to exploit the direct-space strategy for structure solution followed by Rietveld refinement. It is essential that the structural results thus obtained are scrutinised rigorously to ensure that they are correct. He discussed several aspects: validation of the correct structural model for use in direct-space structure solution calculations; and validation of the final structure obtained from Rietveld refinement. Particular care is taken in locating hydrogen atoms, for which solid-state NMR is useful. Synergistic use of information obtained from a variety of techniques is an important part of validating a structure.

In the second talk of the session, Dr **Rainer Schramm** of Fluxana spoke about the use of platinum-free crucibles for fusions. Pt/Au crucibles are commonly used for producing beads by fusion, but samples containing metallic or sulphide-rich particles can attack the crucible material and may actually destroy it. The best alternative is to use quartz crucibles; a research study of the analysis of steel-industry slag samples for 14 elements was successful. To oxidise metallic particles, an oxidising agent was added to the flux.

The final talk of the session was given by **Joanna Collingwood** of Warwick University, who spoke about the use of XRF techniques to investigate the interplay between iron and amyloid in Alzheimer's disease. There is a long-standing debate about whether incompletely-bound reactive iron contributes to toxic processes in such brain disorders. The vast majority of mineralised iron in the brain is normally in a ferrihydrite-like FeOOH form, encapsulated in the protein ferritin. Synchrotron-source XRF was used to show the presence of magnetite (Fe_3O_4) in a region of the human brain exhibiting significant Alzheimer's disease pathology in the form of amyloid plaques. Evidence for the formation of magnetite was also found in a transgenic model of Alzheimer's disease that overproduces amyloid. A complementary set of synchrotron spectromicroscopy techniques, including XRF, allowed them to demonstrate with excellent chemical sensitivity and specificity that both unbound and mineralised iron is chemically reduced at physiological pH to a reactive form when in the vicinity of the aggregating amyloid protein. The suspicion is that this process explains the observation of magnetite in amyloid-rich brain tissue, and that it contributes to the observed toxicity of aggregating amyloid peptides in the brain infected by Alzheimer's disease.



Speakers at the after-lunch session: *Joanna Collingwood* (University of Warwick), *Thierry Théato* (SPECTRO), *Kenneth Harris* (University of Cardiff), *David Beveridge* (Chair) and *Tony Bell* (Sheffield Hallam University).

The final session is reported by
Judith Bain (Alfred H Knight)

The last session of the day mixed some manufacturing advancements with some excellent advice on how to use certain tools for your industry. The experience of these speakers was evident as the techniques **Mike Dobby** (now a consultant) discussed showed that there is a great deal of information often overlooked in a spectrum. The use of diffraction peaks can be useful qualitative information.

Keith Tame of SciMed continued this theme, talking of his experience in putting together XRD and differential scanning calorimetry (DSC) as useful combination research tools, particularly for investigating thermal reactions of solids. Some delegates had differing experience on this, which was interesting to talk through.

The final talk of the day I found very interesting, showing some real initiative. Dr **Graeme Hansford** of the Physics & Astronomy Department at Leicester University described his work, taking a handheld EDXRF instrument and applying back reflection geometry to provide phase composition data on various metal alloys. Many uses came to mind for this as fundamentally producing a handheld XRD instrument opens up some interesting applications for the future. Phase identification and composition, and even texture data, can be obtained in the field.

Speakers at the final session: *Rainer Schramm* (Fluxana), *Mike Dobby* (Consultant), *Ros Schwarz* (Chair), *Kevin Talmage* (Rigaku) and *Graeme Hansford* (University of Leicester).

2017 ACA Annual Meeting

AS is customary in years when there is an IUCr Congress, the ACA meeting took place in late May rather than July. The earlier date makes it convenient to meet in a southern city that would become insufferably hot in mid-summer, and this year the very appealing city of New Orleans was chosen. The venue was the Hyatt Regency Hotel, which is in sight of the Superdome. Residents of New Orleans have experienced great sorrow and joy in the Superdome. In 2005 it became the shelter of last resort for thousands of residents who could not leave the city before Hurricane Katrina struck. It proved to be an imperfect shelter since the hurricane's winds made holes in the roof and tore away cladding, leading to flooding of the field. By 2006 the damage had been made good and the Superdome could again host the city's professional American football team, the Saints. Within 3 years Saints fans could experience the joy of winning their league, followed by a Saints victory in the Super Bowl.

The meeting got off to the best possible start with a fascinating lecture by Nobel laureate Prof. Sir **James Fraser Stoddart** entitled "How Crystallography Helped to Create a New Bond in Chemistry". It was heartwarming to crystallographers to hear such a renowned synthetic chemist express his appreciation of our discipline. He took us on his 50-year journey in science. The starting point was not what one would expect: he was brought up on a mixed arable farm south of Edinburgh that had no electricity until he was 18! Melville College in Edinburgh followed by the University of Edinburgh kindled his interest and gave him the necessary knowledge. His first research was into gum arabic; unfortunately, no two trees in Sudan seemed to produce the same mix of polysaccharides. At the age of 25 he moved to Queen's University in Kingston, Canada, where he developed an interest in the synthesis of the large rings in crown ethers. Moving back to the UK in the mid-1970s, he worked on crown ethers and carbohydrates in Sheffield before spending 3 months with **Donald Cram** in UCLA and taking a 3-year sabbatical with the catalysis group at ICI. He praised the atmosphere at ICI, which offered the opportunity to be highly productive while under low stress. Together with **Howard Colquhoun**, he combined crown ethers with metal complexes as significant as the anti-cancer drug cisplatin. Such work set the stage for MIMs (mechanically interlocked molecules). Analysis of the electron donor-acceptor interactions holding a paraquat cation guest in the crown led to the designed synthesis of a catenane made by creating a cyclobis(paraquat-p-phenylene) tetrapositive ion threaded through bisparaphenylene-34-crown-10. Collaboration with the crystallographers **Alexandra Slawin** and **David Williams** was important to the success of this research. Moving to Birmingham in 1990, Sir Fraser led the synthesis of a molecular shuttle (1991), a molecular switch (1994), and olympiadane (1996), a MIM composed of 5 interlocked macrocycles resembling the Olympic rings. Illustrating the importance of pi-pi, C-H…O and C-H…pi interactions, its crystal structure took David Williams 2 weeks to collect the data but 6 months of perseverance to solve the structure! In 1997 Sir Fraser moved to UCLA, and his research moved into application areas: drug delivery systems, electrochemical switching of a bistable [2] catenane, and a molecular switch tunnel junction. At Northwestern University from 2008, his attention turned from switches, which in principle do no work, to machines, which require an energy source. As a model for carrier proteins that transport molecules across cell membranes, he and his group devised a molecular pump with a viologen at its heart. During redox cycling it first attracts and then repels positively charged rings, enhancing their local concentration. Among his numerous honours Sir Fraser received a knighthood in 2006 and shared the Nobel Prize in 2016. He concluded his talk with the aphorism that to be successful in academia one must have the strength of a horse, the hide of an elephant and the work ethic of a honeybee.

The next day started with a session that matched my research interests particularly well: "Utilization of Small Molecule Crystallography in Pharmaceutical Development". **Bruce Noll** began the proceedings with "Am I Seeing Double? Absolute Configuration and X-ray Crystallography". He reminded us of the amusing observation that the R enantiomer of carvone smells like spearmint, the S like spearmint. Much more seriously, the "wrong" enantiomer of a drug may be ineffective or even toxic. Thanks to advances in data collection techniques, crystallographers can get quick confirmation of absolute configuration. Bruce reminded us of the tests that can be applied. The Flack parameter should be near zero if the enantiomorph is correct but near 1 if it is incorrect. Its uncertainty u must also be taken into account: $u < 0.04$ implies strong distinguishing power but $u > 0.3$ is very weak. Parsons quotients improve the reliability of the Flack parameter. Bruce presented examples of light-atom structures for which the absolute structure can be indicated in minutes and definitively determined in hours.

I was up next with a talk on "Crystal Packing and Pharmaceutical Properties of Salts of Diclofenac."
As part of our research on the structural systematics of amine salts of carboxylic acid drugs we determined the structures of 6 salts of (2,6-dichloroanilino) phenylacetic acid: starting with *t*-butylammonium, expanding the organic moiety and, in another series, successively replacing methyl groups with hydroxymethyl. As usual, the primary ammonium and carboxylate groups create hydrogen-bonded columns. Despite being sequestered between rings, the secondary NH group also hydrogen bonds to $^{-}$OCO. Unsurprisingly, aqueous solubility decreases as the number of carbon atoms increases, and melting point increases as OH groups are successively added to the cation. More surprisingly, after incorporation of one OH group increased the aqueous solubility, further OH groups decreased the solubility – reflecting the power of attractive interactions within the crystal.

Next, **Curtis Moore** from the University of California San Diego talked about "Academic and Industrial Partnerships for the Betterment of All". Curtis led off with some worries about the future of academic crystallography. There are likely to be fewer facilities, and macromolecular and small-molecule laboratories are likely to be consolidated. However, there will be opportunities for well-equipped facilities that can provide

additional services such as crystal growing. Overnight sample delivery is available, and from a crystal to full structure determination can take as little as 10 minutes. Communication with potential users is essential: an informative website that is kept up to date and includes contact information, clarity about one's ability to run a sample (equipment, price, and legality), and a professional report form. Equipment should include a high quality stereo microscope (its cost of $8-10,000 may seem expensive, but it is a small fraction of the cost of X-ray equipment). That equipment should offer bright sources, small beams, low- or no-noise detectors, low temperature, and multiple uses (e.g. powder diffractometry on single-crystal equipment or single-crystal on macromolecular equipment).

With the title "To Solvate or Not to Solvate? A Crystallographic Evaluation of the Isostructural Solvated and Non-Solvated Crystal Forms of an Active Pharmaceutical Ingredient (API)" **Michael Galella** told us about a promising candidate drug that was non-ionisable between pH 2-11 and had aqueous solubility of only 0.04 mg/mL. While an amorphous solid dispersion could provide increased solubility, a stable crystal form is still preferred. Screening resulted in multiple solvated forms, many not suitable. They had similar powder diffraction patterns but a wide range of weight loss in thermogravimetric analysis. There were two sub-classes of crystal forms with the same "structural scaffold" in space group $P2_12_12_1$ and void volume ca. 60 $Å^3$ when solvated and ca. 200 $Å^3$ when non-solvated. Large polar channels form within a bilayered assembly of hydrogen bonded API dimers. Water molecules occupying discrete positions within the channels form hydrogen bonds between layers; without water OH groups move to form the hydrogen bonds. The monohydrate, the anhydrous form and an intermediate hemi-hydrate can be reversibly interconverted. Good crystals of the hemi-hydrate are generated in a slurry of the anhydrous form in methanol/water.

Andrew Brunskill provided another industrial perspective in his talk "Driving Pharmaceutical Development with Small Molecule Crystallography. Not Just a Pretty Picture". Andrew enumerated some questions that are addressed by crystallography in the pharmaceutical context: Confirm the structure. Is it multicomponent? Is it phase pure? Does it rationalise or predict physical properties? How does my catalyst work? What is that HPLC peak? He continued with some case studies. Instability of a molecule was explained by the proximity of an amino group to a vulnerable H atom. Design of an inhaled API required an understanding of the phase behaviour; to de-risk phase changes samples were monitored as they were cycled 40 times between 60% relative humidity and a desiccator. Catalyst design involved a study of the driving forces for the reaction, the enantiomer-determining step, catalyst stability and deactivation. A dissolution study of crystals in a medium containing Tween 80 ended up producing crystals of a Tween solvate. Form I of an API kept in a plastic container changed to Form II by incorporating the dibutyl phthalate plasticizer. A reaction Q → R in hydrobromic acid produced an unexpected product which was shown to be a co-crystal of the hydrobromides of Q and R.

Andrew Maloney concluded the session with "Applying Structural Informatics Approaches to Pharmaceutical Supply Chain Processes". Andrew began by mentioning the Advanced Digital Design of Pharmaceutical Therapeutics project (ADDopt) and asked why we don't design drugs as well as we do aircraft. ADDopt aims to link the wealth of data compiled by manufacturers with the information about molecular and crystal structures in the Cambridge Structural Database (CSD). In a solid-form informatics approach predictive tools are being developed to guide formulation decisions and design robust manufacturing processes based on structural information. By mining the CSD, tools such as Mogul and IsoStar have been developed to indicate preferred molecular conformations and preferred modes of hydrogen bonded and non-hydrogen-bonded interactions. Full Interaction Maps indicate graphically whether a particular structure displays the expected interactions. Unusual conformations or interactions warn that the crystal form under consideration may be unstable relative to another alternative. Effort is now devoted to the steps from crystal form to particle: assuming nucleation has taken place, identifying the faces that are energetically and/or kinetically favoured for growth. Prediction of mechanical properties, and in particular the prediction of slip planes that facilitate compaction, is also an objective.

In the afternoon I chose "Important Science from Small Molecules", which offered a very mixed bag of interesting results presented in shorter talks. **Nick Gerasimchuk** presented "Crystal Structures of Ag(I) and Tl(I) Cyanoximates… " Notwithstanding their different places in the Periodic Table, these monovalent ions have remarkably similar crystal chemistry. Cyanoximates, NC-C(R)-NO^- can coordinate metal ions through two N atoms and one O atom. Ag cyanoximates have unusual colours and great photostability. They can serve as sensors for UV radiation and industrial gases. The poisonous Tl^+ forms crystalline salts readily and is not oxidizing like Ag^+. **Michael Hall** followed with …"Non-innocent Ligands in Transition Metal Complexes". Nickel bis(dithiolene) complexes can exist in three oxidation states $[Ni(S_2C_2R_2)_2]^n$ with n = 2-, 1- or 0, in which the Ni stays dipositive and the ligands are redox-active. The neutral complex can react with an alkene to produce a cis-interligand adduct. Reduction releases the alkene. In the related ruthenium tris(thiolate) complexes with charge 1-, 0 or 1+ the latter form also reacts with alkenes. It is not clear whether oxidation removes electrons from Ru or ligand. DFT calculations for $[RuL_3]^+$ predict a triplet ground state, yet the material is diamagnetic. These complexes have potential as catalysts for releasing hydrogen from methanol according to the overall reaction $CH_3OH + H_2O \rightarrow CO_2 + 3H_2$. **Raul Castaneda** described the "Synthesis of Pyridinium Transition Metal Tetrachlorides"… Pyridinium tetrachloroferrate (III) is a model for perchlorometalate complexes. These can interact with coordinating imidoyl-amidine ligands to form crystalline products. Complexes with 2,6-diaminopyridinium display a broader range of hydrogen bonds. **Alice Brink** told us about "Rhenium Reactivity – Manipulation by Ligand Development". The ultimate objective of this research is to coordinate biomolecules or bifunctional chelators to ^{99m}technetium (I) or $^{186/188}$rhenium (I) for use as diagnostic or therapeutic radiopharmaceuticals. It is important to understand the kinetic effects of ligand binding: if the mechanism is associative, a new ligand binds before the outgoing ligand departs; if dissociative, the outgoing ligand leaves first. In fact, the evidence seems to suggest more or less simultaneous interchange.

After a well-earned tea break **Robin Macaluso** presented "Combining Crystallography and Complementary Techniques to Understanding Small Structural Changes in Intermetallic Compounds and Sulfides". Rare earth – Pt – Ga compounds were prepared by flux growth synthesis with Ga as solvent, at temperatures rising from room temperature to 1150°C for 7 hours, then reduced to 350°C. A compound with formula $Er_{1.33}PtGa_8$ had sites with 33% Ga and 67% Er in a modulated structure. A new one thought to have these elements in a 1:1:1 ratio turned out to be $ErPtGa_{1.27}$. Powder diffraction demonstrated the products from arc melting and from flux

growth are different. Electron microscopy and theoretical calculations were helpful, and elemental composition determinations were essential. Next, **Carlos Murillo** reminded us of "Weak Bonding Interactions, Large Structural Impact". Complexes with metal-metal bonds have been known for about 60 years. Such bonding can be strong: for instance, $[Cl_4Re\text{-}ReCl_4]^{2-}$ has a very short Re-Re bond. However, such strong metal-metal bonds can be affected by seemingly weak crystal packing forces. The Cr-Cr bond length in the red compound $Cr_2(DPhIP)_4$·THF, where DPhIP is diphenyliminopyridine, is 1.858(1) Å, but in the orange $Cr_2(DPhIP)_4$·2THF it is 2.155(1) Å, even though the THF sites are interstitial, not near Cr atoms; and both solids yield the same species when dissolved in THF. **Paul Forster** attempted to solve a long-standing puzzle with "Towards Understanding the Structure of Liquid Transition Metal Oxides through a Joint Experimental and Computational Investigation". Molecular metal oxides stable at ambient conditions are rare, but M_2O_7 molecules are known to exist for M = Mn, Tc and Re. Tc is relevant to the nuclear fuel cycle, where a red substance called "technetium red" has been found but could not be characterized. A model has now been devised and computationally tested which consists of monomers with Tc sites that can interact strongly with adjacent molecules, primarily forming Tc-Tc bonds. **Gertruida Venter** directed our attention to "Rhodium (I) 2-hydroxypyridine N-oxide (hopo) Complexes: Synthesis, Characterization and Reactions". As part of their mechanism of action, transition metal complexes active in homogeneous catalysis may undergo reactions such as oxidative addition, insertion, substitution and reductive elimination. This study concentrated on the first of these mechanisms. Varying the tertiary phosphine ligands PX_3 on Rh in [Rh(hopo)(CO)(PX_3)] manipulated the electron density and/or steric accessibility at Rh, thereby affecting the oxidative addition reaction with iodomethane to give Rh (III) alkyl complexes. Finally, **James Donahue** punctured our complacency with "Element Mis-identification in Crystallography: a Series of Case Studies". The certainty offered by X-ray crystallography really applies to atom *connectivity* rather than atom *identity* since atoms of closely similar atomic number have similar X-ray diffracting power. Even where the diffracting power is very different, mistakes can be made. For instance, a series of structures supposed to be [MCl_2(diazadiene)] with M = Cr, Mo, W were made by a literature procedure and subjected to crystal structure determination. The M-Cl bond distances and unit cell volumes were suspiciously similar and unexpected for crystals of such composition. To get a decent outcome it had been necessary to refine the occupancy factors of the central metal atoms, yielding 0.775 for Mo and just over 0.4 for W. Seemingly no thought had been given to the strangeness of ordered ligands surrounding a void metal site in some unit cells. Multiplying the atomic numbers of Mo and W by the relevant occupancy factors yields values of 32.6 and 29.6, not far from the atomic number of zinc. Careful reading of the synthetic procedure revealed that Zn was used as a reducing agent. Zn^{2+} had formed and replaced the central metal atom! In another case, a tetramolybdenum cluster with dithiooxamide ligands was reported to have some "interesting" properties: a low oxidation state for Mo and diamagnetism. The synthetic procedure used Ag^+, and the properties of the complex are better explained by assuming that it contains the closed-shell Ag^+. These examples show how important it is to document all reagents and solvents.

The next day featured a session on "Porous Materials" that attracted a lot of interest. The two medium-length lectures were given by **Michael Zaworotko** and **Len Barbour**. The BCA had the foresight to invite Mike to give a full-length plenary lecture at our 2016 Spring Meeting. A summary of the ideas behind his research and its spectacular results appeared on page 6 of the June 2016 issue of Crystallography News. Len talked about gas storage media with the difficult-to-achieve property of "Structural Flexibility in the Solid State". He began by reminding us that calculated void volume depends drastically on the size of the probe used. To correlate structural and physico-chemical information on CO_2 uptake by a MOF Len developed a miniaturised pressure cell that could fit on a standard goniometer head. A commercial pressure-ramped DSC apparatus showed a big exotherm as CO_2 pressure passed 10 bar and a smaller exotherm at 18 bar. The crystal structure at 10.5 bar displayed the presence of CO_2, but indistinctly because the CO_2 rattles around. Above 18 bar another CO_2 binds, this time showing up clearly because it occupies a tight space. Len also discussed photo-switchable MOFs. With a bis-benzoic acid co-ligand the MOF develops a blue surface under UV irradiation, reversible with green light. With a more flexible co-ligand there is a shape change.

Two other talks in this session particularly caught my attention. **John MacDonald** took as his research objective the remediation of water sources contaminated with persistent organic pollutants such as benzopyrene, dioxins and pesticides by using "MOFs as Porous Hosts for Generating Singlet Oxygen". MOFs with an aromatic framework are very good at binding aromatics, and porphyrins are very good photosensitisers. The plan was to create a MOF containing these two components in a 2-step process: combine Zn^{2+} with the porphyrin, then add bipyridyl. This MOF was tested with diphenylbenzofuran, a guest well known to react with singlet O_2. A MOF with large pores got rid of it in minutes; with smaller pores it still worked but took longer. Concerns that the bound porphyrin would no longer act as a photosensitiser, or that it would work briefly but undergo photobleaching, were shown to be unfounded. If it is desired to prevent egress of the guest, triphenylacetic acid is a suitable trapping agent. On rotation it traces out a 12.5 Å ring, while the dimension of pores in the MOF is 13 Å. The final lecture in the session was by **Peter Wood** on "Metal-organics: a Rich Seam of Data for Knowledge Mining". Many of us were surprised to learn that, as of the start of 2017, 57% of the structures in the Cambridge Structural Database (CSD) were metal-organic! Nevertheless, they have been the subject of fewer studies than purely organic structures. Pete addressed the need to search for, visualise and analyse metal-organic structures. The search requires easy access to relevant subsets. Visualisation needs easier expansion of networks and availability of a polyhedral display style. Analysis should include calculation of void space, surface areas and pore limiting diameters. The CSD subset most in demand is that of MOFs, but it is surprisingly difficult to define a MOF. Unambiguous search criteria for "MOF-like" structures have been defined and used to create a CSD MOF subset with just under 70,000 entries as of early 2017 [P. Z. Moghadam et al. (2017) *Chem. Mater.* **29**, 2618-2625], which will be regularly updated. MOFs in the CSD were examined, and their chemical structures were incorporated into the definition until all were included. As new types of MOF are added, their chemical diagrams will be added to the definition. Pilot studies have included void space analysis, analysis of disorder, removal of unbound solvent and consideration of labile ligands. A subset consisting only of non-disordered frameworks has been developed.

My second talk was in the enjoyably beer-fuelled "Would You Publish This?" session. For this reason my notes were neither copious nor coherent enough to reproduce here. My own talk

referred back to my earlier presentation on 6 salts of diclofenac. Data had been collected by the National Crystallography Service on world-class equipment according to set criteria; in particular, collecting reflections with MoKα radiation to θ = 27.5°. Three of the data sets were of excellent quality. For the other 3 we had only been able to grow crystals that were very small and/or weakly diffracting, yielding R(obs) values slightly above 10%. The usefulness of this study depended on comparisons of crystal structure with physical properties for the 6 structures. I was concerned that a future researcher might try to retrieve these and other related structures from the CSD with a criterion R <= 10% to exclude the real rubbish, and would therefore throw away much of the significance of our study. However, cutting the resolution for the 3 problem structures to θ = 25.25° reduced the R factors to below 10%, so that they now would pass the R factor test. As I had hoped, this prompted a lively discussion about when, if ever, it is legitimate to throw away data.

My other talk was in the much more serious session on "Standard Practices in Crystallography III: Communicating Crystallographic Results". Since this will be the subject of a separate article, I do not summarise it here.

Carl Schwalbe

New Orleans, the Mississippi River, and Sugar

THE river brings prosperity to New Orleans but constantly threatens the city. At a time when land transport was difficult, the river provided an easier route to ship goods between the American hinterland and the wider world. At New Orleans the Mississippi is about ½ mile wide and almost 200 feet deep, providing an ideal site to transfer cargo and passengers between riverboats and ocean-going vessels. Now it accommodates the longest wharf in the world, just over 2 miles long. Even better for the city in its history, in the delta downstream from New Orleans the river splits into different channels, most of which in places are too shallow for navigation. While experienced river pilots have long known the correct route, a number of foreign invasion forces trying to attack New Orleans from the Gulf of Mexico without such knowledge have had to turn their ships back. In the last battle of the War of 1812, British troops had to land a long way from the city and undertake a debilitating march, partly through sugar cane fields where the recent harvest had left jagged stalks like spikes, contributing to their defeat at Chalmette.

Continued overleaf

Joan and I took a historical cruise on the paddlewheel steamer *Creole Queen* past the competing steamer *Natchez* and downriver to the site of the battle at Chalmette Plantation, which gave us an excellent view of riverside life. One impressive point of interest was the Domino Sugar Refinery at Chalmette, which carries out crystal-growing on an epic scale. Recently the Chalmette refinery processed over 1 million tons of sugar in a single year. According to the website **www.sugar.org** commercial cane sugar is produced in a two-stage process. A sugar mill, usually located near the cane fields, turns sugar cane into raw sugar. Juice is obtained by crushing the washed and shredded cane, clarified by adding calcium hydroxide and carbon dioxide to drag down impurities as calcium carbonate precipitates, and crystallized by evaporation under reduced pressure. The raw sugar, consisting of sucrose crystals coated with molasses, is shipped to a refinery for further purification. There the raw sugar is combined with a sugar syrup to loosen the molasses and centrifuged to remove most of it. Then the crystals are washed, dissolved in water, and clarified again or filtered, resulting in a clear golden solution. After removal of coloured compounds with activated charcoal and concentration of the solution by evaporation, final crystallization takes place. Fine seed crystals of sucrose are added, more water is removed by evaporation under vacuum, the crystals that have grown are dried, and finally they are screened to sort them by size. White granulated sugar is about 99.9% sucrose. If brown sugar is desired, white crystals may be blended with specially prepared molasses syrup, or these components may be boiled together until brown crystals form. Sadly, a significant part of the US economy depends on commodities that have drawbacks, such as coal, tobacco and sugar – but sugar does the least harm and gives a lot of people a lot of pleasure.

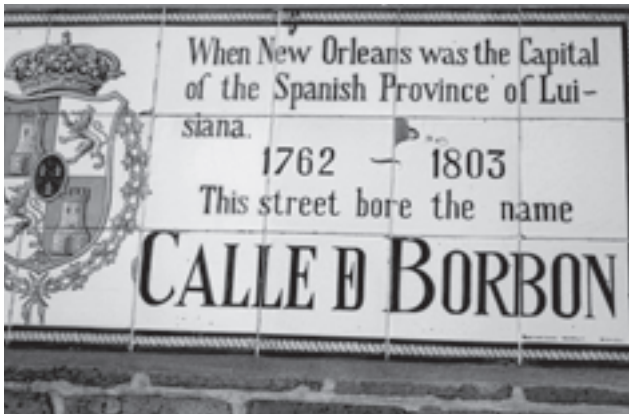
The commentary on our tour included a gripping account of Hurricane Katrina, and from our vantage point on our boat the vulnerability of the city was obvious. With the river level being high, we were looking at the upper floors of riverside buildings. Only the levees kept them dry. At the height of the hurricane there were numerous breaches of levees, either because of inherent structural weakness or because barges broke loose and acted as battering rams. The sugar refinery was hit hard, parts of the site being under 9 feet of water and 8 million pounds of raw sugar turning into a gooey mess. Nevertheless, the staff got the factory up and running again before the end of the year.

Carl Schwalbe

New Orleans Ironwork

NEW Orleans was founded by French colonists in 1718 and named in honour of the Duke of Orléans. It came under Spanish rule for about 40 years before reverting to France and then being sold to the United States in 1803. Most early buildings were made of wood and ramshackle in construction, leading to devastating fires. The Spanish authorities responded by mandating masonry construction. Particularly in the neighbourhood of Bourbon Street, austere Spanish architectural styles became prevalent. As the city prospered under American rule, owners wanted to beautify their properties. The increasingly easy availability of wrought iron (and in later years, cast iron) gave them the means. Pig iron from the smelter contains 3.5 – 4.5% carbon along with silicon and other impurities, rendering it brittle. By heating and hammering, the carbon and impurities were driven off, producing malleable wrought iron with a carbon content reduced to < 0.1%. It was worked by hand into balconies and gates, often decorated with leaves, flowers, French fleur-de-lis and scallop shells associated with Saint-Jacques, featuring a lot of translational symmetry. Some examples photographed by **Joan Schwalbe** are shown here, along with café ambience inspired by it.

Carl Schwalbe



Obituary

Philip Coppens
(1930–2017)

ON June 21, 2017, Philip Coppens, SUNY Distinguished Professor Emeritus and Distinguished Research Professor in the Department of Chemistry, at the University of Buffalo, New York, USA, passed away at the age of 86. He was recognised as a pioneer of X-ray crystallography in the 20th and 21st centuries, making seminal contributions in both experimental and theoretical aspects of the subject. He was among the first to exploit technological developments that allowed him to devise new classes of experiment that were fundamental in changing the perception of X-ray crystallography as a static technique to a truly dynamic one.

Coppens was born in Amersfoort, in the province of Utrecht, in the Netherlands, and obtained both his B. Sc. and Ph D Degrees from the University of Amsterdam. He was attracted to the beauty of crystals in their periodic arrangements, the mathematical aspects of the subject and, not least, the ability of the crystallographic technique to produce unambiguous answers! His Ph D supervisor was **Caroline McGillavry**, who led a vibrant crystallographic laboratory. Among the visitors to McGillavry's lab was **Gerhard Schmidt**, who was setting up an X-ray laboratory at the Weizmann Institute of Science, in Israel. Schmidt had the vision that X-ray crystallography should be used to solve chemical problems and Coppens was fascinated by this approach. McGillavry and Schmidt came to an agreement that Coppens would complete his Ph D at the Weizmann Institute and Coppens moved to Israel in 1956. His research involved studying the interaction of light with crystals, an aspect of crystallography that Coppens pursued throughout his career. **Fred Hirshfeld** was a post doc in Schmidt's lab at the same time as Coppens, and Hirshfeld interested Coppens in charge density analysis which also became a research theme that Coppens was to develop over the next four decades.

On completion of his Ph D Coppens obtained a two-year post-doctoral appointment with **Walter Hamilton** at the Brookhaven National Laboratory (BNL) in the USA. During this period Coppens had the opportunity to develop his own research programme and he made good use of the neutron reactor source, spending much of his time collecting data for structure determinations that was independent of assumptions about atomic form factors. At the end of the post doc Coppens returned to the Weizmann Institute where he collaborated with Fred Hirshfeld on charge density analysis and with **Leslie Leiserowitz** on the accurate evaluation of X-ray absorption corrections by numerical Gaussian integration.

In 1965 Coppens returned to the BNL and used the new, more powerful neutron source to, for the first time, compare X-ray and neutron diffraction data accurately. He showed the limitations of the X-ray spherical-atom scattering factors and constructed the first X-ray-Neutron difference map which allowed the electron pairs on the nitrogen atoms and the bonding electron density between the atoms in s-triazine to be observed. This represented a major development in diffraction analysis and provided new experimentally proven insights into molecular bonding. He also worked with Walter Hamilton on extinction theory and on errors in electron density maps. These contributions to structural chemistry attracted the attention of **David Harker**, who had his own Crystallography Institute in Buffalo, and Coppens was invited to establish a Crystallography Laboratory in the Department of Chemistry at the State University of New York (SUNY) at Buffalo. He gladly accepted, established his own independent group, and pioneered many aspects of experimental and theoretical crystallography for the remainder of his career. His laboratory was quickly recognised as one of the world-leading crystallography laboratories and it remains so to this day.

In the early days at Buffalo Coppens concentrated on the development of charge density analysis and attracted many of the most able researchers to his laboratory. He coded and published one of the first multipole refinement programs that is still used widely today. He then went on to overcome one of the key challenges when comparing experimental and theoretical electron densities, that of thermal smearing which was naturally present in the experimental measurements. He developed a method to smear theoretical densities. Coppens's work on charge densities culminated in the publication of his seminal book *"X-ray Charge Densities and Chemical Bonding"* by Oxford University Press, in 1997, and in subsequent review and perspective articles throughout the early 2000s.

Coppens was among the first to realise the potential of new technologies as they developed and apply them to

crystallography so that whole new classes of experiments could be undertaken. These technologies included the development of high-intensity pulsed lasers, reliable low temperature equipment, faster computers and synchrotron radiation. He was able to return to his first crystallographic love and apply these technologies to *photocrystallography* experiments, a term that he coined in 1997, meaning the use of crystallographic methods to study the interaction of light with crystals. In this way he was able to introduce the dimension of *time* into the crystallographic experiment, and thus monitor chemical processes as they occurred in real time or determine the structures of molecules that had lifetimes down to microseconds. His first study of this type was on sodium nitroprusside which upon photoirradiation at low temperature converted into a metastable linkage isomer in which the bonding mode of the nitrosyl group to the iron atom changed. Largely as a result of this work, sodium nitroprusside was declared to be one of the 10 favourite crystal structures in the first 100 years of crystallography by *Chemical and Engineering News* in their anniversary issue on crystallography published on 11th August, 2014. After this success, Coppens went on to determine the structures of a series of molecules with microsecond lifetimes, at low temperatures, by synchronising laser pulses, with gated synchrotron radiation at various synchrotron facilities in the USA. While much of the work was carried out using monochromated synchrotron radiation Coppens also developed polychromatic Laue techniques to probe species with shorter lifetimes, and to investigate the structural dynamics of doped titanium oxide nanoparticles that are of importance in the photovoltaics industry. Coppens continued to work on the development of the methodology right up until the time of his death.

Coppens's outstanding contributions to advances in crystallography were recognised by awards to him throughout his career. Most notable were the Aminoff Award from the Royal Swedish Academy of Sciences, in 1996, for his contribution to charge density studies, the Ewald Prize, from the International Union of Crystallography, in 2005, and in 2011 he was named as a Fellow of the American Crystallographic Association. Coppens also served the crystallographic community with distinction, in a number of roles, including his term of President of the American Crystallographic Association in 1978, and as President of the International Union of Crystallography between 1993 and 1996.

Coppens's legacy not only includes the new scientific developments that he has pioneered but also by the many students from across the world that he has trained. He was an excellent mentor and teacher. His research group provided a vibrant environment and was always multinational in make-up. Many of his students and co-workers have gone on to take up prestigious appointments in universities across the world and are teaching the methods developed by Coppens to whole new generations of scientists.

Coppens encouraged collaborations and his laboratory had many international visitors who benefitted from his knowledge and expertise. He and his wife, Marguerite, were perfect hosts. I will always remember my own visit to Buffalo in the late 1990s and the kindness and hospitality that they showed me. I am also grateful for all the support that they have given me in subsequent years as I attempted to contribute to the photocrystallography area. Philip Coppens was a true giant in his field and will be sadly missed by the whole crystallography community.

Paul Raithby
University of Bath

Letter to the Editor

In his obituary of **Howard Flack** which appeared in the June 2017 issue of *Crystallography News*, **Mike Glazer** wrote *"Howard had studied Chemistry at Nottingham, if I recall correctly"*. This is indeed correct: Howard was my contemporary, studying at the University of Nottingham from October 1962 until July 1965. He graduated with a First Class BSc degree in Chemistry.

Yours sincerely,
Dr Peter Hubberstey

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, c.h.schwalbe@hotmail.com . Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

3-6 September 2017
7th Cambridge Symposium on Nucleic Acids Chemistry and Biology, Cambridge.
http://www.rsc.org/events/detail/23735/7th-cambridge-symposium-on-nucleic-acids-chemistry-and-biology

3-6 September 2017
ISIC20. 20th International Symposium on Industrial Crystallography, Dublin, Ireland.
http://isic20.com/

3-6 September 2017
AIC International Crystallography School (AICS2017), Pavia, Italy.
http://www.cristallografia.org/aicschool2017/eng/detail.asp?idn=2949

3-8 September 2017
55th EHPRG Meeting: High Pressure Science and Technology, Poznan, Poland.
http://www.ehprg2017.org/

3-15 September 2017
15th Oxford School on Neutron Scattering, Oxford.
http://www.oxfordneutronschool.org/

4-5 September 2017
Advances in Quantum Transport in Low-Dimensional Systems, London.
http://aqt2017.iopconfs.org/home

4-15 September 2017
JCNS Laboratory Course Neutron Scattering, Munich, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/LabCourse/_node.html

5-15 September 2017
EMBO practical course on image processing for cryo-electron microscopy, London.
http://meetings.embo.org/event/17-cryo-em

6-8 September 2017
CCP4 Protein Structure Workshop 2017, Carlisle.
http://www2.le.ac.uk/projects/ccp4/ccp4-protein-structure-workshop

10-13 September 2017
15th Conference on Methods and Applications in Fluorescence, Bruges, Belgium.
http://www.maf15.org/

10-14 September 2017
QMOL. Operating Quantum States in Atoms and Molecules at Surfaces, Ascona, Switzerland.
http://www.qmol.ch/

11-15 September 2017
EMBO Practical Course SAXS/SANS, Grenoble, France.
http://meetings.embo.org/event/17-small-angle-scattering

12 September 2017
Swiss Society of Crystallography Annual Meeting, Geneva, Switzerland.
http://www.sgk-sscr.ch/en/geneva2017/

12-15 September 2017
6th International caesar Conference. Overcoming Barriers: Atomic-resolution and beyond: advances in molecular electron microscopy, Bonn, Germany.
https://www.caesar.de/en/events/2017/6th-international-caesar-conference-overcoming-barriers.html

13-15 September 2017
IWGO 2017. 2nd International Workshop on Gallium Oxide and Related Materials, Parma, Italy.
http://www.iwgo2017.unipr.it/

17-22 September 2017
EUROMAT2017 Symposium: Materials Science with Synchrotron Radiation X-ray, Thessaloniki, Greece.
http://euromat2017.fems.eu/

18-21 September 2017
E-MRS 2017 Fall Meeting, Warsaw, Poland.
http://www.european-mrs.com/meetings/2017-fall-meeting

18-22 September 2017
3D Electron Crystallography for Macromolecular Compounds, Paul Scherrer Institute, Switzerland.
https://indico.psi.ch/conferenceDisplay.py?confId=5525

19-21 September 2017
Methods and applications in the frontier between MX and CryoEM, Barcelona, Spain.
http://www.sbu.csic.es/conference-mx-cryoem-bcn/

20-22 September 2017
European Workshop on Photocathodes for Particle Accelerator Applications / EWPAA 2017, Berlin, Germany.
https://www.helmholtz-berlin.de/events/ewpaa/index_en.html

25-28 September 2017
WIRMS 2017- Infrared Microscopy and Spectroscopy with Accelerator Based Sources Workshop, Oxford.
http://www.wirms2017.com/

25-29 September 2017
Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.
http://www.icdd.com/education/rietveld-workshop.htm

26-27 September 2017
SAXS Excites: The International SAXS Symposium 2017, Graz, Austria.
http://www.anton-paar.com/tu-graz/saxs-excites/

28-30 September 2017
20th Heart of Europe Bio-Crystallography (HEC meeting), Wojanow Castle, Poland.
http://hec-20.iimcb.gov.pl/

2-4 October 2017
Cryo-EM Sample Preparation Workshop, Diamond Light Source, Didcot.
http://www.diamond.ac.uk/Home/Events/2017/cryoEM-Worskhop-October-2017.html

2-6 October 2017
Intermetallics Conference 2017, Bad Staffelstein, Germany.
http://www.intermetallics-conference.de

2-6 October 2017
ic-rmm3. 3rd International Conference on Rheology and Modeling of Materials, Miskolc-Lillafüred, Hungary.
http://www.icrmm3.eu/icrmm.php

4-6 October 2017
6th Joint Workshop on High Pressure, Planetary and Plasma Physics (HP4), Göttingen, Germany.
https://indico.desy.de/conferenceDisplay.py?confId=16402

10-13 October 2017
JCNS Workshop 2017, Tutzing, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/JCNSWorkshops/2017Workshop/AbstractsandRegistration/_node.html

11-13 October 2017
NINMACH2017. 2nd International Conference on Neutron Imaging and Neutron Methods in Archaeology and Cultural Heritage, Budapest, Hungary.
https://indico.kfki.hu/event/518/

15-20 October 2017
6th Accelerator Reliability Workshop. ARW 2017, Versailles, France.
http://www.synchrotron-soleil.fr/Workshops/2017/ARW-2017

16-19 October 2017
25th International Conference on Materials and Technology, Portorož, Slovenia.
http://icmt25.com/en/

16-20 October 2017
10th ILL Annual School on Neutron Diffraction Data Treatment Using The FullProf Suite, Grenoble, France.
https://indico.ill.fr/indico/event/84/

19-21 October 2017
The 75th Annual Pittsburgh Diffraction Conference, Indiana, PA, USA.
http://www.pittdifsoc.org/conference.htm

23-27 October 2017
Structural Bioinformatics, Hinxton, Cambridge.
http://www.ebi.ac.uk/training/events/2017/structural-bioinformatics-1

28 October – 1 November 2017
10th General Meeting of the International Proteolysis Society, Banff, Alberta, Canada.
http://www.ips2017.org/

29 October – 3 November 2017
Advanced Topics in EM Structure Determination: Challenges and Opportunities, New York, NY, USA.
http://nramm.nysbc.org/participants-guide/

6-10 November 2017
62nd Annual Conference on Magnetism and Magnetic Materials. MMM2017, Pittsburgh, PA, USA.
http://magnetism.org/

12-14 November 2017
25th Protein Structure Determination in Industry Meeting, Cambridge.
http://www.psdi2017.org/25117

12-14 November 2017
From Single- to Multiomics: Applications and Challenges in Data Integration, Heidelberg, Germany.
https://www.embo-embl-symposia.org/

13-15 November 2017
Structural biology and biophysics of RNA-protein complexes, Orléans, France.
http://www.lestudium-ias.com/event/structural-biology-and-biophysics-rna-protein-complexes

16-17 November 2017
EMBL Conference: Revolutions in Structural Biology: Celebrating the 100th Anniversary of Sir John Kendrew, Heidelberg, Germany.
https://www.embl.de/training/events/2017/JKS17-01

21-22 November 2017
Design of Crystalline Products. CCG/IG Autumn Meeting, Cambridge.
http://ccg.crystallography.org.uk/2017/02/03/ccgig-autumn-meeting-2017/

26 November – 1 December 2017
2017 MRS Fall Meeting and Exhibit, Boston, MA, USA.
https://www.mrs.org/fall2017

10-15 December 2017
High-Accuracy CLEM: Applications at Room Temperature and in cryo, Heidelberg, Germany.
https://www.embl.de/training/events/2017/LEM17-01/index.html?_ga=2.263148357.87988381.1493825942-1740041149.1491823482

27 January – 2 February 2018
2nd NEUBIAS. The Bioimage Analysis Community Conference, Szeged, Hungary.
http://eubias.org/NEUBIAS/neubias2020-conference/szeged-hungary-2018/

4-8 February 2018
Cryo-EM from Cells to Molecules: Multi-Scale Visualization of Biological Systems (F1). A Keystone Symposium on Cryo-EM, Tahoe City, CA, USA.
http://www.keystonesymposia.org/index.cfm?e=web.Meeting.Program&meetingid=1576

18-23 February 2018
Photoionization & Photodetachment (GRC), Galveston, TX, USA.
http://www.grc.org/programs.aspx?id=12840

27 February – 2 March 2018
ICON Europe 2018. 2nd International Conference on Nanoscopy: Beyond the Diffraction Limit, Bielefeld, Germany.
http://www.icon-europe.org/

26-29 March 2018
BCAA Spring Meeting, Warwick.
http://www.bcaspringmeetings.org.uk/

Design of Crystalline Products

CCG/IG Autumn Meeting
21st-22nd November 2017

Venue: Downing College, Cambridge, UK

Session topics

- Crystal Engineering
- Property Control & Prediction
- Crystallisation & Crystallisability
- Pharmaceutical Product Design
- Early career session with short talks + networking

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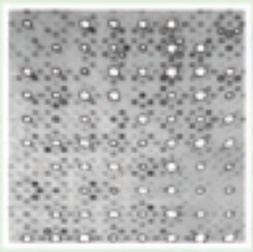
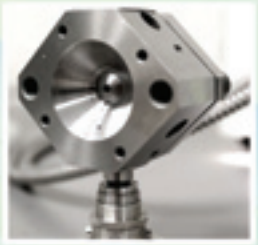
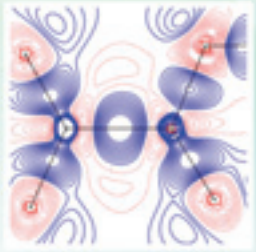


Incommensurates

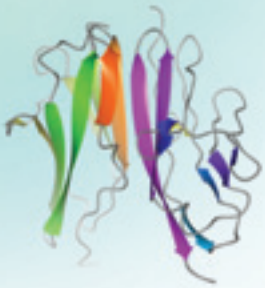


High Pressure



Charge Density

In situ



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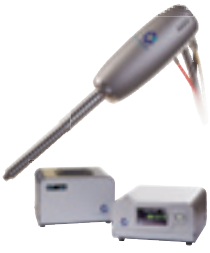
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