Crystallography News

British Crystallographic Association

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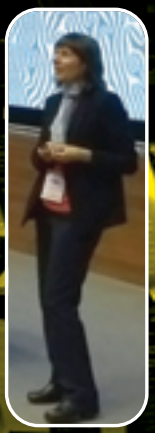

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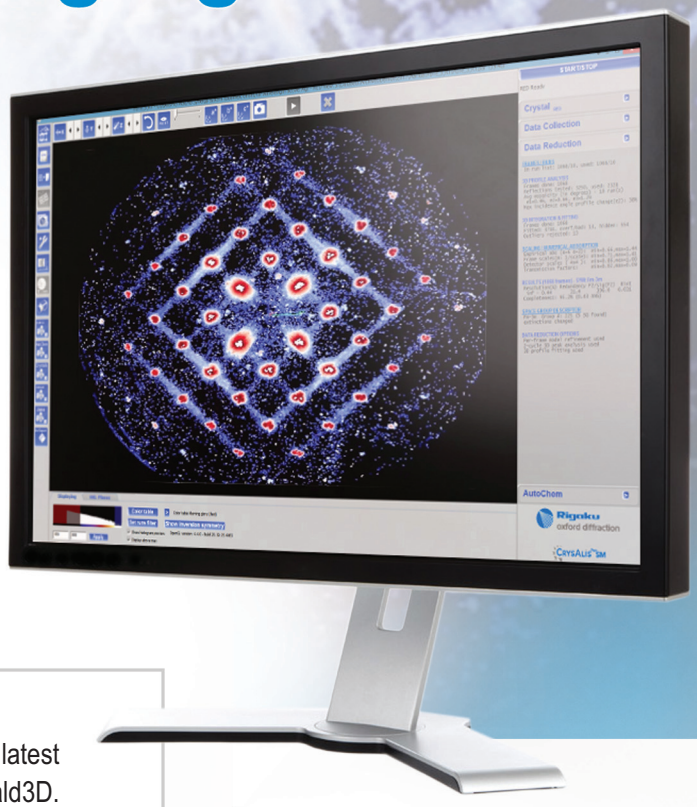

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Thank you to all exhibitors at our

BCA Spring Meeting 2018

BCA 2018

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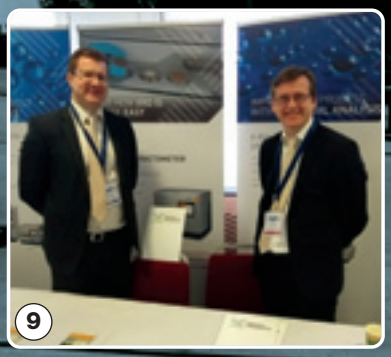
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Crystallography News June 2018

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Honorary Life Membership awards, plenary lecturers, dinner and ceilidh fun, Warwick scenes

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Please ensure that items for inclusion in the September 2018 issue are sent to the Editor to arrive before 25 July 2018.

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From the President

FIRST of all, I would like it say how honoured and delighted I am to be elected as President of the BCA, and I would like to thank the members for electing me. I was not able to attend the AGM, and I would especially like to apologise to all the members who were there, but I was away on an extended, and long planned, trip to Australia. Despite not being there, I hear that the Spring Meeting was a great success and we should thank Leo Brady and his colleagues for organizing and delivering it. I would like to extend my thanks to Lee Brammar for his sterling service as President over the last three years, and it is with some trepidation that I will now attempt to fill his shoes. In addition, thanks are also due to the other officers retiring from Council this year, Mark Senn and Stephen Moggach, for their valuable contributions to the running of the BCA. In the same vein, I must congratulate Cheryl Doherty on her election, Simon Coles on being re-elected, Hazel Sparkes who has agreed to be co-opted to complete Stephen's term, and the Nominating Committee for identifying candidates. I look forward to working with the new Council and the other hard-working committee members.

I should, perhaps, introduce myself a little more, in case not everyone read the election statements in *Crystallography News* in all their gory detail. I had a eureka moment as a chemistry undergraduate at UCL in 1970, at the end of an inspiring week-long practical, starting with mounting our crystals and ending with preparing a photographic print of an electron density map, where I could measure the C-N bond length in hexamethylenetetramine with a six-inch ruler (and it was correct!). I have been sold on crystallography ever since, initially as a small molecule chemical crystallographer working on specific recognition of alkali metal ions by small organic ligands, and topochemical control of photochemically induced reactions of small organic molecules in the crystal. I had a long-standing interest in biology, however, and soon moved into protein crystallography, initially in structure determination and refinement of oxymyoglobin using both X-ray and neutron crystallography at low temperature. Since then I have worked on other metalloproteins, including copper oxidases, magnesium containing nucleases, superoxide dismutase and NiFe hydrogenase. As we all know, crystal structures are essentially static images, or more correctly time and population averages, but function, such as catalysis, often implies dynamics. In order to address this, I have used freeze-trapping methods for observation of catalytic intermediates to try to follow structural changes through reaction cycles, focusing in particular on metalloenzymes. I am also interested in molecular recognition in ligand binding to proteins and drug design, antibody-antigen complexes, how nucleic acid binding proteins recognize specific DNA and RNA sequences in repression, activation, restriction and recombination, and virus structure and assembly. Crystallography has been the continuous theme, but we recently determined a virus structure by cryo-EM, where the quality of the density maps was a real revelation.

We are soon off to try out the Stanford Linear Coherent Light Source (LCLS) free-electron laser to see if it can help our investigation of catalytic intermediates. I hope to report back on how we got on in my column in the next newsletter. At least the weather will be good there in May, although we will probably be underground most of the time.

It's not every day that you turn on the television to watch the BBC 10 o'clock news and see a crystal structure come up on the screen, but that is exactly what happened to me a few days before writing this column. It was the PETase, or "plastic-eating enzyme" as the press would have it, from **John McGeehan**'s lab at Plymouth, where they have a mutant variant with higher activity against the poly(ethylene terephthalate), or PET, commonly used for plastic bottles. The natural enzyme was found in a bacterium living in a Japanese rubbish dump, and happily using plastic bottles as its carbon source. The interesting crystallographic angle is that John and his colleagues used the long-wavelength *in vacuo* beamline I23 at Diamond, with its huge cylindrical detector, to collect data with 2.5 Å X-rays allowing structure solution using the anomalous signal from native sulphur atoms. This was great publicity for crystallography and its relevance in the modern world.

Congratulations are due to other members in the news, including **Richard Henderson**, for the 2017 Nobel Prize for Chemistry, and **Andrew Goodwin**, for the Blavatnik Award 2018. **Elspeth Garman** and **Carl Schwalbe** were elevated to be Honorary Life Members, 2018. I should remind readers here that nominations close for this Honorary Life Members 2019 on August 31st. Nominations should be sent to me at president@crystallography.org.uk, along with a short case for support of not more than 400 words.

I should remind you that there some interesting meetings coming up, including a Joint BCA/RSC XRF Meeting at Sheffield Hallam University on 13th June, and a meeting of the South-West Structural Biology Consortium at the University of Exeter on 21-22nd June. Further afield the ACA2018 meeting is in Toronto 20-24th July and the 31st European Crystallographic Meeting (ECM31) is in Oviedo, Spain, on 22-27th August. Long distance travellers may be interested in the AsCA2018/Crystal32 Conference of the Asian Crystallographic Association and the Society of Crystallographers in Australia and New Zealand in December. At least the weather will be better there, with little chance of a "Beast from the East".

What about the next three years? It seems a daunting task now, but I will work to the best of my ability, on behalf of the members, for both the BCA and crystallography, during my tenure. There are bound to be challenges, and our task will be to meet and overcome them. I would be pleased to hear from any members on their ideas on how make the BCA even better, so please let me know what you are thinking. Crystallography is wonderful, as we all know, and the BCA is a great vehicle for its advancement and promotion. Once again, thank you for your confidence and giving me the opportunity to serve.

Simon Phillips

BCA Council 2018

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

From the Editor

THIS issue reports on another very successful BCA Spring Meeting. For those of us who remember the European Crystallographic Meeting at the University of Warwick in August 2013, the campus presented a different aspect this time. Instead of blazing August sunshine and squadrons of wasps, we had gentle dampness encouraging the masses of daffodils to give their best display, and an atmosphere largely devoid of flying fauna. However, I had promised ducks; and one morning two particularly erudite mallards stood outside the library and beckoned me towards the Science Concourse, which was the meeting venue. I have a variety of people to thank for the pictures, including Amber Thompson, Charlie McMonagle, Maggie White and my wife Joan.

On the cover you will see a picture taken by **Elizabeth Shotton** of three Honorary Life Members receiving their certificates. Since I am one of them, you might well attribute this placement of the picture to boastfulness; but I want to make a special point about my two fellow recipients, **Eleanor Dodson** and **Elspeth Garman**. Eleanor was handed the certificate for a prior year's award, while Elspeth is the other recipient for the current year. According to the BCA website, the award of Honorary Life Membership recognises "significant contributions by the recipient to crystallographic science and to the work of the BCA", and these two have certainly made such contributions. What it doesn't say is how much help and encouragement they have given to so many crystallographers over the years. Although they have been very busy, their unfailing kindness and friendliness has made them the "go-to" people for a wide variety of advice. It is a particular honour for me to be bracketed with them, especially since the "grumpy old man" strand of my research has unearthed a growing number of errors in published structures and may yet turn me into a "mini-Marsh".

I am delighted to include news of an honour for another loyal member of the BCA. The International Centre for Diffraction Data (ICDD) has long supported the BCA, and many of us have enjoyed and benefited from a chat with **Dave Taylor** at the ICDD exhibit at one of our Spring Meetings. Already a Fellow of the ICDD, Dave is one of two people who have just been named ICDD Distinguished Fellows. The ICDD has also recently announced its Board of Directors for 2018-2020. They are presented in this issue.

There was considerable discussion at this year's Spring Meeting about a policy on equality and diversity. Before the meeting many of us expected that it would be a formulaic exercise of no real significance because crystallography had always welcomed women as colleagues and leaders. After all, both named lectures at this year's main meeting (the Lonsdale and Hodgkin lectures) honoured great female crystallographers. The cover picture of Honorary Life Members reinforces this impression: two clever and creative women, and just one man, who perhaps is noted more for dogged diligence. However, the statistics presented below the policy give a cause for concern: 46% of our student members are female, but this drops to 36% for non-student Young Crystallographers and still further to 29% for regular members. Could it be that the factors impeding women in demanding professions may operate in crystallography as well? Therefore it was appropriate to adopt the equality and diversity policy presented in this issue.

I hope that many of you have made plans to attend the European Crystallographic Meeting in Oviedo, Spain this August. There is another meeting just beforehand which you should consider: the European Crystallographic Computing Forum in Mieres, Spain, which will run from 18-22 August. In the words of the invitation poster, "We welcome both beginners and experienced software developers from all crystallographic disciplines…" More information and the link to registration can be found at **https://tinyurl.com/mieres** . Oviedo is located in the beautiful province of Asturias, and the picture from turismoasturias.es adjacent to the poster demonstrates that Mieres is in a part of Asturias that can appropriately be described as "spectacularly beautiful".

A month later there will be another stimulating event. HOT TOPICS IN CONTEMPORARY CRYSTALLOGRAPHY 3 is an advanced workshop for PhD students and postdocs and other researchers in crystallography focussed on three very active areas of modern crystallographic research. This year the topics are Extreme Conditions, Total Scattering and Dynamical Crystallography. The meeting will be held in the town of Bol on the stunningly beautiful island of Brac in Croatia. Sep. 23rd to 27th, 2018. The website for further details is: **http://htcc2018.org/** .

As a benighted small-molecule crystallographer I always enjoy the PDB-101 Molecule of the Month and learn a lot from it. The topic for May is human papilloma virus (HPV) and vaccines. It shows the value of applying both cryo-electron microscopy and X-ray crystallography to a research area, and it helps us to understand the virus, how it can cause cancer, and how we might combat it. Infection by particularly virulent strains of this virus is the leading cause of cervical cancer. Type 16 papilloma virus, the most common cause of such cancer, is under study in PDB entry 3j6r. Cryo-electron microscopy elucidated the structure of its capsid, the preferred target for vaccine development. Coating its capsid with antibodies prevents a virion from infecting a cell. In PDB entry 6bt3 cryo-EM shows the interaction of the Fab antibody fragment with the capsid. The papillomavirus genome encodes two proteins, E6 and E7, which interfere with many cell signalling proteins and in particularly dangerous strains are involved in causing cancer. E6 marks out for destruction protein P53, "the guardian of the genome." Entry 4xr8 is the x-ray crystallographic study of the ternary complex E6/E6AP/p53 complex required for HPV-mediated degradation.

I conclude with a reminder about General Data Protection Regulation ("GDPR") that comes into effect May 25, 2018. If you wish to keep on receiving emails from **bca@hg3.co.uk** about such things as conference registration and abstract submission announcements, reminders and grant information, before this date you will need to click on "Update Settings" and tick the relevant box.

Carl Schwalbe

BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
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For current rates, and to join, please see **www.crystallography.org.uk/membership/**

Puzzle Corner

UNSCRAMBLE the anagrams of 5 methods for solving or determining structures. Note that hyphens or spaces between words have been omitted and capital letters have been made lower case.

omercy
openstart
didectotherms
ourfire
flingapigperch

Answers to March Puzzle Corner

IF you have been watching **Brian Cox**'s *Forces of Nature*, you will have seen his illustration of hexagonal snowflakes forming from interacting water molecules, which are in no way hexagonal. Yet some symmetrical molecules form crystals that do not "use" their symmetry. Of the following molecules, which form(s) crystals with the highest symmetry: cyclobutane, cyclohexane, benzene or cubane.

The space groups for crystalline cyclobutane (ZZZWEO01,02), cyclohexane (CYCHEX,01…07), benzene (BENZEN, 001…17) and cubane (CUBANE) are:

I2/m; C2/c, Fm3m (plastic cubic), $P2_1/n$; Pbca, $P2_1/c$; R-3

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

BCA 2018

WE converged on the Science Concourse of Warwick University in the drizzly aftermath of a low pressure area that passed through a few hours earlier. The corridor linking the conference areas has windows decorated with hexagonal molecules, which looked indistinct in the gloomy daylight. This provided an apt introduction to the Lonsdale Lecture given by Bill Clegg (Newcastle). Ideas about the structure of benzenoid hydrocarbons were similarly vague until Kathleen Lonsdale clarified the situation by determining the structure of hexamethylbenzene (HMB).

Named Lectures and Plenary Lectures

The Lonsdale Lecture

Bill's lecture had the title "Distortions, deviations and alternative facts: reliability in crystallography". He began by reminding us of Kathleen Lonsdale's remarkable achievements. Given that she was one of 10 children, she did not have the easiest start in life. In 1945 she became one of the first two female Fellows of the Royal Society, and she also was the first female President of the International Union of Crystallography. Bill recounted two of her memorable quotations: "The pure scientist seeks facts and accurate deduction from these facts." "A crystal is like a class of children arranged for drill…each individual child is a little fidgety." So why did she choose to work not on benzene, but rather on HMB with all the extra atoms? Importantly, the latter, unlike benzene, is solid at room temperature. Her structure determination settled a long-standing controversy by showing that HMB is flat and the electrons are distributed equally around the ring, not segregated into single and double bonds. But do more modern data confirm that HMB is really flat? There are now 7 CSD entries for HMB and 34 with it in co-crystals. The maximum internal and external torsion angles are 2° and 5° respectively. Bigger substituents lead to bigger torsions. Some monosubstituted benzenes have in-plane deviations that are not credible. There are 141 hits in the CSD with C-C-X angles < 100°, which must be artefacts of such things as unmodelled disorder. Bill also described studies of trigonal bipyramidal $[HgCl_5]^{3-}$. The first structure determination on the cubic crystals gave axial Hg-Cl distances of 2.519 Å which are noticeably shorter than the equatorial Hg-Cl of 2.640 Å. 'this contradicted **Roald Hoffman**'s prediction. However, repeated crystallization 7 years later give thin plates that were no longer cubic. This polymorph actually has axial Hg-Cl distances longer than equatorial! Bill concluded by reminding us that we are well endowed with means of structure validation. It is an overdetermined problem to which we can also apply chemical sense, along with software such as enCIFer, PLATON and MOGUL. Still there are some common sources of errors, starting with mistyped figures in items like cell parameters that still needed to be typed, transformation of the unit cell without matching transformation of reflection indices, and wrongly assigned atom types. Finally, we must be on our guard against deliberate fraud.

PCG Plenary

Nicola Spaldin (ETH Zurich) broadened our horizons to take in the entire universe with her title "From materials to cosmology: Studying the early universe under the microscope." The Grand Unification Transition is believed to have taken place very early in the development of the universe. A homogeneous vacuum changed to a lower symmetry vacuum which can be characterised by one choice of angle, leading to cosmic strings. Slow expansion leads to large regions with the same choice of angle and a low density of cosmic strings. Rapid expansion leads to many small regions with the same angle, and a high density of cosmic strings. Analysis of the cosmic microwave background provides one of the few clues to these mysterious events. However, Nicola and her colleagues have identified a multiferroic material, $YMnO_3$, where a symmetry-lowering phase transition follows the same mathematics of symmetry breaking. Spontaneous symmetry lowering leads to multiple defects. The structure consists of MnO_5 trigonal bipyramids separated by layers of Y. At high temperatures the space group is $P6_3/mmc$ and the behaviour is paraelectric. At low temperatures the space group changes to $P6_3cm$ and the material becomes ferroelectric. The structural transition involves trimerization and tilting. With 3 possible origins and 2 possible orientations there are 6 possible ferroelectric domains. Cooling $YMnO_3$ at different rates and monitoring defect formation allows one to verify that the "Kibble-Zurek scaling" proposed for cosmic string formation also applies to defect formation.

BSG Plenary

Under the title "Protein structure and dynamics using X-ray free-electron lasers" **Ilme Schlichting** (MPI for Medical Research, Heidelberg) began by paying tribute to the remarkable advances in macromolecular crystallography achieved with synchrotron radiation. However, this method encounters problems. Macromolecules can be difficult to crystallize due to their limited range of stability, conformational flexibility and tendency to aggregate. As crystals grow bigger, there is more chance of growth defects. Once a specimen crystal has been obtained and is irradiated, 9 out of 10 X-ray photons cause radiation damage without providing useful data. Global damage leads to decreasing resolution, increasing mosaicity and changes in the cell dimensions. Local damage causes specific chemical changes such as decarboxylation, S-S bond breakage and changes in the oxidation state of metals. What crystallographers want is damage-free data collection, and X-ray free-electron lasers (XFELs) can provide this, albeit requiring some heroic design parameters. For example, the SACLA XFEL has an undulator length of 130m. With their high peak brilliance and fs pulse length XFELs can outrun radiation damage and also enable time-resolved studies. From fs snapshots still images can be acquired and intensities I(hkl) obtained by averaging. However, σ values are also needed, which requires accurate determination of the profile. Introduction of the sample crystals *via* a gas dynamic virtual nozzle liquid jet (GDVN) leads to data collection on an unbroken liquid jet (before it breaks up into droplets). With crystals surrounded by mother liquor at room temperature in a thin jet the background is helpfully weak. Studies using XFEL technology have provided insight into ligand interaction with myoglobin (Mb), specifically CO. MbCO can be photodissociated into Mb + CO with quantum efficiency approaching 1. To investigate the dynamics, decomposition can be initiated with an optical pump pulse and followed with an X-ray probe pulse after a variable time delay. Because the protein concentration in crystals is very high and the optical density is appreciable, rapid and complete photolysis is easier to achieve with very small crystals. XFELs have made it possible to get information from such small crystals and visualise the early events following bond breaking, which are aptly called a "protein quake". Within 0.2 ps the CO is fully dissociated, the haem domed and the Fe atom out of plane by 0.2 Å. Subsequent oscillations have frequencies in agreement with those inferred spectroscopically.

IG Plenary

For a summary of this lecture, please see the report by **Helen Blade** on the IG sessions.

The Hodgkin Lecture

Eleanor Dodson (York) gave this lecture appropriately titled "The joy of seeing—in honour of **Dorothy Hodgkin**." She succinctly summarised such "seeing" as the process of going from crystal to diffraction to a model, and she began by describing 4 outstanding achievements emanating from Dorothy Hodgkin's laboratory. (1) Cholesterol iodide has 27 light (non-hydrogen) atoms along with 1 iodine that gives 75% of the scattering. The iodine atom could be located from the Patterson map and used for initial phase calculation. A projection Fourier map showed some atoms, and successive Fourier maps with improved data eventually revealed the remaining ones. Line Fourier maps provided the third coordinate. (2) The penicillin salt investigated by Dorothy Hodgkin has 23 light atoms and 1 Rb accounting for 55% of the scattering. Successive projection Fourier maps starting with phases from Rb confirmed that penicillin has a 4-membered ring, to the surprise of many chemists. (3) Vitamin B12 with its 112 atoms and just one Co was a much more daunting challenge. Importantly, Dorothy's early adoption of computers made its structure determination possible. (4) Insulin continued the pattern of increasing size and complexity. Eleanor then reminded us that while technology advances fast, the equations remain much the same. She outlined some of the most significant advances. Coot (2008) facilitated fitting a model to electron density. That density could be calculated more rapidly thanks to the Fast Fourier Transform (1968), which reduced calculation time from N^2 to N log(N). Improvements in statistical understanding provided assessments of the accuracy and completeness of the current model and the reliability of the experimental observations. However, no statistics can compensate for missing data. Eleanor illustrated this point with a model of a duck: missing high-resolution data led to a fuzzy duck, while missing low-resolution data gave a hollow duck. Non-crystallographic symmetry can enable averaging to reduce phase errors. Now that we have a large library of known structures, molecular replacement can often provide a starting point for a new structure. Even a tiny model may suffice: PDB entry 1sxv was solved starting with 3% of the atoms. Eleanor concluded with a thought-provoking question: "Speed allows automation, but is this always a good thing?"

CCG Plenary

This lecture is difficult to summarise in words because it was so spectacularly visual, as shown already by the picture on our cover and the illustration on page 74 of the conference booklet. Given by **Jonathan Nitschke** (Cambridge), it had the title "Crystallographic snapshots of soluble metallosupramolecular capsules." A succession of capsules were presented, displaying fascinating structures and a variety of useful properties. Jonathan began by discussing design principles for guest binding in $Fe^{II}_4L_6$ with

aromatic rings as panels. Anion binding induces structural adaptation, enabling anion extraction and recovery. For instance, ReO_4^- can be extracted from a mix of anions and then recovered, allowing the cages to re-form. Large M_8L_{12} cubes can be constructed by building in anthracene rings which are forced to lie flat and parallel to the cube faces, closing them off. In other systems stereochemical plasticity modulates cooperativity: one anion inside a cage repels a second anion, while a fullerene guest changes its conformation but gas can still bind. A capsule in the form of a trigonal bipyramid can effect small molecule fixation, changing CO_2 to CO_2^{2-} and SO_2 to SO_3^{2-} and ultimately SO_4^{2-}. A capsule of composition $Fe^{II}_{12}L_{12}$ has an icosahedral appearance even though there is no true icosahedral symmetry. It is very good for gas binding. Taking advantage of flexibility, dynamic imine exchange can be used as a route to interlocked structures such as a 5-fold interlocked [2]-catenane with S_{10} symmetry. The recurring theme in Jonathan's description of these varied structures was that only crystallography could elucidate the geometry.

Prize Lectures

BSG Prize

The BSG Prize was introduced by **Kate Brown** and awarded by **Marcus Winter** to **Vidya Darbari** (London) for her research including structure-function studies on mycobacterial-host interactions and the structural basis of transcription factor interactions. Core bacterial RNA polymerase (RNAP) together with the σ54 factor provide an ideal model system to study the initiation of transcription because the intermediate can be trapped. Cryo-EM work identified σ54 domain locations. After a lot of effort a crystal structure of RNAP- σ54 at 3.8 Å resolution was obtained, and σ54 was found to interact with various RNAP hotspots.

CCDC/CCG Prize

The CCDC/CCG Prize was awarded by **Peter Wood** to **Claire Hobday** (Bath) for "Exploring MOF flexibility and adsorption with high-pressure XRD and computational methods". Proline is an efficient modulator facilitating growth of high-quality crystals of Zr MOFs. The high bond enthalpy of Zr-O bonds endows such MOFs with strength against shear. Experiments in diamond anvil cells show that methanol can be squeezed into pores at high pressure, stabilising the framework. Initially the framework expands with permeation of MeOH, though compression ensues at higher pressure. MOFs with flexible ligands were found capable of withstanding higher pressure than those with rigid linkers. Diffraction experiments were backed up with single-crystal nanoindentation studies, DFT calculations and molecular dynamics simulations.

PCG Prize

Mark Senn (Warwick), the recipient of the PCG Prize sponsored by the IoP, conveyed insights achieved by studying phase transitions. In a culinary analogy, appropriate for listeners who might be anticipating the delicious conference dinner, he characterised rationalisations as "starters" and predictive control as "mains". He distinguished order-disorder from soft-mode phase transitions. With the latter, at high temperatures the molecules oscillate around central positions, but at low temperatures they "talk to" each other. A local approach is sometimes appropriate to describe charge ordering; in other situations a global approach is better. The first "starter" was the Verwey phase transition in Fe_3O_4, best described locally. Improper ferroelectrics, Ruddlesden-Popper phases, however, are best described globally. The proper ferroelectric $BaTiO_3$ has transitions from rhombohedral to orthorhombic to tetragonal to cubic phases at temperatures around 180 K, 270 K and 410 K. Since symmetry is expected to be lowered at lower temperature, the 180 K transition is unusual. Diffraction data and PDF analysis ascribe the differences in the phases to correlations of local symmetry-breaking distortions.

Carl Schwalbe

Group Reports

BCA session on Electron Diffraction (CCG)

HAVING attended BCA meetings on and off for 18 years, to the best of the author's knowledge, this is the first time the BCA has had a session dedicated to electron diffraction. I used to think there was some electron diffraction exclusion principle where there were only allowed one at a time to speak at a meeting. This hypothesis has now proven to be wrong with an excellent session on electron diffraction, which was well attended and led to active discussion between speakers and audience even after the talks concluded.

The session started with the invited **Xiaodong Zou** (Stockholm University) giving an overview of how the electron diffraction used for structure solution has evolved regarding *ab initio* structure determination of sub-micron crystals. The subject has evolved from collecting low index zone axis diffraction patterns (ZAP) to ZAP with associated images used to phase the reflections. To collect data in three dimensions, both images and ZAPs, took years to acquire sufficiently high-quality data sets. The next step in the subject's evolution is the work of Vincent and Midgley who added precession of the electron beam, to reduce dynamical effects present in ZAP's, finally to the work from the last decade where electron diffraction has followed the lead of X-ray crystallography and emulated or

(L-R) ***Andy Stewart*** *(Limerick),* ***Thanos Galanis*** *(Nanomegas),* ***Alex Hubert*** *(Warwick),* ***Richard Beanland*** *(Warwick),* ***Xiaodong Zou*** *(Stockholm)*

more recently implemented the oscillating crystal method. The subject is now routinely solving nano-crystals from a wide variety of specimens from inorganic and geological all the way through to organic and macromolecular crystals, as was also highlighted in a BCG session with **Tim Grüene**'s invited talk. Xiaodong finished her talk highlighting the next phase in the evolution of electron diffraction where the data collection mode is that of serial crystallography, with one diffraction pattern from one crystal.

The next speaker was **Richard Beanland** from the University of Warwick, introducing a very different type of electron diffraction, Digital Large Angle Convergent Beam Electron Diffraction (D-LACBED). Richard started with a list of issues of why electron diffraction is not practised as frequently as its versatility implies it would be, leading to a discussion of dynamical diffraction and how it can be used to measure the atom potential. D-LACBED is a method for obtaining many LACBED patterns simultaneously made possible by recent advances in computer control of transmission electron microscopes (TEM) and detectors, which lags about a decade or more behind the X-ray world. Richard then went on to explain that although the electromagnetic lens in a TEM gives us many advantages, for diffraction they also introduce more complexity which must be accounted for; once the data has been collected it needs to be processed to assemble the LACBED patterns for each reflection in the diffraction pattern. There is a discrepancy between theory and experiment by a factor of 2 for LACBED patterns. Next was **Alexander Hubert** a PhD student of Richard's at the University of Warwick explaining the challenges in processing the D-LACBED data and the challenges in measuring the electron potential. He started with a discussion on the Debye-Waller factor, where it derives from and what it means concerning electron diffraction patterns for the D-LACBED technique. Alex then went on to describe the processing and quantification of three different datasets with increasing complexity in the unit cell contents (Cu, GaAs, $SrTiO_3$). He explained how the materials' measured data matched theory less and less well the less homogeneous the unit cell was. The discrepancy between theory and experiment alludes to where the breakdown in theory and experiment lies, and where the path to bringing the theory and experiment into closer agreement is to be found. Once this discrepancy can be resolved the atom potentials can be measured, and direct inversion of the diffraction patterns may be possible.

The last speaker of the session was **Thanos Galanis** from the company Nanomegas, introducing the ideas of precession electron diffraction and its many applications, spanning electron diffraction tomography for *ab initio* structure solution on a wide variety of materials to phase orientation mapping. This is a nanoscale alternative to backscattered electron diffraction in the scanning electron microscope, showing copper grain maps down to 7nm, and used to identify lithium uptake in battery materials among other examples. Scanning precession electron diffraction can also be used to map stress and strain in the nanoscale by observing the change in the diffraction pattern between a strained and unstrained reference area; this has a broad range of potential uses for observing stress and strain on the nanoscale. Electron Pair distribution functions (e-PDF) were also discussed for obtaining information about amorphous materials on the nanoscale and how it was significantly quicker to collect them with electrons due to the much stronger beam-specimen interactions.

Dr Andy Stewart
University of Limerick, Ireland

Crystallisation of Macromolecules

THE BSG Session entitled "Crystallisation of Macromolecules" was organised and chaired by Professor Naomi Chayen, Imperial College and who opened the session with a very warm welcome for the Keynote speaker Dr Terese Bergfors from Uppsala University. Terese's Keynote lecture was entitled "Looking for the needle in a haystack: protein crystallisation screening strategies for academic laboratories". Starting from "What screen to use?" Terese described optimisation of a hit but went onto focus on what to do if there was no successful hit. Taking her laboratory's examples from the non-mevalonate pathway in *Mycobacterium tuberculosis* and *Mycobacterium smegmatis* she described the limiting returns beyond 200 chemical conditions, citing Janet Newman's 2005 article (Newman et al Acta Cryst D61, 1426–1431), a former PhD student of Terese's. A key parameter was the protein concentration but also cross seeding from crystals of one protein source to assist crystallisation of another was successful too.

Next Dr **James Birtley** of UMASS MED based in Slough then spoke on "Relieving the bottleneck: simple and rapid optimisation of protein crystals using only sparse matrix screens". James emphasised combining a starter crystallisation condition i.e. with poor-looking crystals or microcrystals to combine with a sparse matrix screen. A volume for volume

continued >>>

Speakers' photo (part group):
(L-R) Naomi Chayen, Liz Blackburn and Terese Bergfors

mix of 85% with 15% he had found to be a good choice documented with numerous examples of successful crystallisations and crystal structures. An audience question and James' answer led to the idea of considering why this works, probably being the increase of the number of chemicals in the crystallisation mix. An analysis of crystal lattice interactions could reveal which would be the best chemical and would be an interesting follow-up study.

Next Dr **Liz Blackburn** of the Edinburgh University Protein Production Facility, jointly with the Roslyn Institute, described her work on lymphostatin, a 366 kDa protein, and a giant virulence factor from pathogenic *E. coli*. The challenge here included using a lot of cells but yielding a small amount of protein such as 0.1 mg with subsequent concentration limited to 2 mg/ml. Liz showed an eye-catching picture of a needle crystal shaped like a sword. This had been very fragile, but led to discussion of the possibility for X-ray study if an X-ray transparent crystallisation plate were to be used.

Finally Prof **Elspeth Garman**, Oxford University spoke on "To cross seed or not to cross seed" and specifically "Why does crystallisation fail?". Elspeth showed that cross seeding yielded crystals where there were none before or were obtained quicker than before. This approach had indeed yielded two new crystal structures for Elspeth. The session I found to be a sparkling illustration of advances in crystallisation science.

John Helliwell
University of Manchester

Industrial Group report

THE theme of this year's Industrial Group sessions was Pharmaceutical hydrates and solvates. 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 was 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.

(L-R) Susan Reutzel-Edens and Cheryl Doherty

The plenary lecture, chaired by **Cheryl Doherty** (Pfizer), was given by **Susan Reutzel-Edens** (Eli Lilly). Susan gave an insightful talk on the challenging field of predicting polymorphism and how through current advances in algorithm development and computational speed, CSP is starting to become more commonplace in drug development. It was shown CSP can be complementary to conventional polymorph screening. Examples were shown how through careful interpretation of energy landscapes better understanding of crystallisation pathways can be achieved and highlight any gaps in the experimentally realized space.

This year's industrial group prize went to **Lewis Morgan** (University of Oxford) and was presented by **Cheryl Doherty** (Pfizer) during the Early Career Research session. Lewis gave a fantastic presentation on the concept of modulated structures and how they are becoming more common in molecular materials. Lewis was selected for the prize due to his presentation style of explaining a complex phenomenon in a clear way that could be understood at multiple levels… and with the use of rubber ducks.

Lewis Morgan

Lewis Morgan being presented with the industrial group prize by Cheryl Doherty

Finally, the IG's main session, Pharmaceutical Hydrates, chaired by **Helen Blade** (AstraZeneca) began with a keynote talk from **Amy Robertson** also from AstraZeneca. Amy outlined the properties of a hydrate, the different types of hydrates that can exist and 'what the problem was' with developing such material as a pharmaceutical when a third of pharmaceutical materials were actually hydrated. Amy talked the audience through two case studies that showed that hydrates were developable with care.

Next, we had **Doris Braun** (University of Innsbruck) who gave an insightful talk on a multidisciplinary approach covering experimental and computational methods to understand the formation of hydrates with non-stoichiometric behaviour. Then **Nadzri Mohd Najib** from Durham University gave an overview of an antiallergic compound, with an extremely rich and complex landscape of hydrates. It was shown that understanding the complicated hydration behaviour of such compounds was required to ensure safe and efficient manufacturing processes. The final talk of the hydrate session was given by **Pete Wood** from the CCDC, here it was shown how hydrates formation is common within pharmaceutical materials. The different types of hydrate co-ordination patterns were presented along with an insight into their frequency, showing that evaluation of hydrate structure can provide understanding and prediction of hydrate formation.

(L-R) Doris Braun, Pete Wood, Amy Robertson and Nadzri Mohd Najib

Helen Blade
AstraZeneca

Chemistry in Action (time resolved crystallography) CCG

THE Nobel laureate Leopold Ruzicka made a disparaging remark that stung crystallographers for a long time: "A crystal is a chemical cemetery". Chaired by Claire Murray, this session demonstrated that very "exciting" things can be going on within a crystal, and by measuring and understanding them we can greatly enhance chemical understanding.

Samantha Chong gave the keynote lecture with the title "*In situ* diffraction studies of porous molecular crystals". She began with the theme of the research being done by her and her colleagues at the University of Liverpool: designing for function. For the function of gas storage, pore size, volume and environment are important determinants. Variation of molecular components and connections within an overarching scheme is a good place to start, but the drawback is that we may end up making a series of closely related molecules with no real breakthroughs. However, the assembly of porous molecular crystals is governed by a variety of competing interactions, including hydrogen bonding, pi interactions, dipole-dipole interactions and halogen bonding. Small changes in their relative strength can lead to entirely different structures. Thus, surprising and interesting new structures can often be obtained; but predicting them in advance is exceptionally difficult. Porosity in molecular crystals can arise in two ways. Extrinsic porosity results from inefficient packing of molecules, leaving voids. Intrinsic porosity results when the molecules themselves contain an inherent void. Samantha then considered specific examples of gas uptake by cages. Cycloaddition of an aldehyde and an amine can produce a porous cage, for example α-CC2. Rietveld refinement based on *in situ* powder diffraction data showed that α-CC2·6(CO_2) does have full occupancy of CO_2. Moreover, when the crystal is xenon-loaded, refinement gives a total occupancy of 2.2(1) Xe per cage, in good agreement with the uptake measured experimentally.

Lucy Saunders (Diamond) presented "Tracking H atom transfer by parametric single crystal refinement". In the solid state, proton transfer can occur across a D-H…A hydrogen bond, so that D^- + H-A^+ is the result. This transfer can influence significant properties such as colour or ferroelectricity. Gradually changing an external variable such as temperature can make it possible to track the H atom along the transfer pathway. For instance, on beamline I19 at the Diamond Light Source data were collected at 25 K intervals from 100 K to 500 K for the test system pyridine-3,5-dicarboxylic acid, whose migration behaviour was already known from neutron diffraction measurements. The high flux from a synchrotron source made it possible to collect the required mass of data easily and rapidly. However, because the signal from hydrogen atoms with X-rays as opposed to neutrons is so weak, it is difficult to track their position reliably. This difficulty was alleviated by using the method of Parametric Refinement in Topas Academic. Normally applied to powder X-ray diffraction data, for the single crystal synchrotron X-ray diffraction data used here it enabled the parameters common across the data sets to be fixed in a consistent model as a rigid body. The resulting reduction in data : parameter ratio led to greater certainty in refined parameters such as H atom positions. Lucy and her colleagues tested key variables to see which gave the best agreement with the "gold standard" neutron structure determinations. These included the refinement protocol (independent *versus* surface), the H atom model and the anisotropic displacement parameters (normal *versus* TLS). It is hoped that in future this methodology will facilitate H atom tracking from X-ray data alone.

Lauren Hatcher (Bath) told us about "Photocrystallographic kinetic studies using time-resolved diffraction methods on beamline I19 at Diamond Light Source". Time-resolved photocrystallographic studies need careful timing between photo-excitation and diffraction data collection, necessitating an understanding of the photo-reaction kinetics. The types of experiment depend on the excited state (ES) lifetime and comprise steady state, pseudo-steady-state and pump-probe studies. Lauren concentrated on solid state linkage isomers, starting with N-bound nitro complexes of metal ions which can be excited to form two isomers of O-bound nitrito complexes. Her specific example was [Pd(Bu_4dien)(NO_2)]BPh_4, which forms robust crystals that diffract well and exhibit no disorder. Solid state UV-visible spectroscopy suggests that irradiation with light of wavelength 390-500 nm would be suitable. Irradiation by LED ring at 400 nm gave 100 % conversion to the nitrito-ONO isomer below 200 K. As such, it was the first Pd- NO_2 system to go to 100 %. The ES has a sufficiently long lifetime that at regular intervals the irradiation could be paused and data collected, yielding good information about the structure of the ES. To study the decay of the ES, data were collected as rapidly as possible after full excitation had been completed. Variable temperature experiments showed that the decay mechanism of nitrito-ONO is strongly temperature-dependent. The information thus gained allows the development of suitable pump-probe protocols.

In her talk "*In situ* continuous segmented flow crystallisation at Diamond Light Source" **Lois Wayment** (Bath) changed our focus from structure of fully formed crystals to crystal growth. She described the design of crystallisers adapted for in-beam operation at Diamond. At set points there are hydrophobically coated Kapton viewing windows that allow the passage of X-rays. Blobs of solution separated by air bubbles are carried past successive windows, enabling the development of crystals to be monitored. Urea : barbituric acid (UBA) in methanol was chosen as a model system. UBA has 3 polymorphs. Crystallisation in MeOH gives a mixture of forms I and III. Another model system, succinic acid in water, typically crystallises as the β polymorph out of the two possibilities.

Daniel Watkins (Sheffield) brought the session to an exciting conclusion with "Continuous flexibility of a hexagonal metal-organic framework". Flexible MOFs are rare. Where they exist, the flexibility is usually between discrete states, open- and closed-pore structures that are determined by the presence or absence of a guest species. The Sheffield group has synthesised two MOFs based on a d^{10} metal centre and two-fold interpenetrated, which display *continuous* flexibility that is guest-dependent. For instance, the MOFs can be prepared with solvents DMF or $CHCl_3$, then gradually heated. Progressive desolvation and gradual alteration of the MOF structure can be monitored by *in situ* powder diffraction.

Carl Schwalbe

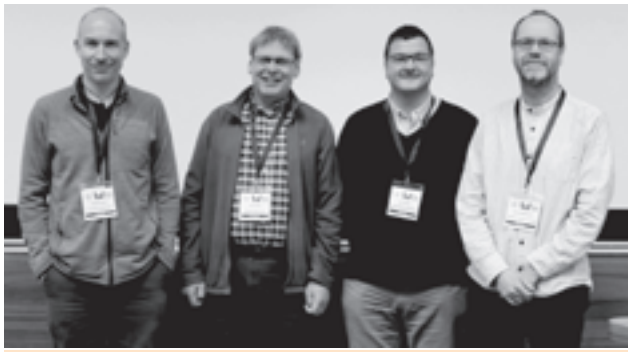
Service Crystallography Forum (CCG)

CHAIRED by William Lewis, this session covered several topics of great importance to anyone providing a crystallography service.

Under the title "When are bad data good data?" **Amber Thompson** (Oxford) shared experiences with us obtained from running a very productive crystallography service. She began by showing pictures that illustrated problems such as badly shaped spots, streaks along rows of spots and gaps in data from a modulated structure. Then she took a good data set and doctored it in ways that represented problems. Cutting the number of reflections to 851 reflections for 281 parameters, or throwing away the strongest 50 % of the full data set still permitted structure determination. While it is commendable to strive for the best resolution and completeness, one should not despair if circumstances make this impossible. Amber reminded us that intensity I is arbitrary and must always be accompanied by σ(I). She showed how plots of I/σ(I) are affected by different schemes for assigning σ. What matters to the chemist is likely to be "Does it solve". "How well does the model fit?" should be the next question.

David Allan (Diamond) brought us up to date about "Remote access on beamline I19: a new approach for structural chemistry studies". The major upgrade at the end of 2015 enabled very rapid data collection with a pixel-array detector in shutterless mode and allowed a remote user to change samples and collect data. Samples are introduced robotically in a puck which can hold 16 crystals. Since a shipping Dewar can hold 7 pucks, a user can send in 112 crystals. Because samples can be mounted and stored at home, and are stable once frozen, no beam time is wasted while fishing for a suitable crystal. However, one must watch out for a phase transition between room temperature and 77K. Remote operation requires a fast and stable internet connection. Given such availability, there is software to transmit sample information for shipping, process data during the experiment and save logs including metadata, and review the data and reprocess if necessary after the experiment.

Horst Puschmann (Durham) told us about "Hirshfeld Atom Refinement from Olex2: too good to be true?" The Hirshfeld partitioning used here has 4 steps: 1. Calculate the molecular wave function by quantum mechanics. 2. Partition the wave function according to the Hirshfeld scheme. 3. Take the Fourier transform of the partitioned wave function for each atom. 4. Use in refinement. A recent paper [M. Fugel et al. (2018) IUCrJ 5, 32-44] showed that refinement against X-ray data by such a scheme gave X-H bond distances that agree well with those from neutron diffraction. Horst gave a convincing demonstration of how easy Olex2 makes this refinement.



(L-R) William Lewis, David Allan, Gary Nichol, Horst Puschmann

Special commendation goes to **Gary Nichol** (Edinburgh) for keeping a cool head in a crisis. Just before the start of his talk "An Edinburgh experience of CSD Communications: publishing the unpublished via an undergraduate project", there was a total failure of the projection system. Not all the king's horses or all the king's men could get it together again. Poor Gary had to give his talk with no visual aids whatsoever, and he did it brilliantly. Fortunately his talk did not involve any description of specific crystal structures. Edinburgh has multiple instruments, enabling the collection of about 450 data sets per year. Inevitably, some chemists planning to present both the chemistry and their crystal structure in the same paper will actually go no further than verifying the connectivity. CSD deposition provides a way to make the rest of the crystallographic information available; it works well and is curated. Because Edinburgh carefully kept an archive of CIFs on a server with sequentially numbered folders, it was feasible for an undergraduate summer student trained by CCDC to run CheckCIF on each unpublished structure, make corrections where necessary and possible, and send them off to CSD Communications. Of course, it was very helpful if comments about problems or non-standard items had been inserted into the CIF when it was first made.

Carl Schwalbe

Bursary Recipients' Reports

I'VE attended all the BCA spring meetings since I started my DPhil and I've enjoyed them more and more for every year. This year, I was particularly excited about the list of plenary and keynote speakers, which looked simply astounding. In addition, I was looking forward to the short travel time to Warwick, relative to the previous year.

As usual, the conference started with the young crystallographers' meeting, where all the three interest groups (chemical, physical and biological) meet. The plenary was given by Dr **Serena Corr**, who gave a humorous and instructive account of lithium ion batteries, followed by interesting talks by students from all over the world. Despite the "B" in "BCA" meaning "British", these meetings are indeed very international. The informal dinner and poster session at the end of the day gave a good opportunity to catch up with fellow crystallographers from other universities.

The main meeting began the following day with a truly amazing talk by Professor **Nicola Spaldin** about the interface between crystallography and cosmology. Who knew that phase transitions in $YMnO_3$ can explain the symmetry lowering of the entire universe after the Big Bang? Subsequently, a range of talks in three parallel sessions ensued. As a physical crystallographer, I mainly attended the physical sessions, where the topics ranged from multiferroics to perovskites to synchrotron/neutron techniques. But BCA gives a good opportunity to widen one's crystallographic horizons and I also very much enjoyed the CCG plenary given by **Jonathan Nitschke** about supramolecular cages and **Xiaodong Zou**'s keynote talk about electron diffraction. Regardless of interest, I think everyone appreciated the Hodgkin lecture, given by **Eleanor Dodson**. She worked with **Dorothy Hodgkin** and hence had several funny stories to tell. Moreover, the talks

given in the early career prize sessions were excellent and covered a range of interests from transcription inhibition to MOF flexibility to solid state phase transitions.

Despite an intense schedule, there were generous breaks, giving an opportunity to view the posters, catching up with friends, compliment speakers on their talks as well as chatting to the more senior academics present. On the last evening, the traditional conference dinner took place, followed by a ceilidh. The venue was spacious, with good food, and our postdoc was particularly excited by the Australian wine. Having lived for four years in Scotland whilst studying for my undergrad degree, I always love to take part in ceilidhs and this year – despite an unplanned elastic collision – was no exception.

All in all, it was a very well-organised and stimulating conference, which both provided an opportunity to learn more about one's own areas of interest and also to learn about the use of crystallography in other fields.

Hanna Boström
University of Oxford

MY BCA Spring meeting 2018 adventure starts very early, 6:00 a.m. precisely, from Belfast. As for myself and Abdessamad, a PDRA who just joined the Edkins group, attending his first BCA, and the second for me, we have to make our way in the cold morning for our flight to Birmingham. As we reached Canley train stop from Birmingham airport, we decided to walk to Warwick University, under a light shower. We managed to arrive just in time for the Lonsdale Lecture given by Prof. Bill Clegg. As a young researcher, it is always inspiring for me to hear about the work of an early crystallographer like Kathleen Lonsdale. I just can't imagine what it would be like for myself working without the aid of a computer, and at the same time ensuring good and reliable data, like Kathleen.

In true BCA style, I hopped between lectures as my interest splits between the physical and chemical group. I found the talk by Dr **Matthew Dyer** from the University of Liverpool on combining computational and experimental crystallography quite impressive, and equally fascinating was the lecture by Dr **Cheryl Doherty** from Pfizer on surfaces and polymorph selection.

The highlight of the meeting for me was definitely the industry group (IG) plenary by Prof. **Susan Reutzel-Edens** from Eli Lily. Coming from the faculty of pharmacy, I found her talk relatable, and at the same time it reiterated the relevance of our work towards understanding hydrate formation. In fact, the whole IG session echoed the message and argument brought forth by Prof. Susan. I am fortunate to have been given the opportunity by the committee to also give a talk in the same IG session, along with prominent researchers in my field like Dr **Doris Braun** from the University of Innsbruck, whose ever detailed and comprehensive work I admire.

I also found the poster session and networking slot engaging, as always. BCA meeting tradition continued with a formal dinner along with awards given to young investigators and poster prizes for students. I also found the lectures on electron diffraction on the final day were equally engaging. As I make my way back to Belfast, back to the lab work and writing, back to pushing through these final few months of my PhD, and hopefully going back home to Malaysia… one thing that I am sure is that this will not be my last BCA!

Mohd Nadzri Mohd Najib
Queen's University Belfast

AS a student member of the BCA, I have been fortunate enough to attend the last two BCA meetings at Nottingham and Lancaster. This year at Warwick I presented a poster as part of the YCG and main meeting poster sessions. The main meeting poster session was well attended and I discussed my research with several of the attendees.

The conference was kicked off with the YCG satellite meeting; the programme for this meeting is always varied with talks covering chemical, physical, biological and industrial aspects of crystallography. The highlights were talks given by **L. Morgan** and **F. Lang** on modulation in materials and silver co-ordination polymers respectively; however, these were just two of the excellent talks given at the YCG this year. In addition I found the two keynotes in the *'When crystals go wrong'* session, given by Prof **Elspeth Garman** and Dr **John Claridge** to be of interest. As an organometallic chemist, I could relate to the crystallisation problems and diffraction quality of protein crystals that Elspeth described in her talk. I often have difficulty growing crystals and on more than one occasion found that it is not the beautiful crystals that give the best diffraction, if the crystals diffract at all.

The YCG meeting always has a great programme and it creates a fantastic networking opportunity due to its relaxed atmosphere. Over the last three years, I have made several lasting connections with other young crystallographers.

There were several sessions to choose from in the main meeting. One of the first sessions I attended was, *'Chemistry in action'*. As someone who has been to Diamond I19 to conduct experiments, it was interesting to find out what other researchers use synchrotron facilities for; the uses are varied and it was fantastic to see the breadth of research carried out.

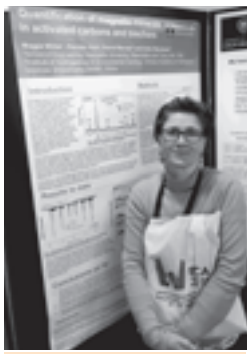
One of my favourite sessions of the main meeting was *'MOFs, molecular machines, rotaxanes and supramolecular chemistry'*. I found the keynote given by Dr **Paul McGonigal** was particularly interesting and there were several analytical techniques described that I can utilise in my own research.

The conference dinner held on the final evening was one to remember, the ceilidh was good fun to watch and participate in. The evening gave another chance to network and build links with other researchers.

I hope to attend future BCA meetings and remain a member of the BCA after I have completed my PhD.

Clare Stubbs
University of Bath

THE programme for the BCA Spring Meeting 2018 at the University of Warwick was packed with a medley of great topics and speakers, with three oral sessions running concurrently during each day of the main meeting and social events during the evening. We were kept busy!



Maggie White and poster

Although sadly no longer a Young Crystallographer myself, there were still plenty of opportunities to enjoy the research posters and speak to researchers from the Young Crystallographers' Group Meeting that preceded the Main Meeting, starting on Tuesday 27 March. First, Professor **Bill Clegg** delivered the Lonsdale Lecture with a charismatic and insightful overview of **Kathleen Lonsdale**'s research and reminded us of the importance of maintaining objectivity in our own work, highlighting various experimental and interpretative issues that are sometimes encountered. Professor **Nicola Spaldin**'s evocative plenary lecture 'From Materials to Cosmology' was followed by a stimulating afternoon of talks covering (amongst many other topics) novel in-situ synchrotron studies to protein crystallography to ferroic and multiferroic materials. Professor **Ilme Schlichting**'s impressive plenary on X-ray free-electron lasers marked the end of the first afternoon's oral presentations.

Tuesday evening comprised a sociable poster session with a buffet and drinks reception and an opportunity to catch up with colleagues past and present and also to speak to the many exhibitors. Particularly useful for me were discussions with colleagues from Malvern PANalytical, Oxford Cryosystems, SciMed and Anton Paar relating to new instrumentation available for non-ambient powder diffraction in controlled environments, which I am keen to acquire for our powder XRD service at Newcastle University.

The oral sessions on Wednesday resumed with the same excellent quality of speakers as the previous day. The Perovskite session, chaired by Professor **Mike Glazer**, was a highlight for me and covered many aspects of emerging research in this field. Professor **Patrick Woodward** delivered an engaging presentation using case studies to showcase the effects that structural distortions can have on the physical properties of perovskites and Dr **Mark Senn** presented a stimulating talk highlighting the various criteria involved in the design of magnetoelectric perovskites.

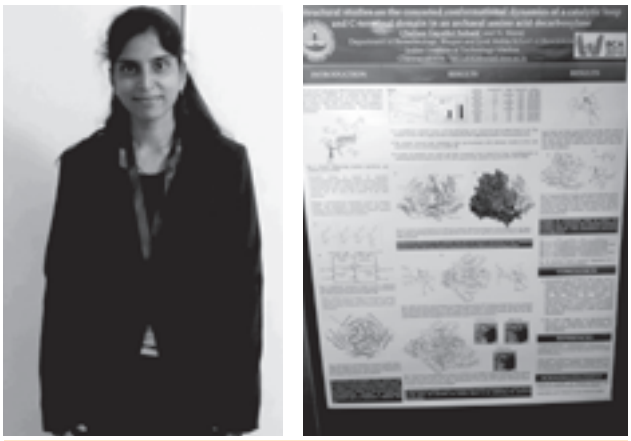
After oral presentations by the Early Career Researcher Prize winners and the Wednesday afternoon sessions, Professor **Eleanor Dodson** closed the day's oral programme with an entertaining but humbling Hodgkin Lecture. We were taken on an intriguing journey through the life and works of the pioneering crystallographer **Dorothy Hodgkin** and reminded of the trials and tribulations of solving crystal structures by hand: far from enviable yet a truly impressive feat, given the luxuries of the instrumentation and software tools that we have access to today, compared to some 70 years ago. By 7.30pm, after a decent-length AGM, we were all ready for the Conference Dinner and an energetic ceilidh!

The Spring Meeting came to a close on Thursday lunchtime after hearing some great oral sessions on electron, neutron and synchrotron techniques followed by 'Hot Topics', headed by an impressive talk on ferroelectric domain structures from Dr **Finlay Morrison**. Dr **Claire Murray**'s account of her impressive secondary school outreach venture 'Project M' using beamline I11 at the Diamond Light Source was both interesting and inspiring, with the project involving a phenomenal degree of organisation!

Finally, I would like to express my gratitude to the ABBF for my award which allowed me to attend this year's BCA Spring Meeting. It was a worthwhile and enjoyable meeting and I look forward to attending again in the future.

Maggie White
Newcastle University UK

THE winner of the American Crystallographic Association (ACA) Journal of Structural Dynamics poster prize at BCA 2018 was Ms Chellam Gayathri Subash from the Indian Institute of Technology in Madras, India. The title was *"Structural studies on the concerted conformational dynamics of a catalytic loop and C-terminal domain in an archaeal amino acid decarboxylase"*. The judging panel was Prof John R Helliwell (Manchester) as Chair along with Prof Ilme Schlichting (Heidelberg) and Prof Xiaodong Zou (Stockholm). This Prize is awarded for excellence in research on structure determination and dynamics of systems, enabled by the emerging new instruments (e.g. XFELs, electron sources, etc.) and new experimental and theoretical methodologies and is open to students (graduate and undergraduate) and post-docs. The journal is published by the American Institute of Physics with the ACA.



Ms Chellam Gayathri Subash from the Indian Institute of Technology in Madras, India, and the winning poster.

Prizes Awarded at BCA 2018

Richard Cooper thanking **Leo Brady** for serving as Programme Chair

BSG David Blow Poster Prize winner **Elizabeth Blackburn**
(prize collected by Atlanta Cook)
The prize was presented by John Berrisford

BSG Prize winner
Rachel Wilkinson
The prize was presented by John Berrisford

RSC CrystEngComm Prize winner
Kiaora Tolmie
The prize was presented by Michael Andrews

RSC CrystEngComm Prize winner
Feifan Lang
The prize was presented by Michael Andrews

Rigaku Prize winner
Natalie Pridmore
The prize was presented by Claire Murray

Durward Cruikshank Prize winner
Claire Hobday
The prize was presented by Elliot Carrington

PCG Prize winner
Tobias Bird
The prize was presented by Paul Henry

Thank you gift to **Sam Horrell** for serving as YCG Chair
The prize was presented by Elliot Carrington

Exhibition Passport winner
Paul Stainton
The prize was presented by Richard Cooper

Other prize winners *(no photographs taken)*
James Bird winner of the YCG "I'm a Scientist Get Me Out of Here" Prize, (Oxford)
Samar Mohapatra winner of the Rigaku-BSG Poster Prize, (IIT Madras)
Zheng Luo winner of a PCG Prize, (Warwick University and Xi'an, China)
Lorella Spiteri winner of a CrystEngComm Prize, (University of Malta)

BCA Equality, Diversity and Inclusivity Policy

POLICY statement modified to include age in list of criteria in section on SPEAKER INVITATION POLICY following discussion at AGM on March 28th, 2018.

BCA Equality, Diversity and Inclusivity Policy

March 2018

The BCA Council is pleased to announce the adoption of the following policy:

CONFERENCE POLICY

The BCA recognizes the positive impact that a conference speaking opportunity has on an individual's track record and visibility. We also recognize that some sections of the scientific community are often under-represented in conference programmes, and that this can affect diversity in the long-term. Our policies are intended to ensure quality and equality.

SPEAKER INVITATION POLICY

The program chairs will ensure the highest quality scientific programme, with speakers that represent the broad diversity of our community. We aim to achieve a speaker and programme chair balance that reflects the make-up of our community without bias with regard to gender, sexual orientation, race, religion, disabilities, age, geography, or national origin.

REPORTING POLICY

We will report and review statistics on the gender balance of the membership, the composition of committees and of invited speakers, selected speakers, session chairs, and attendees of the BCA Spring Meeting.

FEEDBACK

We welcome feedback to president@crystallography.org.uk on this policy and how it might be improved for future conferences to better ensure equality and diversity.

Gender diversity statistics presented to AGM 28 March 2018

Membership (estimated)

Students – 50 female and 59 male:	46% female
YC (not including students) – 20 female and 36 male:	36% female
Standard members – 147 female and 355 male:	29% female

Main Meeting	**2014**	**2015**	**2016**	**2017**	**2018**
Programme Committee:	53%	44%	27%	27%	27%
Plenary speakers:	0%	0%	25%	25%	75%
Keynotes:	17%	28%	11%	18%	28%
Speakers:	12%	35%	31%	24%	38%
Chairs:	53%	22%	23%	42%	43%
YCG Meeting					
Plenary speakers:	50%	50%	50%	0%	50%
Teaching session:	n.a.	0%	0%	66%	n.a.
Speakers:	31%	38%	62%		29%
Chairs:	67%	60%	40%	40%	33%

Plenaries - some improvement recently? **Keynotes** - similar across 5 yrs - needs attention.
Session chairs - good, not much evidence that this helps remove possible bias in keynote selection (may even hinder people from giving invited talks, if they're chairing).
Contributed talks - approximately reflects our membership gender distribution.

ICDD Announces its 2018-2020 Board of Directors

(L-R) Xiaolong Chen, Scott Misture, Terry Maguire, E. Andrew Payzant, Tom Blanton, Robert Dinnebier, Matteo Leoni, Jim Kaduk, Mark Rodriguez, David Rafaja, Vanessa Peterson, Takashi Ida

THE International Centre for Diffraction Data (ICDD) is pleased to announce its new Board of Directors, serving the term 2018 through 2020:

Chairman – **Matteo Leoni**
University di Trento, Department of Civil, Environmental and Mechanical Engineering, Trento, Italy.

Vice Chairman – **Xiaolong Chen**
Institute of Physics, Chinese Academy of Sciences, Beijing, People's Republic of China.

Treasurer – **James Kaduk**
Poly Crystallography, Inc. Naperville, IL, USA.

Corporate Secretary – **Theresa Maguire**
International Centre for Diffraction Data, Newtown Square, PA, USA.

Executive Director – **Tom Blanton**
International Centre for Diffraction Data Newtown Square, PA, USA.

Chairman, Technical Committee – **Mark Rodriguez**
Sandia National Laboratories, Albuquerque, NM, USA.

Directors-at-Large (2016-2020):

Robert Dinnebier
Max-Planck Institute fuer Festkoerperforschung, Stuttgart, Germany.

Takashi Ida
Nagoya Institute of Technology, Ceramics Research Laboratory, Tajimi, Japan.

David Rafaja
Freiberg University of Technology, Institute of Materials, Science Structure Research, Freiberg, Germany.

Directors-at-Large (2018-2022):

E. Andrew Payzant
Oak Ridge National Laboratory, Oak Ridge, TN, USA.

Vanessa Peterson
The Bragg Institute, ANSTO, Lucas Heights, NSW, Australia.

Past Chairman – **Scott Misture**
Alfred University, NYS College of Ceramics, Alfred, NY, USA.

ICDD Distinguished Fellows

THE 2018 ICDD Spring Meeting provided the ideal venue for the Board of Directors to honor two ICDD Fellows by naming them as ICDD Distinguished Fellows. This award was established to further recognize Fellows who have given long and meritorious service to the ICDD. During the Annual Meeting of Members on Thursday, 15 March 2018, ICDD's Chairman, **Matteo Leoni**, had the pleasure of announcing the newest recipients of this prestigious award: **Catharine Foris**, formerly of DuPont, Wilmington, Delaware, and **David Taylor**, formerly of the Pilkington Group, UK.

David Taylor

Current Fellow, **David Taylor**, was also named as an ICDD Distinguished Fellow. Dave became a member in 1999 and quickly became involved in many ICDD activities. He served as a member of the Board of Directors and also as a member of several Committees of the Board. Dave helped bring the awareness of XRF as a complementary technique to ICDD and was instrumental in creating the first XRF Subcommittee. Dave served as Regional Co-Chair for the UK and Ireland for many years. In that capacity, he attended many meetings, particularly the British Crystallographic Association meetings, and hosted many PDF Workshops in that region as an ICDD representative and ambassador.

Dave's most notable contributions emanated from his role as ICDD Treasurer, in which he served for 10 years. He continued to remain active in similar capacities as Chair of the Budget and Review Subcommittee, and currently serves as Chair of the Marketing Committee.

The IUCr OUP Book Series; overview and update

I AM glad of the opportunity to highlight details on the IUCr OUP Book Series and which I presented as a poster at the BCA Spring Meeting held recently in Warwick.

First and foremost let me say that the IUCr OUP Book Series Committee warmly welcomes proposals for new publications and makes its recommendations to the IUCr Executive Committee and to the Delegates of the Oxford University Press (the body responsible for approving all publications handled by the OUP).

TWO TYPES OF BOOK

The sixty books published within the book series stretch back about 20 years, and more than 58000 copies have been sold. They are now commissioned in two categories:

- Monographs on Crystallography
- Texts on Crystallography

IUCr BOOK SERIES COMMITTEE MEMBERS

A diverse, highly experienced, membership of the Committee has recently been assembled and is as follows:

- J.R. Helliwell (Chair, UK)
- G. Chapuis (Switzerland)
- J. Gulbis (Australia)
- R Herbst-Irmer (Germany)
- H. Maynard-Casely (Australia)
- P. Mueller (USA)
- M. Nespolo (France)
- N. Yagi (Japan)
- X. Zou (Sweden)
- K.A. Kantardjieff (USA; ex officio as Chair of Commission on Crystallographic Teaching)
- S. Adlung and H. Kohnishi (ex officio representatives of Oxford University Press)

SUBMISSION OF A PROPOSAL

The procedure to submit a proposal is described here:

http://www.iucr.org/iucr/governance/advisory-committees/book-series/proposals

and basically involves providing:

(a) a presentation of the motivation, aims, scope, level, and readership of the proposed volume;

(b) a detailed Table of Contents (with subheadings);

(c) a short CV of the authors;

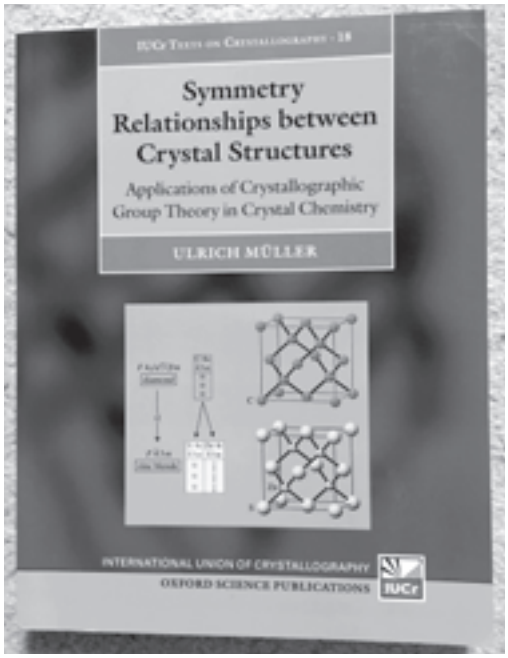
(d) a sample chapter or part of a chapter;

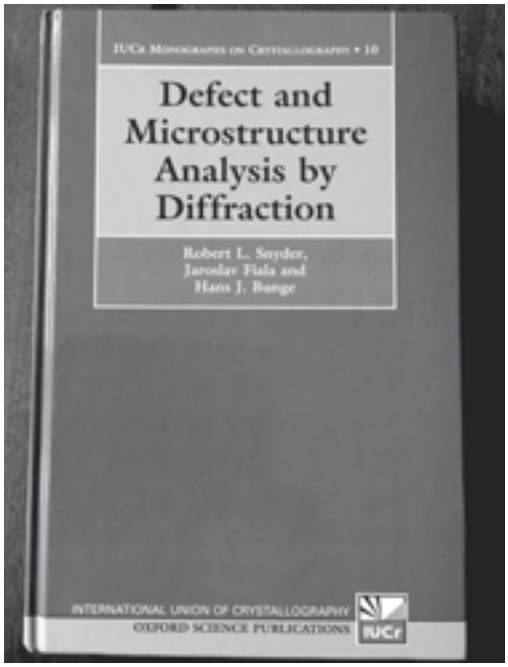
(e) a list of related books and brief comments on how they differ from that proposed.

Example book covers are from:

https://www.iucr.org/publications/iucr-oup

And show a consistent and distinctive style e.g.:-





John R Helliwell, Chair of the IUCr OUP Book Series Committee

A Summer and Autumn Upcoming

THIS upcoming conference 10 to 12 October 2018, Grenoble seems to be rather a milestone. It is jointly organised by the Institut Laue Langevin and the European Spallation Source and is entitled:- European User Meeting (see http://www.neutrons4europe.com/). The conference website describes itself as follows:-

"The neutron landscape in Europe is going through a period of dramatic change. Two major, national facilities will close by 2020 while substantial investment in a new European facility, ESS, will deliver transformative capabilities and extend the technique to new domains by the middle of the next decade. After the Millennium upgrade programmes, ILL is currently executing phase one of the Endurance programme to further enhance its instruments and infrastructure and is now preparing a second, more extensive phase of Endurance that will be the basis of future operations well beyond 2023.

The future of neutron scattering is bright, but both the landscape of facilities and the community of users must take a proactive and strategic approach to navigating and managing these changes in a holistic way, in order to ensure the sustainability and vitality of this important research technique.

ILL and ESS therefore feel that it is timely to review recent achievements and the current status and, above all, look forward to new scientific opportunities with neutrons for the next decade.

The User Meeting programme foresees ten keynote speakers on future directions in neutron science, as well as reports on recent achievements and ongoing work at ILL and ESS. There will be 'focus sessions' in the User Meeting to highlight several key techniques while satellite events, in parallel with the User Meeting, will allow participants to delve deeper into specific areas of neutron science."

The focus sessions, mentioned above, are on:-

- Scientific potential for combined or in-situ neutron spectroscopy;
- Laue Diffraction for Biology;
- Laue Diffraction for Materials;
- Spectroscopy in Biological Systems;
- Imaging.

The satellite events, running in parallel with the user meeting are on:-

- Structure and evolution of thin films and interfaces;
- Magnetism matters;
- Diffraction and energy materials;
- Neutron spin echo spectroscopy – 40 years of NSE user operation;
- Neutron vibrational spectroscopy.

The ESS construction is well underway as these drone photographs from the recent ESS Newsletter shows:-

Photos: Roger Eriksson / ESS

The ESS is also making itself known via its participation for example in helping to organise the Workshop on Neutron Macromolecular Crystallography at the ECM31 upcoming in Oviedo (see **http://ecm31.ecanews.org/en/neutron-macromolecular-crystallography.php**)

That the UK's SRS played a role in helping the development of the neutron Laue method and its instrument provision of LADI and VIVALDi at the Institut Laue Langevin via a synergistic transfer of expertise and analysis procedures, including software, from Daresbury Laboratory is of direct interest to me. Indeed I mention another splendid conference event of much interest to crystallographers and their use of central facilities is happening in late June at Liverpool University and is highlighting all aspects of synchrotron radiation development and is majestically entitled:- ***"50 years of Synchrotron Radiation in the UK and its global impact"***. See:- **http://www.uksr50.org/** . For my submitted abstract I will present as a poster, and which I have already shared an advance draft of on my twitter account **@HelliwellJohn** on May 8th 2018. My contribution is entitled "Integrating X-rays, neutrons and electrons in structural chemistry and biology".

Twitter and drones! Remarkable developments for our science life as well as for our everyday life.

John R Helliwell
University of Manchester.

50 years of Synchrotron Radiation in the UK and its global impact

UKSR50 - 26-29 June 2018, University of Liverpool, UK
www.uksr50.org

ON behalf of the Organising Committee, it is with great pleasure that we extend an invitation for you to attend the UKSR50 to be held in Liverpool during 26-29 June 2018.

The UK Synchrotron Radiation effort started in the 1960's and led to the establishment of the national Synchrotron Radiation Facility (SRF) at the NINA 5GeV electron synchrotron at Daresbury Laboratory via a five-year research grant of six million pounds (in today's value) in 1970. The use of SRF over 5 years persuaded the UK's Science Research Council to design and build the world's first dedicated multi-GeV storage ring that came in operation in 1980.

In 1997 the Synchrotron world received its ultimate recognition in the form of the first Nobel prize for work facilitated by synchrotron radiation (John Walker 1997). An all insertion device third generation source was recommended by the Woolfson review giving birth to a new source that was named DIAMOND in 1995, funded in 2001 and began its operation in 2007 at the Harwell campus in Oxfordshire.

During the past fifty years Synchrotron Radiation, has become an integral part of the UK's academic and industrial science base; and there are now over 70 synchrotron sources and FELs worldwide which facilitate an expanding range of pure and applied science.

We invite you to a conference to celebrate the achievements and explore the future of the light sources (Synchrotrons and FELs) and their applications in the coming decades. It coincides with 70th anniversary of the first publication of the International Union of Crystallography which decided to establish the dedicated Journal of Synchrotron Radiation at its Congress and General Assembly in 1993.

Nearly fifty percent of the invited talks will be selected from the submitted abstracts.

Samar Hasnain and **Richard Catlow**
(Joint Chairs)

Plenary Speakers Include:

Sir Venki Ramakrishnan, Mrc Lmb and The President Of The Royal Society

Sir Mark Walport, Chief Scientist, HM Government (Provisional)

Prof Ian Munro, Emeritus Scientist and Former Director of Synchrotron Radiation, STFC (Daresbury Laboratory)

Sir Tom Blundell, (Cambridge)

Simon Billinge, (Columbia & Nsls)

Mikael Eriksson, (Lund, Sweden)

Tetsuya Ishikawa, (Harima, Japan)

Liu Lin, (Lnls, Campinas, Brazil)

John Spence, (Arizona)

Dave Stuart, (Oxford/diamond)

Moniek Tromp, (Amsterdam, Netherlands)

Bert Weckhuysen, (Utrecht, Netherlands)

Phil Withers, (Manchester)

Registration:

Fees & Early Bird Registration: The following fees will apply:
Standard academic/professionals (1/4/18-15/6/18) **£500** (Student/Retiree **£200**) Accompanying partners **£150** (includes 3 dinners). The fee is inclusive of lunches, refreshments and two evening dinners. In order to make a payment, please visit **payments.liv.ac.uk**

Joint XRF Meeting – Wednesday 13th June 2018

THIS joint XRF meeting is on Wednesday 13th June 2018 at Sheffield Hallam University.

Registration: REGISTRATION CLOSES at 23:59 on Thursday 7th June 2018. You will be asked which morning parallel session you will attend – Beginner or Experienced, Check the programme below now to decide.

Fees: £100 or £50 concessions.
For registrations queries please contact: **Louise Smith**, Tel: +44 (0)1423 529333 Email: louise.smith@hg3.co.uk

This meeting offers a great opportunity for both novice and experienced users to enhance their XRF knowledge and discuss their requirements with major XRF suppliers in the exhibition. The morning has parallel sessions for Beginners and Experienced Users and offers an ideal opportunity for anyone considering adding XRF to their analytical techniques. Attendees of these sessions will be given a certificate of attendance for their Continuing Professional Development.

Pens Sponsored by Spectro UK Ltd.
Pads Sponsored by Datech Scientific Ltd.
Calendar Sponsored by SciMed.

Time	Session 1: Introduction to XRF for Beginners	Session 2: XRF Updates for Experienced Users
09:30	Registration, Exhibition and Coffee – *Sponsored by Malvern Panalytical Ltd.*	
10:00 – 10:05	Plenary Introduction: Welcome, Safety, etc.	
10:10 – 10:35	Nick Marsh – Theoretical Introduction to XRF	Rainer Schramm – The Secret of Getting Multiple XRFs to Provide Equivalent Quantification
10:35 – 11:00	John Martin – Different approaches to XRF: Handheld, ED-XRF, WD-XRF use In oil exploration	Garry Smith – Matrix Influence Correction Methods XRF Calibration
11:00 – 11:20	Coffee-break – *Sponsored by XRF Scientific*	
11:20 – 11:45	Rainer Schramm – Introduction to XRF Sample Preparation: its importance and an overview of the various options	Mike Dobby – Advanced Methods of Sample Preparation for Difficult Samples
11:45 – 12:10	Kevin Talmage – Overview of Typical Applications for XRF	Greg Bale – Latest Developments in
12:10 – 12:50	Sponsor Slot: each supplier to suggest something about their XRF that makes it a useful tool in the analytical lab	
12:50 – 13:50	Lunch – *Sponsored by Malvern Panalytical Ltd.*	
13:50	Plenary Session: The Place of XRF in the Analytical Laboratory	
13:50 – 14:15	Tom Knott – The use of XRF in the Geological Laboratory	
14:15 – 14:40	Jim Barker – The Place of XRF in the Petroleum Industry Laboratory	
14:40 – 15:05	David Beveridge – The use of XRF for Analysis of Coatings and of (mostly) Organic Chemicals	
15:05 – 15:35	Tea-break – *Sponsored by Specac Limited*	
15:35 – 16:00	Chris Vanhoof – Micro-X-ray fluorescence spectrometry (μ-XRF) – Seeing more by looking at less – some dedicated applications	
16:00 – 16:25	Karen Vernon-Parry – Handheld XRF for Analysis of Counterfeit Coins	
16:25	Brief Roundup, Farewell and Finish	

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.

1-10 June 2018
Electron Crystallography. 51st Erice Course, Erice, Italy.
http://crystalerice.org/2018/

1-10 June 2018
First Erice International School on Quantum Crystallography. 52nd Erice Course, Erice, Italy.
http://crystalerice.org/2018/

3-8 June 2018
Three Dimensional Electron Microscopy. GRC, Newport, RI, USA.
https://www.grc.org/three-dimensional-electron-microscopy-conference/2018/

4-5 June 2018
Applied Crystallography, London.
http://crystallography.euroscicon.com/

4-8 June 2018
4D Workshop: Deep-time Data Driven Discovery and the Evolution of Earth, Washington, DC, USA.
http://www.4d-workshop.net

4-8 June 2018
Quasicrystals: pattern formation and aperiodic order, Edinburgh.
http://www.icms.org.uk/workshops/quasicrystals

4-8 June 2018
ICDD Clinic on X-ray Powder Diffraction: Session I – Fundamentals of X-ray Powder Diffraction, Newtown Square, PA, USA.
http://www.icdd.com/education/xrd.htm

6-8 June 2018
2nd Meeting on Porous Molecular Solids (PoMoS), Vietri sul Mare, Italy.
http://www.pomos.org/

10-14 June 2018
ISXB3. 3rd International Symposium on Halogen Bonding, Greenville, SC, USA.
http://isxb-3.org/

10-16 June 2018
FEBS 2018: Advanced Methods in Macromolecular Crystallization, Nove Hrady, Czech Republic.
https://macromolcryst2018.febsevents.org/

11-13 June 2018
Fourth international SPHIRE workshop, Dortmund, Germany.
http://sphire.mpg.de/

11-14 June 2018
55th Annual Meeting of the Clay Minerals Society, Urbana-Champaign, IL, USA.
http://conferences.illinois.edu/cms/

11-15 June 2018
ICDD Clinic on X-ray Powder Diffraction: Session II – Advanced Methods in X-ray Powder Diffraction, Newtown Square, PA, USA.
http://www.icdd.com/education/xrd.htm

11-16 June 2018
13th International Conference on Synchrotron Radiation Instrumentation (SRI 2018), Taipei, Taiwan.
http://sri2018.nsrrc.org.tw/site/page.aspx?pid=901&sid=1157&lang=en

13 June 2018
Joint BCA/RSC XRF Meeting, Sheffield.
https://sites.google.com/site/bcaxrf/meetings/13-june-2018

14 June 2018
Exploiting Disease Genomics to Catalyse New Medicines, Oxford.
https://www.thesgc.org/tep-symposium-2018

18-19 June 2018
UK-Israel Summer School 2018 on NanoScale Crystallography for Bio and Materials, Tel-Aviv, Israel.
http://nano.tau.ac.il/Summer-School

18-21 June 2018
PCG Intensive School in Physical Crystallography: From Phonons to Phase Transitions
Cosener's House, Abingdon, Oxfordshire.
http://pcgschool2018.wordpress.com/

18-22 June 2018
2018 E-MRS Spring Meeting and Exhibit, Strasbourg, France.
https://www.european-mrs.com/meetings/2018-spring-meeting

18-26 June 2018
The 14th European Summer School on Scattering Methods Applied to Soft Condensed Matter, Carcans-Maubuisson, Gironde, France.
https://indico.ill.fr/indico/event/86/page/2

19-22 June 2018
MLZ Conference 2018 "Neutrons for Culture and Arts", Lenggries/Munich, Germany.
https://indico.frm2.tum.de/event/56/

21-22 June 2018
2018 Atomic and Molecular Interactions Group (AMIG) Summer Meeting, London.
https://www.iopconferences.org/iop/frontend/reg/thome.csp?pageID=759914&eventID=1240

24-28 June 2018
American Conference on Neutron Scattering (ACNS 2018), College Park, MD, USA.
http://www.mrs.org/acns-2018

24-28 June 2018
Ultrafast X-ray Summer Seminar (UXSS), Menlo Park, CA, USA.
https://app.certain.com/profile/web/index.cfm?PKwebID=0x1008141abcd

24-29 June 2018
10th International Conference on the Occurrence, Properties, and Utilization of Natural Zeolites – Zeolite 2018, Krakow, Poland.
http://zeolite2018.org/

24-29 June 2018
Crystal Engineering (GRC), Newry, ME, USA.
https://www.grc.org/crystal-engineering-conference/2018/

25-27 June 2018
Artificial Water Channels: Faraday Discussion, London.
http://www.rsc.org/events/detail/26212/artificial-water-channels-faraday-discussion

25-27 June 2018
Science@FELs, Stockholm, Sweden.
https://indico.maxiv.lu.se/event/476/

25-28 June 2018
DSL2018. 14th International Conference on Diffusion in Solids and Liquids, Amsterdam, Netherlands.
http://www.dsl-conference.com/

26-29 June 2018
Electrochemistry at Nano-interfaces: Faraday Discussion, Bath.
http://www.rsc.org/events/detail/26816/electrochemistry-at-nano-interfaces-faraday-discussion

26-29 June 2018
UKSR50. 50 years of Synchrotron Radiation in the UK and its global impact, Liverpool.
http://www.uksr50.org/

29 June – 1 July 2018
14th TOPAS Users Meeting, Edinburgh.
https://www.bruker.com/pt/events/users-meetings/x-ray-diffraction-and-elemental-analysis/topas-users-meeting.html

1-4 July 2018
EPDIC16 – The 16th European Powder Diffraction Conference, Edinburgh.
http://epdic16.efconference.co.uk/

2-6 July 2018
Combined Analysis in XRD by using MAUD software: 9th Workshop, Caen, France.
http://maud.radiographema.eu/

3-6 July 2018
Polarized Neutrons for Condensed Matter Investigations (PNCMI) 2018, Abingdon,
http://www.pncmi2018.org/home

4-6 July 2018
EMAG2018: Applications of Electron Microscopy to Beam Sensitive Materials, Coventry.
http://emag2018.iopconfs.org/home

8-13 July 2018
Aperiodic 2018, Ames, IA, USA.
https://register.extension.iastate.edu/aperiodic2018

8-13 July 2018
Geoanalysis 2018, Sydney, Australia.
http://ccfs.mq.edu.au/Geoanalysis2018/

8-13 July 2018
Sagamore2018, Halifax, Nova Scotia, Canada.
http://www.sagamore2018.ca/

9-13 July 2018
SIAM Conference on Mathematical Aspects of Materials Science, Portland, OR, USA.
http://siam.org/meetings/ms18/

10 July 2018
Nano-medicine and characterisation, London.
https://www.iopconferences.org/iop/frontend/reg/thome.csp?pageID=737559

11-13 July 2018
Methods and applications of crystal structure prediction: Faraday Discussion, Cambridge.
http://www.rsc.org/events/detail/24508/methods-and-applications-of-crystal-structure-prediction-faraday-discussion

15-20 July 2018
15th International Conference on Applications of Quasielastic Neutron Scattering – QENS2018 - WINS2018, Hong Kong.
http://qens-wins2018.com/

16-20 July 2018
Workshop on Diffuse Scattering and Structure Simulation, Erlangen, Germany.
https://www.icsp.nat.fau.eu/neder-group/discus-home/

20-24 July 2018
ACA 2018, Toronto, Canada.
http://www.amercrystalassn.org/2018-meeting-homepage

22-27 July 2018
XAFS2018. 17th International Conference on X-ray Absorption Fine Structure, Krakow, Poland.
http://www.xafs2018.com/

23-27 July 2018
18th International Conference on High Pressure in Semiconductor Physics (HPSP18) and Workshop on High Pressure Study on Superconducting (WHS2), Barcelona, Spain.
https://congresses.icmab.es/hpsp18-whs2/

23-28 July 2018
Particle based methods in materials science, Edinburgh.
http://www.icms.org.uk/workshops/particlebasedmethods

25-28 July 2018
χ-mag 2018, Nara, Japan.
http://www2.pe.osakafu-u.ac.jp/pe8/kai_mag2018/kai_magn2018_index.html

26-28 July 2018
In situ Methods in Cell Biology and Cellular Biophysics. EMBO workshop, Berlin, Germany.
http://meetings.embo.org/event/18-insitu-methods

28-29 July 2018
Diffraction Methods in Structural Biology (GRS), Lewiston, ME, USA.
https://www.grc.org/diffraction-methods-in-structural-biology-grs-conference/2018/

29 July – 3 August 2018
Diffraction Methods in Structural Biology (GRC), Lewiston, ME, USA.
https://www.grc.org/diffraction-methods-in-structural-biology-conference/2018/

5-9 August 2018
Microscopy & Microanalysis 2018 (M&M 2018), Baltimore, MD, USA.
https://www.microscopy.org/MandM/2018/

5-9 August 2018
ZMPC2018. International Symposium on Zeolites and Microporous Crystals, Yokohama, Japan.
http://www.jaz-online.org/ZMPC2018/

6-10 August 2018
Denver X-ray Conference, Westminster, CO, USA.
http://www.dxcicdd.com/

12-17 August 2018
Goldschmidt, Boston, MA, USA.
https://goldschmidt.info/2018/

13-17 August 2018
IMA XXII, Melbourne, Australia.
https://www.ima2018.com/

18-22 August 2018
European Crystallographic Computing Forum, Mieres, Spain.
https://www.mrc-lmb.cam.ac.uk/harry/ecacomsig/mieres.html

19-22 August 2018
3rd International Workshop on Biological Membranes, Helsinki, Finland.
https://www.helsinki.fi/en/conferences/international-workshop-on-biological-membranes

19-24 August 2018
XRM2018: 14th International Conference on X-ray Microscopy, Saskatoon, Saskatchewan, Canada.
http://xrm2018.com/

22-27 August 2018
31st European Crystallographic Meeting (ECM31), Oviedo, Spain.
http://ecm31.ecanews.org/en/index.php

26-30 August 2018
7th EuCheMS Chemistry Congress, Liverpool.
https://www.euchems2018.org/

27-30 August 2018
15th Biennial Meeting of the Society for Geology Applied to Mineral Deposits, Glasgow.
https://www.sga2019glasgow.com/

27 August – 1 September 2018
BCA/CCP4 Summer School in Protein Crystallography, Didcot (Diamond).
http://www.diamond.ac.uk/Home/Events/2018/BCA-Summer-School.html

28-31 August 2018
Workshop on subtomogram averaging with Dynamo, Basel, Switerland.
https://wiki.dynamo.biozentrum.unibas.ch/w/index.php/Basel_Dynamo_Workshop_2018

29 August – 2 September 2018
AIC International Crystallography School 2018, Bari, Italy.
http://www.cristallografia.org/aicschool2018/eng/detail.asp?idn=3129

2-6 September 2018
SMARTER6, Ljubljana, Slovenia.
https://smarter6.ki.si/index.php/smarter6/

2-6 September 2018
XXIV Conference on Applied Crystallography, Bieszczady Mountains near Przemyśl, Poland.
http://www.cac.us.edu.pl/

2-7 September 2018
MATRAC 1 School: Application of Neutrons and Synchrotron Radiation in Materials Science, Lauenburg and Hamburg, Germany.
https://www.hzg.de/ms/summerschool/058651/index.php.en

3-6 September 2018
Photon 2018, Birmingham.
http://www.photon.org.uk/516760

3-7 September 2018
XTOP2018. XIV Biennial Conference of High Resolution X-ray Diffraction and Imaging, Bari, Italy.
http://www.ba.ic.cnr.it/xtop2018/

3-7 September 2018
Synchrotron Radiation and Neutrons in Art and Archaeology, Portsmouth.
http://www.diamond.ac.uk/Conference/SR2A-2018.html

3-14 September 2018
22nd Laboratory Course Neutron Scattering, Juelich and Garching, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/LabCourse/_node.html

9-13 September 2018
29th Annual Meeting of the European Society for Biomaterials (ESB2018), Maastricht, Netherlands.
http://www.esb2018maastricht.org/

9-14 September 2018
19th International Microscopy Congress. IMC19, Sydney, Australia.
http://imc19.com/

10-11 September 2018
Scottish Centre for Macromolecular Imaging – Symposium and opening, Glasgow.
https://www.facebook.com/SCMICryoEM

13-14 September 2018
10th International Workshop on Radiation Damage to Biological Samples, Brookhaven, Upton, NY, USA.
https://www.bnl.gov/rd10/

13-16 September 2018
ESCG2 Second European School on Crystal Growth, Varna, Bulgaria.
http://escg2.eu/

16-19 September 2018
8th Conference on Electron Tomography, Les Diablerets, Switzerland.
https://www.colorado.edu/symposium/etm2018/

16-19 September 2018
Neutrons and Biology, Carqueiranne, France.
https://sites.google.com/view/bioneutrons2018

16-20 September 2018
ECCG6 Sixth European Conference on Crystal Growth, Varna, Bulgaria.
http://eccg6.eu/

16-21 September 2018
ECCG6 Sixth European Conference on Crystal Growth, Varna, Bulgaria.
http://eccg6.eu/

16-21 September 2018
Synchrotron Radiation School (SR school 2018), Oxford and Diamond Light Source.
http://www.diamond.ac.uk/Home/Events/2018/SR-Summer-School.html

20-22 September 2018
HEC 21. 21st Heart of Europe Bio-Crystallography Meeting, Quedlinburg, Germany.
http://hec21.uni-halle.de/

22-25 September 2018
SEG2018. Metals, Minerals and Society, Keystone, CO, USA.
http://www.seg2018.org/

23-27 September 2018
Hot Topics in Contemporary Crystallography – HTCC, Bol (island of Brač), Croatia.
http://htcc2018.org/

24-28 September 2018
ICDD Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.
http://www.icdd.com/education/rietveld-workshop.htm

24-28 September 2018
MDANSE: Molecular Dynamics and Lattice Dynamics to Analyse Neutron Scattering Experiments, Puerto de la Cruz, Tenerife, Spain.
https://www.isis.stfc.ac.uk/Pages/MDANSE-2018.aspx

26-29 September 2018
7th Murnau Conference on Structural Biology, Murnau, Bavaria, Germany.
http://www.murnauconference.de/conference_2018/index.php

5-7 October 2018
9th International Conference of the Hellenic Crystallographic Association, Patras, Greece.
https://sites.google.com/view/hecra2018/home

7-12 October 2018
SAS2018. XVII International Conference on Small-Angle Scattering, Traverse City, MI, USA.
http://sas2018.anl.gov/

8-14 October 2018
ASMOSIA XII - Association for the Study of Marble & Other Stones in Antiquity XII, Izmir, Turkey.
http://asmosia2018.com/

16-19 October 2018
Neutrons and Food 5, Sydney, Australia.
http://www.ansto.gov.au/Events/Neutronsandfoodconference2018/index.htm

29 October – 1 November 2018
JCNS Workshop 2018, Tutzing, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/JCNSWorkshops/2018Workshop/_node.html

13-14 November 2018
BCA-Industrial Group Autumn meeting, Durham.
bca@hg3.co.uk

2-5 December 2018
AsCA 2018/Crystal32: 15th Conference of the Asian Crystallographic Association and 32nd Conference of the Society of Crystallographers in Australia and New Zealand (SCANZ), Auckland, New Zealand.
http://asca2018.org/

European Crystallographic Computing Forum

Mieres, Spain, 18th - 22nd August 2018

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Helen Ginn (CPPXFEL)
James Parkhurst (DIALS)
Randy Read (PHASER)

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