Crystallography News

British Crystallographic Association

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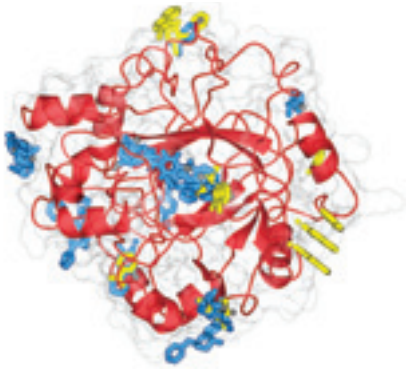
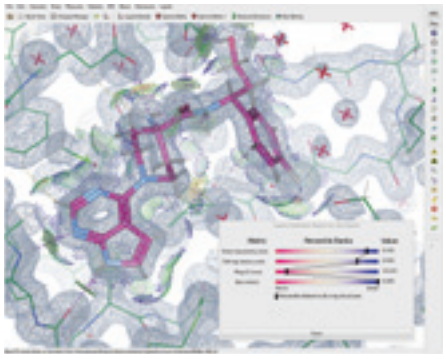
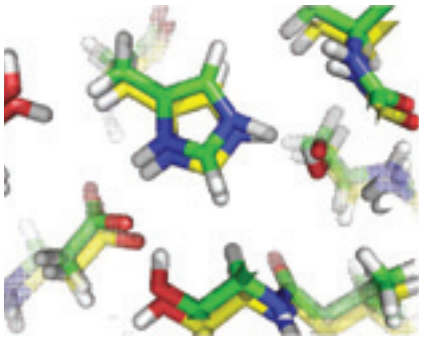

Spring Meeting and CCP4 Highlights

The University of Nottingham

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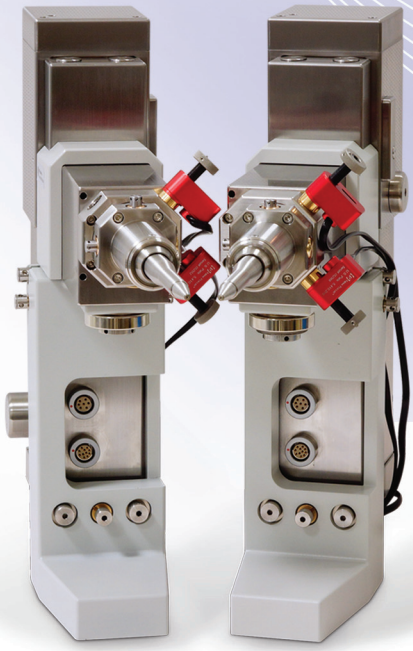

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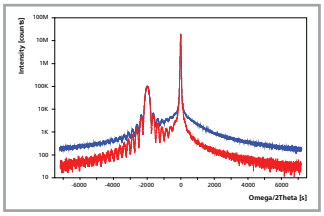

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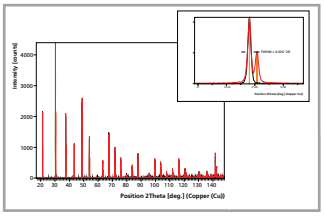

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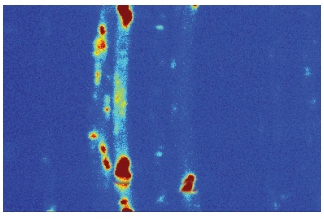

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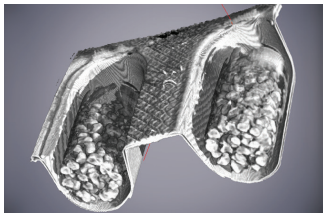

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Crystallography News June 2016

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by Bowmans, Leeds. Text should preferably be sent electronically as MSword documents (any version - .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.
Please ensure that items for inclusion in the September 2016 issue are sent to the Editor to arrive before 25 July 2016.

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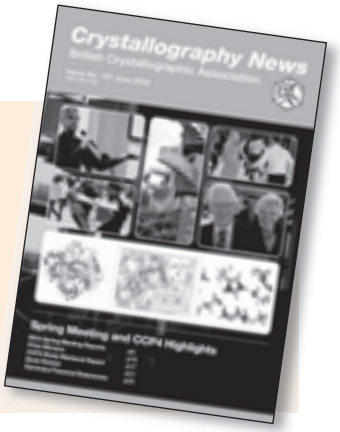
This month's cover:

Spring Meeting scenes; Figures 2, 4 and 6 from CCP4 report



From the President

IT'S a good time to reflect on an excellent Spring Meeting in Nottingham. Feedback from those who attended was very positive, concerning both the scientific programme and the venue. Attendance was 250+ for the second consecutive year. It was also a pleasure to meet Stephen Wallwork, a founding member of the BCA, and his wife Marion, who were guests of the BCA and University of Nottingham School of Chemistry at the banquet.

The future of all organisations and scientific disciplines depends on the involvement and development of students and early-career researchers, so it was very encouraging to see an attendance of 118 at this year's YCG satellite meeting. I am also pleased to see that the **Early Career Prize Lecture Symposium** is now firmly established as an important part of the BCA Spring Meeting and would like to congratulate the winners of the four awards: **Mark Warren** (Diamond Light Source) winner of the CCDC Chemical Crystallography Prize, **Paul Saines** (University of Kent) winner of the IoP Physical Crystallography Prize, **Matthew Gold** (University College London) winner of the BSG Prize – sponsored by Rigaku Oxford Diffraction, and **Clare Stubbs** (University of Bath) winner of the IG–YCG Prize.

The PCG plenary lecture in Nottingham was given by **Bill David** (ISIS Facility, University of Oxford). His talk, entitled *120 Years of Powder Diffraction*, allowed him to look back on a century of progress in this technique, but also to think about what the future may bring in this field. Bill is one of the more well-known and distinguished members of the BCA community, having presented the inaugural BCA Prize Lecture in 2002, the Lonsdale Lecture in 2007 and one of the Bragg Lectures associated with the Centenary celebrations in 2013. Bill has been an Honorary Life Member of the BCA since 2002, and I'm very pleased now to be able to offer my congratulations on his election to Fellow of the Royal Society (https://royalsociety.org/people/william-david-12857/). I am delighted also to see the election to FRS of **Russell Morris** (University of St. Andrews), whose work in solid-state chemistry, notably zeolites and metal-organic frameworks, has always made strong use of diffraction methods, particularly powder diffraction (https://royalsociety.org/people/russell-morris-12886/).

I would like to congratulate **Richard Cooper** (Vice-President), **Claire Wilson** (Secretary) and **Anna Warren** (Ordinary Member), who were elected to the BCA Council at the AGM in April. Richard and Claire were re-elected to their positions and Anna, although new to the committee as an Ordinary Member, has been involved with the BCA for a number of years though the YCG and the BCA Education and Outreach activities. I would like also to thank **Jeremy Cockroft** for allowing his name to be put forward for election, and would like to encourage more nominations for positions on BCA Council in future. My thanks also go to **Dave Keen** (Past-President) and **Andrea Thorn** (Ordinary Member) for their contributions as their terms on Council come to an end.

The planning cycles for BCA Spring Meetings move smoothly from one to the next. The programme committee for the 2017 Spring Meeting at University of Lancaster is in place (a full list of committee members is on the BCA website), and will be in good hands under the leadership of **Andrew Bond** (Cambridge). Just after this Newsletter is in print, the 2017 planning meeting will have been held at Lancaster (June 2nd), symposia topics will be in place and invitations to plenary and keynote speakers will be going out. We have tried to encourage more input in terms of programme suggestions from the BCA membership via the programme committee members and I hope you have taken the opportunity to provide such input and will do so in future. Planning for the Autumn/Winter 1-day meetings organised by the BCA Groups is also getting underway.

As many of us in academic settings are trying to look past the blocks of exam marking that are on the near horizon towards a summer that will involve the opportunity to attend and present work at national or international conferences, I'll draw your attention to ECM30 in Basel (28th Aug – 1st Sep) and the 66th ACA Meeting in Denver (22-26th July), both of which have prominent UK speakers, **Simon Parsons** as keynote lecturer in Basel and **Elspeth Garman** as Fankuchen Prize winner in Denver.

Have a great summer.

Lee Brammer

BCA Council 2016

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(The dates in parentheses indicate the end of the term of office).

Full committee details on the BCA website

www.crystallography.org.uk

From the Editor

OUR recent Big Event was the Spring Meeting in Nottingham, which elicited a very positive response from participants. The venue was the Business School (South) building on the Jubilee Campus of the University of Nottingham. Although the architects meant business, subconsciously they must have thought of crystallography as well. The helical staircases on the outside of the building, which show up prominently in the cover picture, must have brought delight to all practitioners of macromolecular and supramolecular crystallography. The layout of the campus was almost too convenient. Our hall of residence, the breakfast cafeteria and the lecture and poster rooms were just a few minutes' walk apart. Therefore I didn't have to burn off the calories from a Full English Breakfast getting from A to B; and there was always the temptation to pop back to my room for a quick nap. The presentations were far too stimulating to afford any chance of a quick nap during a lecture!

Pictured on our cover is **Christer Aakeröy**, who gave our BCA Prize Lecture and presented the CCDC Chemical Crystallography Prize as well. Besides the honour of giving this prestigious lecture, Christer must be a contender for "longest-distance traveller", coming all the way from Kansas State University. Springtime in Kansas is a precious but fairly brief interlude between cold winter and hot summer weather. We can be grateful that he sacrificed some of it to be in Nottingham.

Credit for such an interesting Spring Meeting goes to the hard-working Programme Committee and, in particular, **Phil Lightfoot**, its Chair. Phil modestly told Council just before the start of the Spring Meeting that it had required surprisingly little effort and surprisingly few sleepless nights from him. To my mind, that is the distinguishing characteristic of someone who is good at delegating and pro-active at anticipating problems before they become serious.

This issue includes reports on the named, plenary and prize lectures, summaries of selected symposia together with our bursary recipients' impressions of the meeting. I am most grateful to them for these perceptive reports. As usual, a lot of high-quality research was presented in imaginatively designed posters, receiving recognition by the awarding of poster prizes at the conference dinner. In past years I have attempted the difficult task of photographing the winners receiving their prizes while also noting down their names. If a prize-winner was shy and departed quickly, the combination of my slow reaction time and the shutter delay of my camera sometimes meant that I only got a photograph of a retreating back. One year, after I had written the names on the back of an envelope, I set this envelope down in a small patch of spilled red wine. It became a challenge to discern the names among the paper-chromatographic bands. This year you will find beautifully sharp photographs thanks to the skill of **Alex Griffin**. Our cover shows that she even managed to capture a clear view of our whirling ceilidh dancers. I also had the reassurance of an accurate list of names supplied by **Steph Bryant**. I give both of them my sincere thanks.

It was a particular delight to see **Stephen** and **Marion Wallwork** (pictured on the cover) at the conference dinner. Stephen had a distinguished career at the University of Nottingham from 1949 to 1982. The BCA owes him a big debt of gratitude: he served on the Working Party to set it up, and he became a Founder Member. Well into his retirement he has continued to support *Crystallography News* with enjoyable articles reminding us about crystallographic history. Our December 2014 issue had an article on pages 22 and 23, modestly entitled "A Crystallographic Dinosaur", and earlier he had given us a lucid explanation of Beevers-Lipson strips (June 2010, pages 26-29). We hope that he will have had a happy 91st birthday this May.

We don't have long to wait for the next important meeting. On 15 June the joint BCA/RSC XRF meeting will take place at the University of Leicester. Full details are available at https://sites.google.com/site/bcaxrf/meetings/15-june-2016 .

Don't forget the European Crystallographic Meeting in Basel from 28 August to 1 September. While "early bird" registration is no longer available, and the regular registration fee is now about 12% higher, it still pays to register before 6 July so that you don't become a "late bird" and have to pay still more. The microsymposia listed elsewhere in this issue will be well worth attending at whatever price!

Looking further into the future, we can start to plan for the 24th Congress of the International Union of Crystallography, which will take place in Hyderabad, India, from 21-28 August 2017 at the International Convention Centre there. The Congress website is http://www.iucr2017.org/ . The first glimmerings of plenary lectures and satellite meetings now appear on this website; keep checking it for additional developments.

An important feature article was published by the IUCr this April: C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward (2016) *Acta Cryst.* B**72**, 171-179; doi:10.1107/S2052520616003954 . This article provides much more than just an updated literature reference to the Cambridge Structural Database. It precisely delineates the coverage of the database in terms of chemical species and types of data. It includes interesting statistics about the growth of the database and the size and complexity of the structures in it, and it describes the journey of a structure from submission as a CIF to inclusion in the database. A final section considers the future. Methods for obtaining three-dimensional structural information are evolving beyond just X-ray and neutron diffraction. More of the estimated 85% of determined but unpublished structures need to be deposited. Links between repositories need to be developed.

Carl Schwalbe

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Puzzle Corner

THE clues identify a chemical symbol and sometimes a city as well. These symbols also form the first one or two letters of the venues for American, British, European and International crystallographic meetings between 2017 and 2013; identify them too.

The first of all

Beginning of a series – a rare treat

It's inert, but the start of a lively venue

Named for a prize-giver whose fame endures, but it is very short-lived

It's heavy, but this one's a real getter

Like the first one, but heavier

Builds teeth and bones, just like cream cheese

Not an element, but an organic group; here it's often exposed to UV radiation and NaCl solution

From Sweden, it's not a rare earth but acts like one; the English city was influenced by Vikings

A stalwart for generating X-rays and excitement

A good metal for aircraft, but you don't want too much of its salts in your water

First and third letters this time: the last rare earth

Good in filaments; it's a well-used venue

A rare earth that's hard to isolate, but Sherlock would have identified it

March Puzzle Corner Answer

The crystallographic concept and crystalline substances are underlined.

The two seven-letter words are:
LATTICE, TACTILE.

Sixteen other words are:
ACE, ACT, CAT, ICE, LAC, TIC, CITE, LACE, TACT, TALC, ATTIC, CLEAT, ECLAT, ILEAC, TACIT, CATTLE –

but maybe you can think of more!

BCA Spring Meeting Reports
University of Nottingham, 4-7 April 2016

Plenary Lectures

Lonsdale Lecture

*(L-R) **Arwen Pearson** with Sam Horrrell*

The Lonsdale Lecture forms the bridge between the Young Crystallographers' Satellite Meeting and the main meeting. As such, it is expected both to present research and to promote education. This year's lecture, "Visualising molecules in motion: crystallography as a tool to probe structure and dynamics" given by **Arwen Pearson** from Hamburg, did just that. With respect to a macromolecule, Arwen raised four questions that a crystallographer might have. (1) How does it work? (2) Why has it gone wrong? (3) Can I fix it? (4) Can I make it do something else? She reminded us of the criticism of Kendrew's initial proposal to carry out macromolecular crystallography: "crystals don't wriggle; and if it doesn't wriggle, it's not biology". In fact, macromolecules are dynamic and flexible. An ensemble measurement takes an average over all conformations at once. Because many enzymes retain catalytic activity in the crystal and remain crystalline during turnover, it may be possible to derive useful mechanistic information, not least because the reaction may be slower within the confines of a crystal. Intermediates may be cryotrapped, or full turnover prevented by altered conditions, altered substrates or mutants. If trapping of intermediates is not possible, pump-probe experiments can initiate the reaction by absorption of a strong light pulse. The structure is then examined after a suitable time interval. The experiment must be repeated many times to build up sufficient signal, and different time intervals can be chosen. The use of Hadamard matrices optimises the signal-to-noise ratio. If neither the biomolecule nor the substrate can be activated by light, the reactants can be held apart until the right moment by enclosure in a photolabile cage based on groups such as nitrobenzyl, coumarinyl or p-hydroxyphenyl.

CCG Plenary Lecture

Mike Zaworotko from the University of Limerick gave this lecture with the title "Crystal engineering: form to function". Holder of the Bernal Chair of Crystal Engineering, Mike began by paying tribute to **J. D. Bernal**, who was born in Nenagh, about 30 km from Limerick. From determining the structure of graphite in 1924, to the first diffraction pattern of a protein in 1934 to suggesting a crystallographic database in the 1950s, Bernal made numerous important contributions to crystallography. Mike then quoted the infamous but totally accurate editorial by **John Maddox** (*Nature*, 1988, 335, 201) to the effect that "crystal engineering" was an oxymoron. Now

crystal engineering has become a reality. Mike defines it as "the field of crystallography that studies the design and properties of new crystals". He showed us how co-crystals of neutral and ionic species can improve the properties of drugs. Lithium salts are useful for conditions such as bipolar disorder, but the margin between effective and toxic doses is small. A 1:2 co-crystal of LiCl and leucine gives improved delivery to rat brain without tissue accumulation. Porous materials that selectively capture gases are badly needed. Carbon capture requires something that does not yet exist: a cheap, robust material with CO_2/N_2 selectivity around 2000 and CO_2/H_2O selectivity around 100. A series of MOFs with a range of pillars and metals named "SIFSIX" (because the pillar is hexafluorosilicate, SiF_6^{2-}) shows promise: SIFSIX-3-Zn gives CO_2/N_2 selectivity close to 3000 but water vapour remains a challenge. Purification of ethylene is another technologically important application of gas capture. At about 150 million tonnes per year, ethylene is the most produced commodity in the world. As obtained by cracking hydrocarbons, it is accompanied by 1-2 % of acetylene, which needs to be removed or it will poison catalysts. A different SIFSIX material has the highest C_2H_2/C_2H_4 selectivity yet.

IG Plenary Lecture

The 2016 Industrial group plenary was given by Dr **Rolf Hilfiker**, from Solvias (Switzerland), with the title "Using Co-Crystals to Optimise Solid Properties". Rolf started by illustrating the various reasons that co-crystals are interesting to the pharmaceutical industry: they may have better solubility, morphology and stability, be less hygroscopic or avoid "problem polymorphs". They may provide crystals of the quality needed for purification, resolution or structure determination. Next Rolf explored the differences in regulatory approach between the EU and US authorities. He exemplified crystal engineering strategies that can be exploited to screen for suitable co-crystals. The importance of understanding the ternary phase relationship was clear and the relative solubility differences between the co-formers were shown to be vital to developing a successful crystallisation route. The simplest form of phase diagram contains A (the API), B (the co-former) and the desired co-crystal AB; appropriate fractions of A and B can

be chosen to give a final composition in the region AB, the "red region" on the phase diagram. A wide "red region" is desirable because it broadens the tolerance of variations in concentration. Rolf provided case studies for co-crystals which proved essential for a variety of purposes: superior physical properties, improved morphology and an example valuable as intellectual property.

BSG Plenary Lecture

This lecture was given by **Susan Lea** from Oxford with the title "The use of hybrid structural methods to study the protein complexes required for export of proteins from bacteria". As the organism in which this important topic is to be studied, Susan has chosen the Gram-negative bacterium *Shigella flexneri* for two reasons. (1) Its proteins are properly functional but stripped-down versions of proteins found in other bacteria, making them easier to study. (2) Dysentery caused by *Shigella* species kills around a million people per year. These bacteria invade intestinal epithelial cells, multiplying within them and then killing them. In many respects *Shigella* bacteria resemble the well-known and generally harmless *Escherichia coli*, but they have a Type 3 secretion system (T3SS) that injects targeted proteins into the host cell, rendering it hospitable to invasion. The apparatus is assembled, its "needle" is inserted into the host, secretion is turned on and then off again. A nonameric ring formed from MxiA is important: without it, assembly is incomplete and no secretion occurs. It is very similar to a protein in flagella. By combining information from X-ray crystallography and electron cryo-tomography it has been possible to suggest some mechanistic details. A chaperone is probably recognised by the secretion system; a chaperone-effector complex is recruited to an ATPase complex, and partially folded substrate passes into the MxiA cage. The intra-membrane complex is now under investigation.

PCG Plenary Lecture

Bill David from the Inorganic Chemistry Laboratory, Oxford and the ISIS Facility had the daunting task of giving the PCG Plenary Lecture first thing on Thursday morning to an audience who had liberally enjoyed food, drink, conversation and dancing the previous evening. His topic "120 Years of Powder Diffraction" was a winner, encompassing both a long and distinguished history and substantial recent advances. Already mentioned as a possibility by Laue in his 1915 Nobel lecture, powder diffraction was implemented in Germany the next year by **Peter Debye** and **Paul Scherrer**, and independently in the USA by **Albert Hull**. Hull's success is surprising: he studied Greek at Yale with physics only as a supplementary course. Nevertheless, he was offered a scientific job by General Electric. Not knowing that determining the structure of iron was supposed to be difficult, he obtained and interpreted diffraction from a sample of iron filings, and in 1917 he published the structure of 9 elements. For a long time powder diffraction was used mainly as a "fingerprint" identification technique. **Hugo Rietveld** made modern structure determination possible when he devised the method for matching calculated and observed profiles even for overlapping peaks – yet, when he displayed a poster about it at the IUCr Congress in Moscow in 1966, everybody just walked by! Obtaining a suitable trial structure for the start of Rietveld refinement remained a major obstacle. In 1997 David, Shankland *et al*. presented a much faster method for doing this. Bill recounted that "If we had claimed 50% improvement, we would have been believed and honoured; but because our method was 5000-fold faster, we were called Mystic Druids". This work culminated in the program DASH. Modern powder diffraction can solve technologically important but perplexing problems. Bill discussed one of his studies of LiBH4 which is a superionic conductor with a paradoxical structural story. Pair distribution function methods indicate short-range disorder while Rietveld analysis asserts long-range order. The conundrum was resolved both experimentally with a "golf ball" model involving 37 symmetry-independent "atomlets"and computationally using DFT molecular dynamics. In the future, drawing on the increasing capabilities of computational modelling, bigger, more complex problems as large as the materials science of proteins will come into the domain of powder diffraction.

BCA Prize Lecture

This is always one of the highlights of a Spring Meeting. As well as educating and inspiring us, it has to put us in a good mood for the sometimes arid discourses in the Annual General Meeting that follows it. On the topic "From molecular sociology to functional materials" **Christer Aakeröy** from Kansas State University gave a talk that was funny at times and fascinating throughout. As a synthetic chemist, he reminded us that supramolecular synthesis is restricted to one-pot reactions, unlike organic synthesis. One seeks to design a molecular assembly process based on a hierarchy of interactions. A

(L-R) Christer Aakeröy with Lee Brammer

higher electrostatic potential (ESP) implies a stronger bond and more efficient assembly. Isonicotinamide provides an example. It has two sites attractive to a carboxylic acid, the amide group and the pyridine N atom; in fact, the COOH forms a hydrogen bond to the ring N atom and the amide group forms hydrogen-bonded dimers. Changing the ring to pyrazole with its small negative potential reduces its attractiveness, so that the COOH group now interacts with the amide. Along with the well-established field of hydrogen bonding, the "new kid on the block" is halogen bonding. Many drugs are halogenated, and the "tip" of the halogen atom has positive ESP, which is related to polarizability, so I > Br> Cl. Thus the halogen atom can be an acceptor of electron density. Calculations give remarkably similar ESP for the acidic terminal H atom in phenylacetylene (157 kJ mol^{-1}) and an iodine atom replacing it (168 kJ mol^{-1}). Hydrogen and iodine really can do the same thing! Christer then applied these concepts to make predictable changes in the properties of materials, often to increase the solubility of a variety of pharmaceutically relevant compounds. It can also be desirable to *decrease* the solubility of a pesticide with basic N atoms by cocrystallisation with a "greasy" dicarboxylic acid so that one application can last a long time without polluting watercourses. The explosive ethylenedinitramine is tractable; but if it corrodes metal, the resulting metal salts can be dangerous. Co-crystallisation with 4,4'-bipyridine reduces impact sensitivity moderately and stops corrosion of copper.

Carl Schwalbe and **Cheryl Doherty**

Prize Lectures

Early Career Prize Lecture Symposium

NO parallel lectures were scheduled to compete with these presentations – a wise move because these lectures were so exciting.

(L-R) Christer Aakeröy with Mark Warren

The CCDC Chemical Crystallography Prize for Younger Scientists 2016 was awarded to **Mark Warren** from Diamond. He presented his research under the title "Watching chemistry happen", and he addressed the question "What are the intermediates in a reaction?" An example is linkage isomerism, where an N-bound nitro ligand is converted photochemically to an O-bound nitrito group. Sufficient irradiation is provided by a ring of LEDs. At 100K Ni(dppe)(NO_2)Cl is converted 50% after 10 minutes. The lifetime of Ni(dppe)(NO_2)$_2$ can be tuned by varying the temperature. For short-lived intermediates one can use pump-probe techniques, for which the Diamond facility is well-equipped. The use of a chopper is no longer necessary since the Pilatus detector can be gated. It becomes possible to probe numerous time series from one pump and collect an entire series in about 2 hours.

(L-R) Phil Lightfoot with Paul Saines

The winner of the Physical Crystallography Group prize sponsored by the Institute of Physics was **Paul Saines**, who spoke to us about "Probing magnetic interactions in coordination frameworks". Functional materials are critical for technology. Within this field Paul has interests covering metal oxides and MOFs. Having metal ions close enough to communicate, hybrid coordination frameworks exhibit features of both these entities. Small ligands enable strong magnetic interactions. Powder neutron diffraction probes both the arrangement of magnetic spins and the light atom (H,D) positions. Co(adipate) shows unusual behaviour upon cooling below 20K: the *b* and *c* axes decrease rapidly, while *a* (the pillar direction) expands. There is an effect of magnetic interactions, especially a super-exchange pathway in the *b*-*c* plane.

(L-R) Cheryl Doherty with Clare Stubbs

The Young Crystallographers Prize selected by the IG was awarded to **Clare Stubbs**, who told us about "New Platinum Pincers for a variety of sensing applications". Platinum (II) was chosen because, in its d^8 configuration, the dx^2-y^2 orbital is of high energy. Use of a strong field ligand such as CN^- prevents population of this orbital, which would join in antibonding interactions, while it facilitates dz^2 intermolecular interactions. Pt is N-C-N coordinated by a 2,6-dipyridylbenzene ligand; varying the group (X) at the 4-position of the phenyl ring renders the complex susceptible to solid-state vapochromic, solvochromic and mechanochromic behaviour.

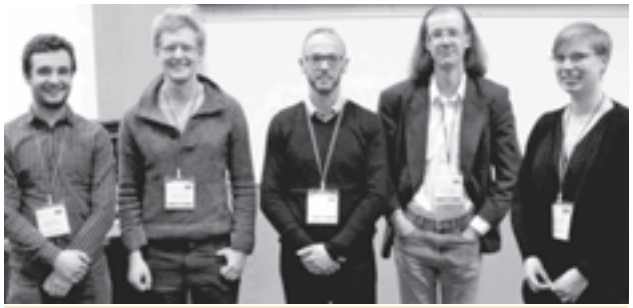
(L-R) Tadeusz Skarzynski (Rigaku) with Matthew Gold

Matthew Gold, the winner of the BSG Prize sponsored by Rigaku Oxford Diffraction, told us about his research on "Structural investigation of a signalling protein complex that regulates synaptic strength". Memory formation is thought to involve changes in synaptic strength. Paradoxically, Ca^{2+} drives changes in both directions; and cyclic AMP (cAMP) plays an important role. A key finding is that the receptors for such second messengers occupy specific locations within cells. A-Kinase Anchoring Protein 79 (AKAP79) is believed to anchor the Ca^{2+}-sensitive phosphatase calcineurin. It dimerises and binds 2 copies of calcineurin. Because of its flexibility, it is hard to study crystallographically. Cross-linking helps with the elucidation of binding sites.

Carl Schwalbe

Selected Sessions

From Amorphous to Crystal



(L-R) Jerome Wicker, Christopher Jones, Ivan Marziano, Colan Hughes, Katherina Edkins

THIS session, chaired by **Katharina Edkins** (Durham) and **Ghazala Sadiq** (CCDC), was the first of a pair jointly organised by the Chemical and Industrial groups. **Ivan Marziano** (Pfizer) gave us a perspective from the pharmaceutical industry by way of 3 case studies. The impact of solvent on particle shape can be predicted by quantifying the affinity of process solvents for different crystal faces. Inconsistent dissolution of a milled product can be explained by differences in exposure of hydrophobic and hydrophilic faces. Different polymorphs of a drug may differ in their ability to purge impurities during crystal growth. Attempting to answer the question "(When) will it crystallise?", **Jerome Wicker** (Oxford) applied a machine learning approach. Molecules were assigned "feature vectors" of molecular descriptors and classified as crystallisable or not. The Cambridge Structural Database provided a large set of molecules absolutely certain to crystallise, and a complementary set was taken from the ZINC database of purchasable compounds. Size and flexibility were found to be key attributes.

Colan Hughes (Cardiff) demonstrated the utility of *in situ* solid-state NMR in elucidating crystallisation processes. The relevant spectrometers are sensitive to samples in both solid and liquid phases, and amorphous phases can be distinguished by peak width. Systems that have been studied include glycine in water, methanol and water/methanol mixtures, m-aminobenzoic acid and DL-menthol; in the latter case, as a melt cools, sharp liquid peaks change to broad amorphous peaks and then to sharp crystal peaks. **Christopher Jones** (Durham) described the remarkably diverse behaviour of molecules containing two or more urea functional groups. They tend to form tapes, which may then associate in crystals or gels (fibres, vesicles, rods, etc.); in Christopher's work, unbranched fibres are typical. The crystals display 7 different network topologies; and while the gels lack long-range order, they have a locally ordered lamellar structure.

Carl Schwalbe

Interactions and Materials

(L-R) Cheryl Doherty, Elna Pidcock, Hamish Yeung, Lauren Agnew, Bob Docherty, Graham Tizzard

THE Interactions and Materials session was a joint session by the Chemical and Industrial groups, chaired by **Graham Tizzard** (Southampton) and **Cheryl Doherty** (Pfizer). Keynote speaker **Bob Docherty** kicked off the session by highlighting the importance of understanding the key features of the structure and function of a pharmaceutically active molecule. He went on to discuss the usefulness of designing in desirable behaviour and function from an early stage. The ultimate aim is to allow a digital definition of drug product design. **Lauren Agnew** followed up with her description of polymorphic control via a continuous crystallisation process as part of the CMAC group. Lauren presented the effects of templating in a continuous process to allow the crystallisation of the metastable polymorph of Paracetamol (Form 2).

Elna Pidcock from the CCDC gave the third presentation. Elna ably illustrated the value of investigating packing trends in large numbers of crystal structures. She highlighted unusually prominent packing networks and described the insights to be gained by this in depth assessment of symmetry and interactions. The session was completed by **Hamish Yeung** from NIST, Hamish presented his quest to create new functional organometallic materials. Hamish covered the successes and challenges in understanding a complex family of 8 polymorphs of a metal-organic system including mapping out the reaction energy landscape for the formation of his materials.

Cheryl Doherty

Complementary Techniques

CHAIRED by **Helena Shepherd** (Kent) and **Andrew Stewart** (Limerick), this session showcased a variety of techniques that provide valuable additions to traditional crystal structure determination. **Graeme Day** (Southampton) described the great progress that has been made in crystal structure prediction (CSP). In the usual procedure a 3-D molecular structure is optimised by quantum mechanics, then incorporated into trial crystal structures which are screened and lattice energy minimised. Typically, the crystal energy landscape shows several minima which may be isolatable polymorphs if their energy range is within 10 kJ mol^{-1}. Furthermore, it is now possible to predict terahertz spectra from lattice dynamical calculations. Anthony Reilly (CCDC) evaluated the success of CSP in

(L-R) Andrew Stewart, Sarah Gurung, Anthony Reilly, Graeme Day, Claire Hobday

(L-R) Natalie Johnson, Horst Puschmann, Iain Oswald, Mike Probert, Patrick Shaw Stewart, David Allan

the most recent (6th) Blind Test against newly determined but secret structures. This time there were 25 distinct submissions, many of which performed well on this challenging set. Computationally intensive ranking methods appeared to help; 12 groups used DFT. The Cambridge Structural Database (CSD) itself can provide valuable guidance for structure generation and prediction: for Z'=1 systems there is usually an analogue in the CSD that reproduces the observed form.

Sarah Gurung (Reading) showed how photophysical methods complement crystallography in the study of DNA i-motifs (four-stranded structures made of cytosine-rich DNA sequences, which can be found in promoter regions). With the aid of synchrotron radiation the crystal structures of $d(CCCT)_4$ and $d(TAACCC)_4$ have been determined. The stability of such i-motifs as a function of temperature and pH has been evaluated with high-throughput ultraviolet and circular dichroism spectroscopy on Diamond beamline B23. **Claire Hobday** (Edinburgh) introduced pressure as another variable to manipulate. Zeolitic imidazolate frameworks (ZIFs) with various small substituents at the imidazole 2-position are isostructural and can take up guest molecules such as N_2 or methanol. As the pressure increases, some but not all of these ZIFs change from a "closed" to an "open" structure by ring rotation. Grand Canonical Monte Carlo calculations with polar interaction represented by point charges and nonpolar by Lennard-Jones potentials yielded values of the energy penalty for ring rotation that rationalised these observations.

Carl Schwalbe

Tips, Tricks and Trials

THIS multifaceted session was chaired by Mike Probert (Newcastle) and Iain Oswald (Strathclyde). First, David Allan (Diamond) described the technique of using a diamond anvil cell and outlined the advantages of growing crystals at high pressure. The hierarchy of interactions (van der Waals, hydrogen bond, ionic, covalent) may change as pressure alters the interatomic distances; in the case of ice, variation of both pressure and temperature leads to 16 different structural phases! Substances that are liquid at ambient pressure may crystallise under high pressure. Raising both pressure and temperature can simulate conditions deep within the interior of Earth and other planets. Patrick Shaw Stewart (Douglas Instruments) introduced us to random Microseed Matrix-Screening (rMMS) and stated that it should be part of normal protein crystallisation workflow. Without seeding, one must exercise exquisite control over concentrations, starting out in the nucleation zone but migrating into the metastable zone when some seeds (but not too many) have formed. By adding seeds, one can operate entirely within the metastable zone, achieving better crystals and the right number per drop. Furthermore, cross-seeding can be employed, leading to epitaxial growth.
Next, **Horst Puschmann** (Durham) took us downstream to the creation of a CIF. Horst used the epithet "pesky", because that is how we sometimes perceive it. Actually, we should be very grateful to it: it has rigorous syntax, clear definitions, easy data interchange, and best of all, it is human-readable. Originally the "F" stood for "file", but a better word now is "framework". Ideally, every step of the structure determination should be documented in the CIF. Finally, **Natalie Johnson** (Newcastle) discussed the "integration game". We may collect data from a top-quality crystal on the best possible equipment, but data processing by default "because we always do it this way" may degrade the data. In particular, a choice between simple summation and profile fitting needs to be made case-by-case. Often the simple option is best. In the ensuing discussion **John Helliwell** mentioned that a round-robin organised at the time of the 1981 IUCr Congress in Ottawa showed that profile fitting was most useful for sets with a large fraction of weak data, where "the weak can learn from the strong" [J. R. Helliwell *et al.* (1981) *Acta Cryst.* A37, 311-312].

Carl Schwalbe

Bursary Reports

ON the 4th April, as spring was just beginning, the attention of people across Britain, and even many abroad, turned towards the East Midlands. Not for the remarkable successes of the underdogs of Claudio Ranieri, Jamie Vardy *et al*. but for the 2016 edition of the BCA spring meeting.

The meeting began, as is now traditional, with the program of the Young Crystallographers Group, which contained fascinating talks on subjects as varied as how to control thermal expansion in Ruddlesden Popper layered oxides

(**Sarah Craddock**) to developing methods for collecting data on tricky to crystallise membrane proteins (**Katharine Jungnickel**). **Jonny Brooks-Bartlett** enthused the audience with his drive to show the public the thrills of crystals in his Parkin Lecture. The YCG also gained a little more appreciation for the classics with Prof **Paul Raithby** speaking about how we actually were able to measure diffraction patterns in the past – and Prof **Mike Glaze**r gave a great introduction to the stereographic projection: useful both for perovskites and piloting a plane.

After a brief break, the main meeting began with the Lonsdale Lecture given by Prof **Arwen Pearson**, demonstrating that we can now begin to measure protein crystals while they function. The exciting potential of photocrystallography was further demonstrated later in the meeting by **Mark Warren**'s CCDC Chemical Crystallography prize lecture, where he spoke about tracking photochemical changes on an incredibly fast timescale. The Lonsdale lecture was followed by the CCDC plenary given by Prof **Mike Zaworotko**, who showed that mixing in inorganic salts can be a very powerful route for creating both new pharmaceutical cocrystals and metal-organic frameworks with remarkable gas sorption properties.

After these plenaries the full spectrum of crystallography erupted, with talks on a huge range of topics. The number of interesting presentations meant that coffee sessions were taken up by discussions of the talks that you had missed. Nevertheless, some personal highlights included Prof **Susan Lea**'s description of the intricate machinery of bacterial protein secretion in her BCG plenary and Prof **Christer Aakeröy**'s entertaining comparative studies of both crystal engineering applications and transatlantic politics. Back-to-back talks on metal ammonium formates and cyanides (**Anthony Phillips**) and technetium oxides (**Emily Reynolds**) demonstrated that physical crystallographers will never let danger get in the way of a good phase transition. Perhaps worryingly for experiments – a number of talks demonstrated the fantastic successes of crystal structure prediction, for both organic (Prof **Sarah Price** and Prof **Graeme Day**) and inorganic (**Andrew Morris**).

In amongst this diversity of talks, an important theme that ran through the BCA spring meeting was time. Sessions throughout the three days, and even in the YCG satellite session on classic techniques beforehand, reflected on the evolution of crystallographic methods, questions and understanding and pointed towards where we could and should develop. Prof **Bill David** in his PCG plenary lecture gave his on the long and storied history of powder diffraction, leavened with some pointers toward the future of this powerful technique. A session on the 'Future of Structural Science' asked fundamental questions about the direction of our discipline, including talks on free electron X-ray lasers (Prof **John Spence**) and their role in macromolecular structure determination; the history and importance of neutron diffraction (Prof **Dave Keen**); time-resolved gas-phase electron diffraction (Prof **David Wann**) and some predictions of the future of structural databases – and next-generation dancing (**Pete Wood**). One thing is certain about the future though: there will be surprises. Now, where did I put that Premier League betting slip?

Matthew Cliffe
University of Cambridge

Biology at the BCA

THIS year's BCA spring meeting was held in Nottingham, a very familiar city to the structural biology community through the annual CCP4 study weekend. As my fourth BCA meeting and first as a post doc this was my busiest conference to date, chairing two sessions, running for YCG chair, a poster to present and the aftermath of being elected YCG chair.

My meeting started with the Young Crystallographers' satellite meeting. As a biochemist by training I had never given much thought to metal organic frameworks before attending a BCA meeting, but thanks to the YCG I now have a much greater understanding of MOFs than any biologist probably should. The YCG AGM saw many changes in the committee including my election to the position of chair. Based on this I suspect my fifth BCA is going to be even more hectic. The first day closed out with one of my favourite sessions of the meeting, the flash poster presentations, which I chaired with the help of **Jonny Brookes-Bartlett**.

Speaking of Jonny, the second day of the meeting began with a well-deserved and masterfully presented Parkin Lecture on the joys of outreach and how you can and should get more involved with science communication. Watch this space for more outreach activities from our vice-chair and education and outreach officer.

The main meeting opened with the Lonsdale Lecture, awarded to **Arwen Pearson** who presented a fascinating look into the techniques used in real time crystallography to observe molecules in motion and better understand enzyme dynamics. This also marked my first time chairing at the main BCA meeting, which was nerve-racking at first but turned out OK in the end.

The rest of Tuesday (for me at least) was followed by a number of interesting biological talks covering antimicrobial resistance and the development of new therapeutics to counteract it, with the University of Oxford showing up in force for the latter. The usual slew of GPCR's were presented along with a very impressive mutlidrug efflux pump solved using Cryo-EM by **Dijun Du** from the University of Cambridge.

The BSG's first session on Wednesday looked into the future of structural biology, with **John Helliwell** sparking a lively debate on the merits of publishing raw diffraction data. The afternoon session continued this theme, focusing on honouring the work of the next generation of crystallographers with the Early Career Prize Lecture Symposium. Wednesday ended as always with the conference dinner and a ceilidh where I had the honour of receiving the ACA poster prize, as well as the unique experience of giving **Scott McKellar** a giant piece of ham as thanks for his service as YCG chair. A tradition I hope to see continued by the YCG in the years to come.

The meeting closed on Thursday with an interesting series of talks on molecular machines, the subject that first sparked my interest in studying structural biology after a lecture series of the same name during my undergraduate degree at the University of Leicester. With that we have come full circle and all that is left to say is thanks to the ABBF for awarding me a bursary to attend and I look forward to seeing you all again next year.

Sam Horrell
University of Essex

FIRSTLY I'd like to thank the BCA for awarding me an ABBF bursary to attend the BCA spring meeting 2016, and what a meeting it turned out to be! A small cohort of us from Sheffield made the short one-hour drive down to Nottingham Tuesday morning to attend, and arriving early meant we could acquaint ourselves with the campus and all the interesting architecture.

The meeting was kicked off by the new chair of the Young Crystallographers' group **Sam Horrell**, handing over of the YCG from the previous day, with introduction of the Lonsdale lecturer Prof **Arwen Pearson**. Prof Arwen's lecture on studying molecular motion using a clever beam chopping technique and Hadamard matrix allowed unprecedented movements to be observed by X-ray diffraction, such as a CO molecule leaving a heme group, and promises some very exciting results in the future.

The first BSG session showcased a good breadth of senior and junior researchers, with some very large multicomponent macromolecules being studied through complementary methods. Overall the session was an inspiration and gave me some nice future experiment ideas for my own work, a bonus! The final talk of the day was from Sheffield's very own Dr **Claudine Bisson**, a cautionary tale of chiral promiscuity even in chirally selective enzymes.

Tuesday was wrapped up with a lovely buffet dinner and poster session with wine reception. I particularly enjoyed the Poster session, as it's a great time to showcase results, network, and gain insights from others in the field, very valuable indeed.

Wednesday morning was abuzz with discussion of the lectures the previous day over breakfast. The buzz continued into the first lecture of the day given by Prof **Susan Lea** from Oxford, on the Type 3 secretion system, a monster of an assembly which threw up a nice conundrum on how such a large assembly can make itself, and then post proteins through the needle, something we spent the following coffee discussing between ourselves.

The BSG lecture series for the day then looked at the future of structural science, with some great lectures and some food for thought on access to, and storage of raw diffraction data from Prof **John Helliwell**.

Dr **Matthew Gold** gave a great lecture as the winner of the Early Career Researcher Prize, on the investigation of signalling protein complexes in shaping synaptic strength, with some interesting crosslinked mass spec to determine fragments that are involved in interactions between proteins in the complex.

Finally that evening was the conference dinner and entertainment. The meal was fantastic, and the Ceilidh went on to the wee hours of the morning.

The final day consisted of two final sessions of BSG talks, this time focusing more on cell signalling and attachment, a nice reminder of the overall biology such as neuronal networking mediated by these atomic scale molecules. A particular highlight for me was watching the movement of the dynein motor during the power stroke.

With the end of the conference upon us, we grabbed a lunch and headed back up to Sheffield, full of inspiration, feeling relaxed, and with a nice bonus of the Blue John trophy in tow, which made its return to Sheffield since its introduction in 1989. A fantastic week indeed!

Finally thanks to all the organisers of this great event! This is the second time I've attended, and will continue to do as such when the quality and quantity of talks is as brilliant as this year's organisers have managed.

Jason Wilson
University of Sheffield

I HAD arranged a ride to Nottingham with some other students attending the BCA meeting from Oxford. However, there was a feeling in the back of my mind that something wasn't right. Arriving at the conference and seeing the word "poster", I realised that mine was still in Oxford… Quel désastre! Nevertheless, I was still excited for a week of good science and seeing old friends.

The range and depth of science on show from young scientists at the YCG satellite meeting was impressive. A highlight for me was **Franziska Fischer**'s talk on *in situ* XRD-Raman studies on ball milling reactions – working in the *in situ* XRD field, I had read the papers but didn't realise that there would be a delegate at BCA. I also enjoyed **Sarah Craddock**'s talk on the control of negative thermal expansion, a subject close to my heart as it was the subject of my PhD. Outside the talks, I must give particular thanks to **Nicola Peel** of Hg3, who during the breaks printed for me several copies of my poster in A4 so that I at least had something to stick to the poster board. The day rounded off with some light relief in the form of the flash poster presentations.

The next day saw the end of the YCG satellite and the start of the main meeting. Despite my studious avoidance of biochemistry (since reading it as an undergraduate major), I couldn't help but be impressed by **Arwen Pearson**'s Lonsdale lecture on time-resolved protein crystallography using the Hadamard transform. (This, amongst other subjects, was also later expanded on by **Mark Warren** in his excellent CCDC prize lecture). Working on MOFs, I also enjoyed **Mike Zaworotko**'s plenary – always exciting to see high-impact work pre-publication. Later that day, I ran between sessions to see talks by **Matt Cliffe** and **Hamish Yeung**, both great collaborators whom I had worked with on *in situ* XRD. After dinner and posters, the day ended in the bar with ping pong, pool and lively debate, scientific and otherwise.

Wednesday brought another raft of great talks including the BCA prize lecture from **Christer Aakeröy**, who no doubt has a promising career in comedy should he ever leave science. We then saw democracy in action at the BCA AGM before heading to the conference dinner. After dinner the poster prizes were announced and I was shocked to find that I had been awarded two prizes! Perhaps the posters had been judged on the criterion of "less is more"? The rest of the night then progressed in the traditional post-conference-dinner manner.

I woke up the next morning after a good four hours' sleep but none the worse for wear. I particularly enjoyed **John Evans**'s demonstration of using genetic algorithms to 'evolve' symmetry mode distortions – a simple but powerful concept. **Natalie Johnson** also gave a thought-provoking presentation on how

different SCXRD integration methods can provide quite different results.

All in all, an excellent conference and full of surprises to the very end – for anyone passing the car park, half of the YCG trying to push start a professor's car must have been an unexpected sight!

Yue Wu
University of Oxford

The Young Crystallographers' Satellite Meeting

THE first session of the 2016 Young Crystallographers' Satellite meeting was chaired by Natalie Johnson from Newcastle University and began with the Chemical Crystallography Group plenary talk from Prof Sally Price from UCL who delivered an interesting lecture on whether the polymorphs a crystal form can be predicted computationally, and if it was possible to determine which of the plausible structures generated could be crystallised.

Thomas Roseveare from the University of Sheffield was the first young crystallographer to take the stage, explaining how intermolecular interactions such as halogen bonding could be used to design flexible porous systems. He used a combination of single crystal and powder X-ray diffraction techniques to monitor the changes to the material during gas uptake.

Franziska Fischer from the BAM Federal Institute of Materials Research and Testing spoke next describing her work on monitoring crystallisation during mechanical reactions. She described a new and interesting *in situ* set-up which allowed the grinding based reactions to be monitored by both powder diffraction and Raman spectroscopy.

Next up was **Gurdeep Minhas** from the University of Oxford who presented our first biological talk of the session explaining his work on the peptide transporters PepT1 and PepT2 to determine the mechanism by which these highly versatile peptide transport proteins are able to bind approximately 8000 peptide substrates in a single binding site with a view to aid in rational drug design.

Clare Stubbs was next to take the stage delivering a talk on her work on the development of Platinum Pincers which would go on to win her the coveted IG – YCG award and the opportunity to present her work at the main meeting in the Early Career Prize Lecture Symposium.

Alistair Overy from the University of Oxford went on to talk about strongly-correlated disorder within crystalline materials. He identified key classes of these aperiodic procrystalline materials and demonstrated how the characteristic effects seen in materials diffraction behaviour could be reproduced computationally.

Patrick McIntyre from the University of Leicester closed the first session of the meeting with an interesting talk explaining his work on the Aurora-A/TPX2 binding interface and how this interaction might be blocked through disruption of any of three high affinity binding sites to provide novel anti-cancer drugs.

* * *

The second session of the meeting was chaired by **Claire Hobday** from the University of Edinburgh and began with the Biological Sciences Group Plenary talk from Dr **James Errey** from Heptares Therapeutics. James gave an in-depth look into the use of structure based drug design in the development of novel drugs to target the ever prevalent GPCR family.

Shiyuan Zhang from the University of Limerick followed the plenary lecture giving a talk on his work developing a new crystalline sponge material. He showed how various small molecule structures, typically ones unable to be crystallised by normal methods, could be determined by including them as guests inside a porous crystalline chiral framework material.

Rachael Skyner from the University of St Andrews was up next and went on to talk about her work on solubility prediction methods. She showed us the power of big data, by developing a solubility dataset from the CSD and trying to identify trends in solubility induced by molecular changes, with the goal of improving solubility by design.

This was followed by a talk from **Alycia Yee** from The Institut Laue-Langevin who combined neutron and X-ray diffraction experiments in an attempt to better understand how the hydrogen bonding network in two mutant forms of Transthyretin affect complex formation and the development of Transthyretin amyloidosis.

Sarah Craddock from the University of Oxford spoke next, discussing her work on tuning the negative thermal expansion properties of a family of layered perovskite materials known as the Ruddlesden Popper Oxides. This was achieved through doping of the materials allowing chemical control of two competing phases.

The penultimate talk of the session was delivered by **Phillip Tucciarone**, another University of Oxford student, on the remarkable behaviour of ZrW_2O_8. The material is known exhibit negative thermal expansion (NTE), however, this new work shows that upon hydration the material also undergoes negative expansion of 10 %. Tucciarone used *ab initio* methods and structural flexibility models to uncover the mechanism of the NTE and hydration driven collapse.

Sarah Makin from the University of Reading closed session two with an interesting talk on her work investigating how the inclusion of germanium in solvothermal reaction mixtures impacts on the formation of Gallium sulfide based solid state materials.

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The YCG AGM saw a significant change in the committee with many new faces joining the ranks. For a full account of the new committee members and their research interests please visit the YCG website at www.ycg.crystallography.org.uk/the-committee/.

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Day one of the YCG meeting ended with session three, the Flash Poster Presentations, where all YCG poster presenters are invited to sell their poster in thirty seconds. The session was chaired by **Sam Horrell** from the University of Essex and **Jonny Brookes-Bartlett** from the University of Oxford. The YCG flash poster presentation prize was awarded to **Yue Wu** from the University of Oxford for his excellent salesmanship.

* * *

Session four was chaired by **Scott McKellar** from the University of Edinburgh and started with the Parkin lecture, awarded to **Jonny Brookes-Bartlett** for his unparalleled list of outreach activities over the course of his PhD, including his time in FameLab and winning "I'm a Scientist get me out of Here". Jonny delivered a very engaging talk on the joys of outreach and how you could and should get involved in science communication in your field.

Joanna Baker also from the University of Oxford then went on to present her work on the production and use of photoswitchable materials. Using a host such as deoxycholic acid or metal-organic frameworks that have porous channels, she can trap photoswitchable materials such as stilbene and azobenzene and carry out cis-trans isomerisations.

Katharina Jungnickel completed the University of Oxford triple with an interesting talk on the development of serial synchrotron crystallography at PETRA III and its application to membrane proteins grown in lipidic cubic phase.

As has become tradition at the YCG satellite meeting the final session is devoted to teaching. This year's theme was dubbed "Forgotten Methods in Crystallography" and was chaired by **Jerome Wicker** from the University of Oxford. Sadly our first speaker Prof **Bob Eady** from the University of Liverpool was unable to attend and his talk on Protein Purification Before the His-tag era could not be delivered.

Therefore the first speaker of the session was Prof **Paul Raithby** from the University of Bath who gave a fascinating talk on the developments in crystallography during his career. This included advances in the detectors used to collect data and the revered crystallographers that he worked with.

The final talk of the session and meeting was delivered by Prof **Mike Glazer** from the University of Oxford and University of Warwick who explained the ins and outs of plotting three-dimensional information in two dimensions by taking us on an aeroplane ride from New York to Delhi using a Wulff net and some tracing paper.

Sam Horrell
University of Essex

Obituary

ON 12 February 2016 our much-esteemed colleague Prof Dr Theo Hahn died, a few weeks after his 88th birthday.

Between 1963 and 1993 Theo Hahn was Professor of Crystallography at the Technical University of Aachen and director of the Institute of Crystallography that he founded. As an outstanding academic teacher and scientist who made highly significant contributions to the areas of theoretical crystallography and symmetry, he enjoyed great international recognition. From 1972 to 2009 he was editor and author of the International Tables Vol. A, and from 1972 to 1983 and again from 1993 to 2003 Chairman of the International Tables Commision of the IUCr.For the new edition of Volume A of the International Tables for Crystallography he composed the section on point groups and symmetry classes.

Theo Hahn was an Honorary Member of the German Crystallographic Society (DGK) and was awarded the Carl Hermann Medal in 2001. In addition, he received the Abraham Gottlob Werner Medal of the German Mineralogical Society (DMG) in 1997. From 1984 to 1987 he was President of the International Union of Crystallography, and from 1982 to 1984 Chairman of the DMG.

The international community of crystallographers, especially those who could personally experience the dynamic and pleasant manner in which he approached scientific themes and questions, will painfully miss him.

Susan Schorr, Chair of the DGK.
Gernot Heger and **Georg Roth**, Institute of Crystallography, RWTH Aachen.
Ulrich Bismayer, Representative of the DMG in the Council of the DGK.

To this tribute by Theo's German colleagues I can add my own reminiscences. I became well acquainted with Theo when I retired and joined the Senior Crystallographers General Interest Group (GIG2-SC) of the European Crystallographic Association. Theo was a real inspiration to me. Although he was a decade and a half older, his zest for crystallography, travel and culture showed me that retirement does not have to equal idleness. Joan and I remember an enthusiastic and perceptive conversation with him about art and music in the Rodin Museum when we were in Paris for the start of the International Year of Crystallography. Theo had a delightfully self-deprecating sense of humour that I can only describe as English in spirit. At one GIG2-SC meeting he recounted his experience of studying with Carl Hermann in Marburg. (Carl Hermann was both a brilliant theoretical crystallographer and a brave and generous man; some biographical details about him and his French co-worker Charles Mauguin appeared in the December 2010 issue of *Crystallography News*.) Carl Hermann presented to the class an extremely complicated derivation of certain subgroups in higher-dimensional space. As the number of dimensions increased, the number of members in the set increased from 4 to 8 to 16. Then he asked how many members there would be in the next higher dimension. The class started frantically scribbling equations, to no useful effect. Then Theo, relying on the evident geometric progression, raised his hand and said "32", which was correct. Carl Hermann beamed and said "Herr Hahn has demonstrated a deep understanding of symmetry theory." While that may not have been strictly true on this occasion, it certainly became true during Theo's career. Our copy of Volume A of the International Tables that he edited became an indispensable resource for my research group. After a colleague borrowed it to study while spending a weekend beside the River Avon, only for it to get soaked when the river suddenly flooded his accommodation, we carefully dried every page as if it were a priceless medieval manuscript.

Carl Schwalbe

Scenes from

BCA Spring Meeting 2016












BCA Prize Winners

BSG Poster Prizes
sponsored by Protein Data Bank Europe:

*Matthew Conroy (PDBe) presenting the first prize to **Jason Wilson** (University of Sheffield)*

*Matthew Conroy (PDBe) presenting the second prize to **Hayley Owen** (University of Sheffield)*

*Sam Horrell presents a giant ham to **Scott McKellar** for his service as YCG chair.*

*Pete Wood presenting the CCG poster prize to **Feifan Lang** (University of Sheffield)*

*Pete Wood presenting the CCG/CrystEngComm poster prize to **Merina Corpinot** (UCL) – Target crystals/materials*

*Pete Wood presenting the CCG/CrystEngComm poster prize to **Daniel Harcombe** (University of Oxford) – Properties*

*Pete Wood presenting the CCG/CrystEngComm poster prize to **Yue Wu** (University of Oxford) – Techniques/methods*

*Anthony Phillips (Queen Mary, University of London) presenting the PCG poster prize to **Mia Baise** (UCL)*

*Anthony Phillips (Queen Mary, University of London) presenting the PCG/RSC Solid State Chemistry poster prize to **Matt Dunstan** (University of Cambridge)*

*John Helliwell presenting the ACA Structural Dynamics Journal poster prize to **Sam Horrell** (University of Essex)*

*Sam Horrell presenting the YCG Best 30 Second Flash poster presentation to **Yue Wu** (University of Oxford)*

Bill Clegg impartially drawing the Exhibitor passport prize

*Lee Brammer awarding the Exhibitor passport prize to **Alex Cousen** (Bath)*

*Sam Horrell presents the Durward Cruickshank prize to **Scott McKellar***

***Andrew Cairns** receiving the PANalytical Thesis Prize from Phil Lightfoot*

CCP4 Study Weekend at Nottingham 2016

THE annual Collaborative Computational Project in Macromolecular Crystallography (CCP4) Study Weekend was held at the East Midlands Conference Centre at the University of Nottingham on January 8-10, 2016. This year's meeting, entitled "Protein-Ligand Complexes: Understanding Biological Chemistry", provided a comprehensive overview of the processes involved in sample generation, data interpretation and validation of crystal structures obtained from proteins containing small molecule-type ligands. The scientific programme was organised by Judit Debreczeni (AstraZeneca, UK) and Paul Emsley (MRC Laboratory of Molecular Biology, UK). Registered participants numbered 380, from a diverse range of academic and industrial institutions in the UK and from 13 other European countries as well as China, India, Japan, Mexico and the United States.

Figure 1a. Bernhard Rupp from (k.-k. Hofkristallamt, Vista, CA, USA. (Image provided by STFC).

The meeting opened with a keynote seminar by **Bernhard Rupp** (k.-k. Hofkristallamt, Vista, CA, USA). In his talk entitled "Introduction to protein-ligand complexes – the twilight experience," he began by setting the scene of how protein-ligand crystal structure can provide insights into fundamental protein function and in applied research such as drug design. However, interpretation of ligand structures within proteins is still challenging. He pointed out that recent surveys of protein-ligand crystal structures suggest that as much as 12% of the approximately 70,000 structures lack solid evidence to support the ligand presence or orientation (referred to as "pose") in these complexes. He then illustrated, with examples drawn from the literature, difficulties associated with ligand modelling in crystal structures. These include: small contributions to total scattering, low site occupancies, and less restrained B-factors. Dr. Rupp further discussed how more attention needs to be paid to the protocols using for refinement of ligands and the types of electron density maps used to interpret ligand structures. Utilization of validation tools for ligand structures is also important, as well as visual inspection of electron density and a solid understanding of the stereochemistry of the ligand and its interactions within the environment of the protein. The message here is that implementation of more robust procedures that are specifically focused on ligands in proteins should improve the reliability of interpretation of these complexes in the future.

The second session, "Sample Preparation", immediately followed with **Ilke Mueller** (BioFocus, Saffron Walden, UK) presenting "Classic ligand complex sample preparation techniques." She opened her talk by explaining the impact of solving crystal structures of protein-ligand complexes in translational research involving drug discovery programs. Not only are these structures used as part of the optimization of lead compounds for drug efficacy, but they are also increasingly playing a role in target validation. Using a wide range of examples, Dr. Mueller explained how design of expression constructs and the use of ligands in purification can yield higher success rates for obtaining diffraction quality crystals. She discussed the pro's and con's of different strategies used to obtain "crystallizable" protein-ligand complexes, with particular emphasis on when ligands are introduced (e.g., during crystallization or soaking) or exchanged, particularly for studies aimed at developing compound with high binding affinities.

The final talk of this session was from **Patrick Collins** (Diamond Light Source, Didcot, UK) who spoke on "Emerging techniques for ligand complex crystal preparation and data collection". Dr. Collins spoke about the latest capabilities of streamlining the screening of protein-ligand complexes on the I04-1 beamline at the Diamond Light Source. The I04-1 beamline has recently developed the XChem facility, a novel pipeline for medium-to-high throughput screening of small molecule fragments bound to well-diffracting crystals. The pipeline includes all steps from crystal soaking, harvesting, mounting, data collection and data analysis. Currently, 1000 datasets can be collected from 1000 crystals in under 40 h. This remarkable throughput has been facilitated in part by the use of acoustic waves to eject solutions containing small molecule fragments in low volumes (≤ nanoliter quantities) in crystal soaking/rapid crystallographic screening experiments (see Figure 2 for an example of the output). In combination with the bright synchrotron source and fast detector for data collection, the XChem facility should provide a more rapid route to structure-based identification of compounds with potent activities and/or high affinities.

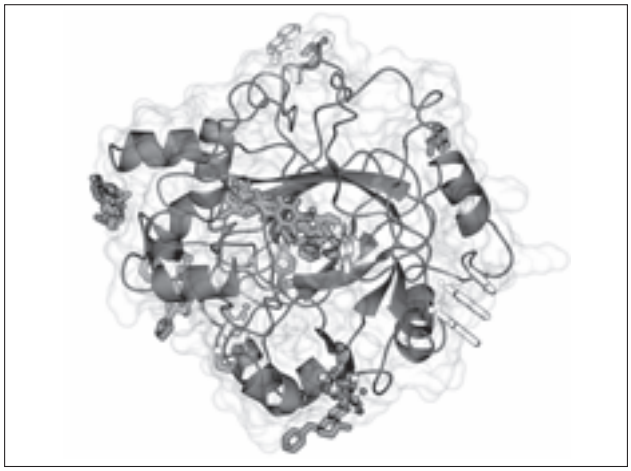


*Figure 2. **Typical readout from the XChem facility at Diamond Light Source.** Small molecule "fragments" bound to the surface and binding sites of JMJD2D, a human histone demethylase. Protein-ligand complexes were obtained using acoustic droplet ejection techniques for rapid crystal soaking. **(In colour on the front cover)** (Image provided by Dr Patrick Collins, Diamond Light Source, Didcot, UK).*

A second keynote seminar was presented by **Stephen Burley** (RCSB Protein Data Bank, Rutgers, USA) whose talk was entitled, "Small-molecule ligand/drug representation and

Figure 1b. Stephen Burley from RCSB Protein Data Bank, Rutgers, USA.
(Image provided by STFC).

validation in the Protein Data Bank." He stated that since the establishment of the Protein Data Bank (PDB) in 1971, beginning with just seven X-ray crystallographic structures of proteins, the global PDB Archive holds more than 113,000 experimentally determined three-dimensional structural models of biological macromolecules. Some 76% of these entries include at least one non-polymeric small molecule ligand. He encouraged experimentalists to use the anonymous wwPDB Validation Server (**http://wwpdb-validation.wwpdb.org/**) during structure determination and refinement to evaluate structure quality prior to deposition.

Roberto Steiner (Kings' College London, UK) opened the second session, "Refinement and Restraints", with his talk "Restraints in macromolecular crystallographic refinement." He emphasized that in macromolecular crystallographic refinement X-ray data alone are not sufficient to lead to chemically reasonable structures. Therefore, the correct use of stereochemical restraints is critically important. He briefly described the concept of restraints from a historical perspective and discussed the implementation of 'restrained refinement' in crystallographic software including examples of the various types of restraints used at different experimental resolution ranges.

Julie Tucker (University of Newcastle, UK) discussed "Dictionary generation software through the ages: a user's perspective." She explained how the generation of dictionaries of crystallographic restraints for novel molecules have evolved rapidly over recent years leading to improvements in model quality and throughput. These changes have been driven in part by the particular needs of researchers engaged in structure-based drug design. In her talk she introduced the basic steps involved in ligand restraint derivation and compared methods employed by about half a dozen software solutions that are currently in use. Examples of 'difficult' cases were given.

Garib Murshudov (MRC Laboratory of Molecular Biology, Cambridge, UK) concluded this session with "AceDRG – a tool for generating small molecule descriptions." He stated that Libcheck in the current CCP4 was not designed to generate ligand coordinates, only descriptors, therefore the development of a new tool was necessary. This tool is AceDRG. It uses the Crystallography Open Database (COD) to derive atom types, and uses the observed values of bonds and angles between atoms in order to generate dictionary (restraint) files for new ligands. The program accepts various input file formats, including SMILES string, SDF molfile, SYBIL MOL2 file, and mmCIF restraints dictionary.

The final session of the first day focused on methods for "Ligand Fitting". **Rob Nicholls** (MRC Laboratory of Molecular Biology, Cambridge, UK) presented excellent overview to "Ligand Fitting in CCP4." He acknowledged that the quality of ligands in macromolecular models deposited in the PDB has been lacking, with many ligands being fitted with poor geometry. This complex process depends on various factors, including data resolution, model quality, and the ligand's structural flexibility. He described the various tools distributed as part of the CCP4 suite, including: Coot, JLigand, AceDRG and REFMAC5.

Joana Pereira (European Molecular Biology Laboratory, Hamburg, DE) presented "Automated ligand identification and building with ARP/wARP." She explained how ARP/wARP is used to identify and build small-molecule ligands into density regions that are not accounted for by the protein structure. A pipeline for this process is shown in Figure 3. The program generates a mesh of free atoms in the target density region to be matched to the topology of the ligand. In cases when the density region is known but the identity of the ligand is not, ARP/wARP can evaluate the shape of the density and propose a candidate ligand from a database of about 80 common small molecules.

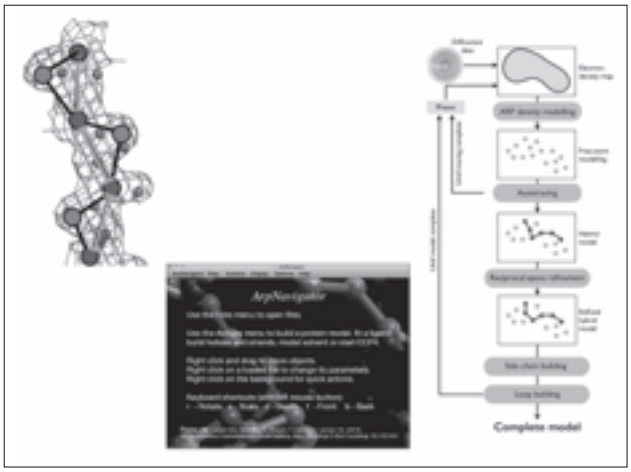


*Figure 3. **Pipeline for automated protein model building with ARP/wARP.** (Image supplied by Joana Pereira, European Molecular Biology Laboratory, Hamburg, DE).*

Nicholas Pearce (Structural Genomics Consortium, Oxford, UK) presented "PANDDAs: multi-dataset methods for ligand identification in X-ray crystallography". He presented a novel computational method for identifying electron density arising from a ligand. The method uses F_o-F_o maps derived from datasets obtained from non-isomorphous crystals. The method has been most effectively applied in cases involving crystallographic screening of fragment libraries soaked into ligand-free crystals. In these experiments, analysis of the resulting electron density maps shows that the majority show little evidence of fragment binding. The PANDDA method, which stands for PAN-Dataset Density Analysis, averages these "empty" datasets and generates a very accurate electron density map of the ligand-free structure. This structure can then be used to more effectively analyse F_o-F_o maps. This analysis can reveal weak electron density indicative of a weakly bound fragment and also reduces the potential for misinterpretation of electron density.

Paul Adams (Lawrence Berkeley National Laboratory, CA, USA) concluded the first day of the workshop with his talk, "What's in my blob?" He explained that it is commonplace to discover unexpected and/or difficult to interpret electron density features in crystallographic maps. In come cases, this density may be due to the presence of ligands, solvent or metals/ions that were not anticipated or identified during initial model building. He illustrated the challenges of ligand identification with a number of visual examples and then described tools that have been implemented in the *Phenix* crystallographic suite of programs that focus on ligand modelling. These tools include the Guided Ligand

Replacement (GLR) module, which uses graph theory to generate a coordinate set for a ligand. The module has additional features to better define ligand restraints in refinement and to improve ligand placement in a complex structure. For high throughput screening of ligand-complexes, an automated pipeline for ligand binding and refinement is also available. Challenges and developments for identification and orientation of metals and metal ions in proteins structures were also discussed.

The first session of the second day of the workshop, "Validation", was opened by one of the organizers, **Paul Emsley** (MRC Laboratory of Molecular Biology, Cambridge, UK) who spoke about "Ligand visualisation, validation and scoring." He primarily spoke about the new tools for assessing the quality of ligand structures in protein-ligand complexes that have been developed in the molecular-graphics software application *Coot*. These tools will improve the quality of modelled ligands deposited in the wwPDB by providing a means to assess and correct ligand quality during refinement and deposition. For example, *Coot* scores ligand structures modelled in protein complexes for the quality of correlations with direct and difference electron density maps. *Coot* can also interface with the Cambridge Crystallographic Data Centre program *Mogul*, to assess molecular distortion in terms of a quality indicator known as a Z-score. These quality indicators are then given a percentile rank against ligands of the PDB and, as shown in Figure 4, are displayed with sliders in a similar fashion to best practices recently recommended by the Validation Task force (see Adams *et al.,* 2016, *Structure*, **24**, 502-8).

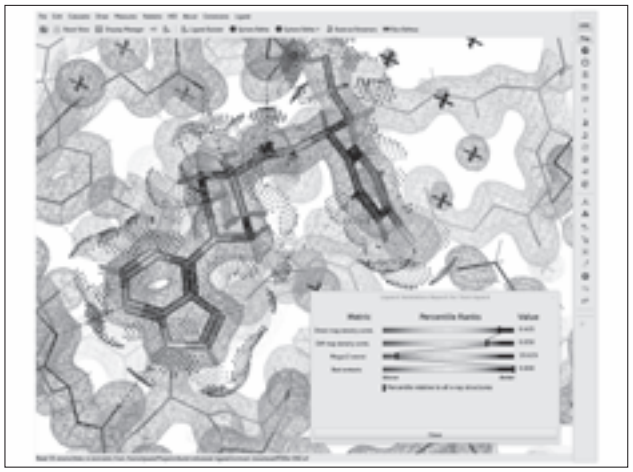


Figure 4. ***Tools for assessing the quality of protein-ligand complexes in Coot.*** *The structure of typical ligand (4gv1) is displayed, along with its electron density, its non-bonded contacts with the protein and the representation of the related metrics shown as sliders.* ***(In colour on the front cover)***
(Image provided by Dr. Paul Emsley, MRC Laboratory of Molecular Biology, Cambridge, UK).

Jon Agirre (University of York, UK) followed with "Automated detection, building and validation of carbohydrates – Privateer." Privateer is a new software package in the CCP4 suite of programs aimed at the detection and correction of anomalies in the refinement of carbohydrates present in protein structures. As mentioned in the previous talk, it has been recognized that poor refinement of ligand-type structures results in incorrect ligands (including carbohydrates) being deposited into the wwPDB. It is estimated that more than 30% of carbohydrate/sugar ligands are incorrect, corresponding to more than 7,000 deposited structures. Dr. Agirre explained how Privateer can be used to aid the crystallographer in building carbohydrate structures with more sensible region- and stereo-chemistries and conformations. Real-space correlations using appropriate electron density maps are a key element of the software that is used to guide and correct carbohydrate structures during refinement processes. Examples of this are shown in Figure 5. Automation of carbohydrate model-building using Privateer was also presented and will soon be included in future distributions of CCP4 package.

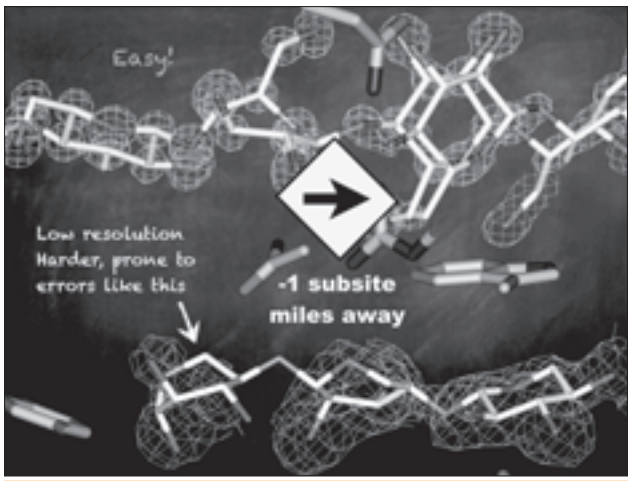


Figure 5. ***Sugar model validation.*** *The sugar-enzyme complex in the upper part of the image, which shows a snapshot of the hydrolysis done by a cellulase on cellobiose, has been determined to atomic resolution and there is little doubt that the enzyme is distorting the glucose from its minimal energy chair conformation to a boat in order to achieve catalysis. In the lower part of the slide, another structure shows a xylanase with bound xylotetraose. On the left, a xylose sugar in a boat conformation is aligned with the -3 subsite of the enzyme. An omit electron density map shows very little density for it, with the high energy boat conformation arising as a consequence of refining the model with a very low observation:parameter ratio. At lower resolutions, more restraints are required to increase this ratio.*
(Image provided by Jon Agirre, University of York, UK).

The third talk in this session was given by **Heping Zheng** (University of Virginia, USA) on "Validation of metal and other single atom binding sites in macromolecular structure." He introduced the 'CheckMyMetal' web server, which checks the binding site for types of coordinating ligands, valence of the site, geometry and data consistency (bond lengths and angles). He showed several examples of the program's use. He also showed the H20 server, which uses deep-learning (neural network) techniques to identify the correct metal at a site.

The final talk in the session was given by **Jason Cole** (Cambridge Crystallographic Data Centre/CCDC, Cambridge, UK), "Using 810,296 small molecule crystal structures to aid in protein structure refinement and analysis," which primarily focused on how the CCDC can be used to design restraint libraries for novel ligands. The 2016 release of the CSD has over 800,000 entries of small organic and metal-organic structures. He showed how the CCDC uses its tools (Mogul) to define the chemistry of new structures from previously deposited structures.

The next session was entitled "Tracking Hydrogen Atoms", and opened by **Ben Bax** (GlaxoSmithKline, UK) who presented, "Getting the chemistry right: protonation, tautomers and the importance of hydrogens in biological chemistry." He introduced tautomers, explaining these occurred where there could be hydrogen movement to produce different structures with the same chemical content. He proceeded to show three examples of DNA Gyrase bound to the inhibitor QPT1. In each example the binding mode of the QPT1 is different due

to tautomerism. He also illustrated how neutron protein crystallography can be used to better define hydrogen positions by showing a comparison between the X-ray and neutron crystal structures of a complex between trypsin and bovine trypsin protease inhibitor (Figure 6). He finished the talk by reminding us of the story of how Jerry Donohue helped Watson and Crick solve the structure of DNA, by pointing out the correct tautomeric binding mode of the bases.

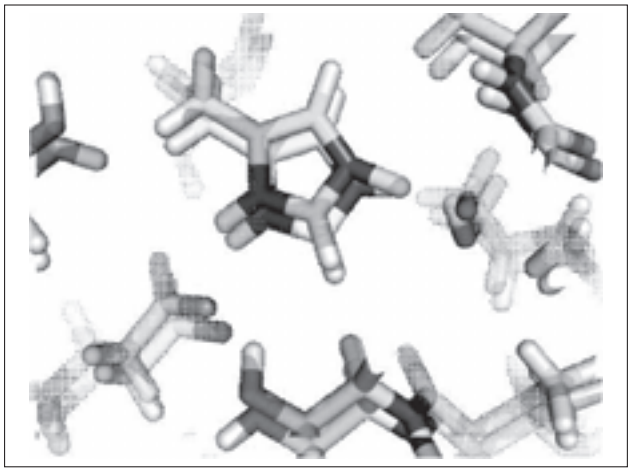


Figure 6. ***Comparison X-ray and neutron protein crystal structures of the trypsin-BPTI complex.*** *A superposition of experimentally determined (see reference) hydrogens (green carbons) with those placed automatically (yellow carbons). Note that although the positions of most hydrogens are determined from the positions of the heavy (non-hydrogen) atoms the positions of some hydrogens are not simply defined by the heavy atom positions (e.g hydrogens on the serine side-chains – in the figure). (Reference: Kawamura et al., 2011, Acta Crystallogr. D. Biol. Crystallogr.* ***67****, 140-8.* ***(In colour on the cover)*** *(Image provided by Ben Bax, GlaxoSmithKline, UK).*

The second talk in the session was given by **Greg Warren** (OpenEye Scientific Software Inc., USA) on "Placing those ghostly hydrogens: computational methods for assessing tautomer states in structural biology." He explained that the fact that hydrogens are rarely fitted leaves a lot of information out of the model, which can cause problems for modelling enzyme processes. His company has software which can generate all the possible tautomers of a structure and then use QM/MM techniques to decide which are the most probable. He showed two examples, AZM (which binds to human carbonic anhydrase) and uric acid (which binds to urate oxidase), which have 15 and 43 different possible tautomeric states, respectively, and showed which were the most probable.

The last talk was given by **Oliver Smart** (Global Phasing Ltd., Cambridge, UK) on "Assessing ligand strain energy in BUSTER protein-complex structure refinement." In this method, restraint dictionaries are not used to restrain the ligand. Instead the ligand is refined using force fields (MMFF94). This refinement strategy yields results that are equivalent to using high-level QM methods, but at a fraction of the computational cost. The ligand strain energy can also be used as an extra validation tool, where high ligand strain energies are indicative of errors in the ligand structure.

* * *

The workshop concluded with a final session called "Application of protein-ligand complexes." **Colin Groom** (Cambridge Crystallographic Data Centre, Cambridge, UK) began this session with a lively presentation titled, "Using ~~801,296~~ 815,527 small molecule crystal structures to complement ~~113,971~~ 114,741 biological macromolecular structures" to address affinity, selectivity, bioavailability and solubility. The crossed-out numbers in the title emphasize the dynamic nature of both the CCDC and the wwPDB (the figures he cited were the number of depositions as of 10/01/2016), and the versatility in the way that small molecule crystal structures can be mined for information – particularly relevant to structure-based drug development studies. Not only can structural information about specific ligands or fragments be easily obtained, but tools have been developed that take advantage of studying a collection of entries. For example, comparisons of structures and their interactions in a crystal lattice can provide deeper insights into understanding the energetics of molecular conformations of ligands, or interactions responsible for molecular recognition in protein-ligand complexes. Similar analyses of inter- and intra-molecular interactions, along with information about crystallization conditions, can also provide additional predictive power about the solubility and bioavailability of specific ligands or fragments. For structural biologists, developing more familiarity with the computational and molecular graphics tools in the CCDC could improve the quality of refined structures of ligands in proteins. Increased knowledge about these tools could also improve investigations requiring an understanding of the molecular interactions critical for protein-ligand complex formation.

Peter Moody (University of Leicester, UK) followed with his presentation, "Neutron diffraction and in situ spectroscopy" (Figure 7). He presented examples of different techniques for using protein crystals to elucidate molecular information for understanding enzyme mechanisms. First, he explained that the function of some enzymes can be analyzed using spectroscopic techniques, in some cases by by taking advantage of X-ray irradiation to trigger a reaction or follow the structure of photo-reducible ligand such as flavin. Using single crystal spectrophotometry, reaction intermediates in enzyme can be characterized for their presence during X-ray data collection. Dr. Moody showed how this methodology has been successfully used to study the reduction of an enzyme-bound flavin and reaction intermediates (Compound I and II) in heme peroxidases. In addition, hydrogens often play key roles in enzyme mechanisms but the presence of hydrogen is usually modelled, rather than observed, in X-ray crystal structures. Dr. Moody showed how neutron crystallography

Figure 7. ***Peter Moody, University of York, speaking at the CCP4 Study Weekend 2016 in the East Midlands Conference Centre, University of Nottingham.***
(Image provided by Jon Agirre, University of York, UK).

allows direct visualization of protonation states within the active site of cytochrome c peroxidase, and how these data could be used to develop a revised hypothesis about how O-O bonds are cleaved by heme enzymes. This study demonstrated the potential of neutron crystallography for providing key data for understanding molecular processes in enzyme catalysis. This work also suggests that such an approach could be very generally beneficial for understanding how molecular interactions influence ligand binding and/or catalysis in many other proteins.

Charlotte Deane (University of Oxford, UK) then spoke about "WONKA and OOMMPPAA – analysis of protein-ligand interaction data to direct structure based drug design." Dr Deane leads a bioinformatics group that combines theoretical studies and empirical analyses of problems involving protein structure prediction and protein interaction networks. In her talk she first introduced WONKA, a computational tool for analyzing ensembles of protein structures. For complexes, WONKA analyzes ligand structure within a protein and identifies whether binding modes of the ligand are unusual or even erroneous. In the program OOMMPPAA, three-dimensional matched molecular pairs from structures or sub-structures are identified. Three-dimensional ligand conformations are then generated and associated with relevant activity data. This information is visualized in a pharmacophore-type of presentation, involving both the ligand its local protein structure environment. OOMMPPAA is a particularly useful tool for analyzing large volumes of structural and functional date generated in high throughput ligand or fragment screen. Both WONKA and OOMMPPA are freely available to use and download at: http://commppa.sgc.ox.ac.uk/OOMMPP/ and http://wonka.sgo.ox.ac.uk/WONKA/.

The final talk of the workshop was presented by **Martin Noble** (University of Newcastle, UK), "From high volume data to knowledge: tools to tame the torrent of structures in a drug discovery campaign at home and at the synchrotron." It is widely recognized that new software is needed to cope with the analysis and interpretation of data generated from high throughput structural biology research programs, particularly for downstream applications such as drug discovery. Dr Noble's talk focused upon describing computational tools developed for the CCP4 suite that can be used to organize and analyse large volumes of data. He began by describing how the XChemExplorer program is being used to organize results arising from the high throughput fragment-pipeline at the I04-1 beamline at Diamond. Additional examples followed that descriptions of the i2Archive and CCP4mg programs. i2Archive program facilitates the transfer of structural data and related information between different research groups using the CCP4i2 graphical user interface. CCP4mg provides users with a range of functionalities that enable users to create high quality images and movies, with specific features that enable animation and superpositions of structures. A key message of the talk is that provision of effective computational tools for use with structure-based compound screening experiments is essential for generation of drug development models with genuinely predictive capabilities.

Finally, this year's CCP4 workshop ran smoothly and successfully due to the dedicated and professional support provided by the UK Science and Technology Facilities Research Council (STFC) team comprised of **Karen McIntyre**, **Shirley Miller**, **Laura Johnston**, **Ville Uski**, and **Charles Ballard**. A/V support, including photography, was provided by **Stuart Eyres**. In addition, this meeting benefited greatly from the support of the UK-based sponsors: the STFC, the Biotechnology and Biological Sciences Research Council (BBSRC), the Medical Research Council (MRC) and Diamond Light Source.

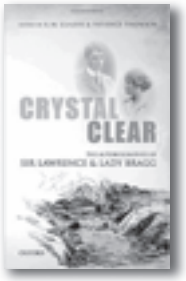
Prepared by members of the Biological Structures Group Committee and edited by **Katy Brown** (BSG Chair).

Book Review

Crystal Clear: the Autobiographies of Sir Laurence and Lady (Alice) Bragg

Edited by A M Glazer and Patience Thomson

(Oxford, OUP, 2015, 427 pp)



PREVIOUSLY unpublished (in full) autobiographies of the younger of the pioneer crystallographers, William Laurence Bragg (WLB 1890-1971), and his beloved but very different wife, Alice Grace Jenny nee Hopkinson (1899-1989) have been gently edited by A. Mike Glazer, now also a crystallographic historian, and Patience Thomson, younger daughter of WLB. Both authors were, among their attributes, accomplished artists and the volume is illustrated by many sketches by WLB as well as a few photographs.

With several biographies and many shorter accounts available about the young Nobel prizewinner, one might have thought that most details of the lives of WLB (especially) and Alice Bragg would be well known. One would be wrong. These two partial autobiographies contain immense amounts of intimate and inside detail, carefully edited, about the thoughts and doings of the authors, especially about Alice and her happy childhood. William Henry Bragg (WHB) took the month of August off, in different places each year, seaside or country, with the family making their own amusements walking, swimming, climbing, cycling. Obviously, for Alice there was neither of the planned language stays in France and Germany but instead, in addition to academic studies in preparation for

Cambridge, Alice learned to sing, play the piano, sew, and drive; she also ran a Girls' Friendly Society club once a week.

WLB first proposed marriage, after a brief acquaintance, when Alice Hopkinson was aged 19 (not her first proposal) enjoying her first May week at Cambridge, mainly accompanying recently demobbed naval officers (Patrick Blackett was deemed the most attractive). This was when women wore hats to lectures and formally could not receive degrees. Alice was in the Student Christian Movement and went to their Swanwick conference, did social work in the Camberwell Settlement, and also took part in reading parties. During that first Long Vac, WLB and Alice walked and punted, eating meals with the Hopkinsons (WLB was a close friend of Cecil, Alice's cousin), and Alice learned about the wide knowledge of Nature of the serious WLB. It was another two years without communication with WLB, before Alice took Finals in History (and managed a 2nd), that WLB asked again and was accepted. He was already an FRS. The Hopkinsons were aware of career structures whereas WLB took things as they went (except for his pursuit of Alice). After marriage on 10 December, 1921, and an 'enchanting' honeymoon in Somerset, Paris and Cannes, she went into a 'charming' house in Didsbury, Manchester, where dinners and calling cards were exchanged with much older wives of professors, doctors, etc. After ten years in Didsbury, they moved to the big Windy Howe house at Alderley Edge. In the 1930s at the RI, WHB had on his staff people who would become eminent X-ray crystallographers including Astbury, Bernal, Cox, Lonsdale, Megaw, Muller, and Shearer; both WHB and WLB had a relatively high proportion of women in their research students. Alice says she kept a diary for only three periods: the year she became engaged, the year at beautiful Bushey House (1937, when WLB was running the NPL), and the time when she was Mayor of Cambridge (1946-48). Evidently she had a good memory and she wrote very long letters to relatives, e.g. 60 pages on the Nobel prize trip to Scandinavia! Several times she mentions only selecting the highlights of an event so more should be available.

As for the relations between WHB and WLB, Alice thinks the difficulties have been exaggerated; the two minds worked in the same way. Certainly her father-in-law did not find it easy to communicate especially about feelings (when moved, he would raise his feet from the ground). As a result of this limited interaction, WLB would sometimes tend to overemphasise the contributions of research students to joint research; also Alice discouraged son Stephen from becoming a third generation physicist (he became an engineer).

During World War II (WLB had trenches dug at the NPL in 1938), Lady Reading directed Alice to run the Women's Voluntary Services in Cambridge (looking after Belgian refugees, for example); there followed the CD committee and then Independent town councillor for Newnham. (no elections during the War). This led to being asked, despite being a woman, to be the Mayor, which WLB persuaded her to accept (WHB had been Mayor of Manchester) and was proud of her achievement. This involved three-hourly council meetings (50 men, 4 women) but the worst worries seem to have been flying in a Tiger Moth (to open the airport) and marching the WVS under Sgt Brown in the Victory Parade. In 1941, WLB recounts, he was scientific liaison officer (before the USA was in the War, based at the NRC, Ottawa, travelling out (together with 17 mannequins) aboard the 4,800 ton *Baltrover* and returning from Gander to Hendon by four-engined bomber.

The lengthy vacations may raise a contemporary eyebrow. The August holiday was often spent at Hickling Broad or Blakeney, with much sailing, but sometimes near Aviemore or Donegal, but there were also Easter and autumn stays, including Abersoch and Abergele. WLB liked traveling abroad but much preferred small gatherings to big conferences (hence rather few appearances at BA meetings). Thus they enjoyed the lavish hospitality of the 1948 Solvay Conferences (Alice's first) in Brussels which was followed by a US tour based on Pittsburgh. Alice soon found that she was expected to give talks as well, including local government and magistrates courts. Much earlier, at the Volta Celebrations in Como and Rome they met Mussolini who said a few words to each scientist in his own language. In 1931, they went by Russian boat (no bath plugs or lavatory locks), helped by the Kapitzas, to a conference (cancelled before it began) attended by several eminent British scientists in shabby Leningrad. In Moscow (50 pages of letter to family before writing articles for *The Yorkshire Post*), amid the fleas, poverty and queues, was a five-year plan of growth in the developing USSR.

Pregnant with Patience, she read for the bar (aiming to be a poor man's lawyer), passing all except for Finals, and took a course in journalism, with homework checked by WLB, but WW II stopped these. WLB concentrated on sound-ranging (disappointed that so little had been done between the Wars) and ASDIC, continuing to advise at Portland Head after the War. In 1960, they had a round-the-world tour (including a short talk on the plane on protein research!), prompted by the Rutherford Memorial Lecture in Nelson , New Zealand, but covering Auckland to Christchurch, followed by a month in Australia.

Mike Glazer and Patience Thomson have edited a captivating book that reflects on 50 years' happy loving relationship between two distinctive, intelligent, accomplished, mutually interacting people. Each author includes interesting footnotes but, for WLB's autobiography in particular, every time a (usually distinguished) character is mentioned the name is repeated in full with dates of birth and death. This collection is in itself a valuable resource. From Niels Bohr's biography, also written separately by two authors, some have concluded that his (younger) wife, Margrethe, played a considerable part in the formulation of Bohr's conclusions in his papers, 'a midwife to the quantum atom'. Meeting them in 1922 only a few months after her marriage (a decade after Margrethe's), Alice felt that the enchanting Margrethe, mother of six sons, would be an international model for all physicists' wives.

Derry W Jones
University of Bradford

Summary Financial Statements for year ended 31 December 2015

Examining Accountant: R A Young, BSc. FCA
The Young Company, Ground Floor, Unit 2b Vantage Park, Washingley Road, Huntingdon, Cambridgeshire PE29 6SR.

These are consolidated accounts based on the unaudited financial statements and include the BCA, BSG, IG, CCG, CCG School funds and YCG, expressed in pounds sterling (£)

INCOMING RESOURCES:

	2015	2014
Grants and sponsorship	21,506	10,524
Donations	705	203
Annual conference (5)	89,923	66,042
Meetings of groups	43,154	8,738
Crystallography News	17,149	10,338
Membership Subscriptions	18,916	19,860
Investment income	5,582	6,063
Interest received	54	50
TOTAL INCOME	**196,989**	**121,818**

EXPENSES:

	2015	2014
Direct charitable expenditure (2)	174,628	120,222
Management and administration (3)	12,563	13,103
TOTAL EXPENDITURE	**187,191**	**133,325**

	2015	2014
NET INCOME/(LOSS):	**9,798**	**(11,507)**
Unrealised (losses) on investment assets	(5,822)	(1,533)
NET MOVEMENT IN FUNDS	**3,976**	**(13,040)**
Balances brought forward at 1 January 2015	244,744	257,784
Balances carried forward at 31 December 2015	248,720	244,744

ASSETS:

Fixed assets	2015	2014
Tangible assets	-	5
Investments	132,863	135,723
Total	**132,863**	**135,728**
Current assets		
Debtors	2,068	18,507
Cash at Bank	128,843	105,722
Total	**130,911**	**124,229**

CREDITORS:

Amounts falling due within 1 yr	(14,010)	(14,410)
Amounts falling due after 1 yr	(1,044)	(803)
NET ASSETS	**248,720**	**244,744**

INCOME FUNDS:

	2015	2014
Restricted funds (4)	130,745	127,116
Unrestricted funds (4)	117,975	117,628
Total	**248,720**	**244,744**

NOTES TO THE SUMMARY FINANCIAL STATEMENTS

1. ACCOUNTING POLICIES

These summary statements are based on financial statements which have been prepared under the historical cost convention, with items recognised at cost or transaction value unless otherwise stated in the relevant notes to the accounts. The financial statements have been prepared in accordance with the Statement of Recommended Practice, (SORP 2015) "Accounting and Reporting by Charities" and applicable accounting standards.

All incoming resources are included in the Statement of Financial Activities when the charity is legally entitled to the income and the amount can be measured reliably. All expenditure is accounted for on an accruals basis and has been included under expense categories that aggregate all costs for allocation to activities. Investments are stated at market value at the balance sheet date.

Tangible fixed assets are stated at cost less depreciation. Depreciation is provided at rates calculated to write off the cost of fixed assets, less their estimated residual value, over their expected useful lives.

2. DIRECT CHARITABLE EXPENDITURE

	2015	2014
Subscription to International bodies	10,660	10,970
Annual conference (5)	92,561	72,067
Meetings of groups	6,680	9,806
Crystallography News + Newsletters	14,034	14,783
Course fees and accommodation	45,156	2,292
Grants and sponsorship	1,634	8,204
Awards & bursaries	1,903	900
Arnold Beevers Bursary Fund	2,000	1,200
Total	**174,628**	**120,222**

3. EXPENDITURE ON RAISING FUNDS

	2015	2014
Administration fees	4,627	4,604
Administration expenses	1,534	1,499
Accounting fee	4,800	5,100
Insurance	599	566
Bank and security charges	181	87
Special Interest Group Administration	228	545
Council members' expenses	477	613
Website Costs	112	89
Depreciation – tangible fixed assets	5	-
TOTAL	**12,563**	**13,103**

continued overleaf

4. STATEMENT OF FUNDS	Brought Forward	Incoming Resources	Resources Expended	Transfers	Gains (Losses)	Carried Forward
UNRESTRICTED FUNDS						
General Fund	**117,628**	**137,116**	**(130,947)**	**-**	**(5,822)**	**117,975**
RESTRICTED FUNDS						
Arnold Beevers Bursary Fund	6,946	-	(2,000)	-	-	4,946
IUCr bursary fund	28,631	-	-	-	-	28,631
Dorothy Hodgkin prize fund	8,705	-	-	-	-	8,705
Chemical group teaching school	33,616	46,901	(45,897)	-	-	34,620
Chemical group fund	5,763	3,030	(1,246)	-	-	7,547
Industrial group fund	28,087	8,417	(2,965)	-	-	33,539
Biological Structures group fund	13,785	25	(2,876)	-	-	10,934
Durward Cruickshank fund	1,531	-	(250)	-	-	1,281
Young Crystallographers Group Fund	52	1,500	(1,010)	-	-	542
Subtotal	**127,116**	**59,873**	**(56,244)**	**-**	**-**	**130,745**
Total of Funds	**244,744**	**196,989**	**(187,191)**	**-**	**(5,822)**	**248,720**

5. Spring Meeting 2015 University of York	
INCOME	
Conference income	89,923
Total	**89,923**
EXPENDITURE	
Venue exp. (accom, meals)	62,671
Hg3 fee	11,320
Conference expenses	5,234
Printing & stationery	3,262
Travel & subsistence	253
Bank charges	2,113
Staffing costs	2,400
Exhibition commission	2,338
Storage costs	540
Courier charges	212
Meeting insurance	617
Planning meeting exps	1,601
Total	**92,561**
TOTAL INCOME	**89,923**
TOTAL EXPENDITURE	**92,561**
MEETING DEFICIENCY	**2,638**

Treasurer's Report 2015

OVERALL we had a surplus of £3,976 during the year ended 31 December 2015, and the Association has no material guarantees or commitments which could affect its future solvency.

The general fund had a surplus of £347 including a decrease of £5,822 in the value of the investments. The reserve funds operated by the Groups and the Association had an overall surplus of £3,629. The income from our investments brought in £5,636 this year, a small decrease on last year due to a decrease in yields on the investment portfolio.

The major risks to which the Association is exposed are with regard to the cost of the Spring Meeting and its effects on the Association's major reserves. To mitigate those risks the Association has all its investments placed with an independent professional management company. Our investment portfolio was valued at £132,863. Bank interest rates continue to be at historically low levels, so income from interest is substantially lower than a few years previously. The Council's review of the reserves indicates that we should always be striving to generate more income to enable us to plan and encourage even higher levels of educational and scientific activity.

Crystallography News continues to contribute to the income of the BCA. We are grateful to its advertisers and sponsors who have continued to generously support our activities. We are as always grateful for those who contribute to the newsletter and to **Carl Schwalbe**, **Dave Allan** and **Tony Hopps** for editing and overseeing its production.

Subscriptions to international bodies were £10,660, covering our membership of the IUCr and also our subscription to the European Crystallographic Association.

I would like to thank everyone who has helped me in my role this year, in particular the other Officers, members of Council, **Nicola Peel** and the team at Hg3, and our accountant **Ray Philpott** at The Young Company for all their help throughout the year.

Pamela Williams
Treasurer

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.

10-13 June 2016
13th TOPAS User's Meeting, Bari, Italy.
http://www.bruker.com/events/users-meetings/x-ray-diffraction-and-elemental-analysis/topas-users-meeting.html

12-15 June 2016
15th European Powder Diffraction Conference (EPDIC15), Bari, Italy.
http://www.ba.ic.cnr.it/epdic15/

12-15 June 2016
RNA structure meets function. EMBO Workshop, Stockholm, Sweden.
http://events.embo.org/16-rna/

12-15 June 2016
The biochemistry and chemistry of biocatalysis: From understanding to design, Oulu, Finland.
http://events.embo.org/16-biocatalysis/

12-15 June 2016
Synchrotron Radiation to Study Atomic Layer Deposition, Bellaterra (ALBA), Spain.
https://indico.cells.es/indico/event/63/overview

13-14 June 2016
Synchrotron Resources for Future Investigations of Thin-Film Growth, Processing, and Characterization, Ithaca, NY, USA.
http://meetings.chess.cornell.edu/sciworkshops2016/Workshop3.html

13-17 June 2016
OPPF - Workshop on frontiers of recombinant multi-protein complex expression in insect and mammalian cells, Didcot.
http://www.oppf.rc-harwell.ac.uk/OPPF/public/courses/oppf2016.jsp

13-17 June 2016
REXS2016. Resonant Elastic X-ray Scattering, Hamburg, Germany.
https://rexs2016.desy.de/

15 June 2016
BCA Industrial Group XRF Meeting, Leicester.
https://sites.google.com/site/bcaxrf/

15-17 June 2016
The Future of X-Ray and Electron Spectroscopies, Uppsala, Sweden.
http://www.delegia.com/app/attendee/default.asp?PageId=41261&MenuItemId=36856&ProjectId=6979

19-22 June 2016
74th Device Research Conference (DRC 2016), Newark, DE, USA.
http://www.mrs.org/drc-2016/

19-24 June 2016
European Conference on X-Ray Spectrometry EXRS2016, Gothenburg, Sweden.
http://www.exrs2016.se

20-21 June 2016
Protein Modelling and Structure-Based Function Prediction, Liverpool.
https://www.biochemistry.org/Events/tabid/379/View/Programme/MeetingNo/TD010/Default.aspx

20-21 June 2016
Hard X-ray Spectroscopies and Imaging. CHESS-U Workshop, Ithaca, NY, USA.
http://meetings.chess.cornell.edu/sciworkshops2016/Workshop4.html

22-24 June 2016
58th Electronic Materials Conference, Newark, DE, USA.
http://www.mrs.org/58th-emc/

26-30 June 2016
CGOM12 and BACG2016, Leeds.
http://www.crystalgrowth2016.co.uk/

26-30 June 2016
DSL2016. 12th International Conference on Diffusion in Solids and Liquids, Split, Croatia.
http://www.dsl-conference.com/

26 June – 1 July 2016
7th European Charge Density Meeting (ECDM7), Warsaw, Poland.
http://ecdm7.chem.uw.edu.pl/

27-28 June 2016
D3: Defects, Distortions, and Dynamics in complex materials, Ithaca, NY, USA.
http://meetings.chess.cornell.edu/sciworkshops2016/Workshop5.html

27 June – 2 July 2016
Advanced Methods in Macromolecular Crystallization VII, Nove Hrady, Czech Republic.
http://www.crystallography.fr/mathcryst/antwerp2016.php

27 June – 2 July 2016
International School on Fundamental Crystallography with Applications to Electron Crystallography, Antwerp, Belgium.
http://www.crystallography.fr/mathcryst/antwerp2016.php

2-7 July 2016
ICCBM-16. 16th International Conference on the Crystallization of Biological Macromolecules, Prague, Czech Republic.
http://www.iccbm16.org/

3-8 July 2016
6th international conference on NANOstructures and nanomaterials SElf-Assembly (NANOSEA), Giardini Naxos, Italy.
http://www.nanosea2016.imm.cnr.it/

4-6 July 2016
Faraday Discussion: Nanoparticles with Morphological and Functional Anisotropy 2016, Glasgow.
http://www.rsc.org/events/detail/16842/

4-8 July 2016
3rd International School on Aperiodic Crystals, Antwerp, Belgium.
https://www.uantwerpen.be/en/summer-schools/aperiodic-crystals/

4-9 July 2016
Integrative modelling of biomolecular interactions. EMBO Practical Course, Barcelona, Spain.
http://events.embo.org/16-biomol-interact/

6-7 July 2016
Scanning Probe Microscopy Meeting, Warwick.
http://www.rms.org.uk/discover-engage/event-calendar/scanning-probe-microscopy-meeting.html

6-8 July 2016
British Biophysical Society Biennial Conference, Liverpool.
www.bbs2016.co.uk

6-10 July 2016
Ribosome Structure and Function, Strasbourg, France.
http://events.embo.org/16-ribo/

9-10 July 2016
Ion Channels. Gordon Research Seminar, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?id=15311

10-14 July 2016
American Conference on Neutron Scattering, Long Beach, CA, USA.
http://www.mrs.org/acns-2016/

10-14 July 2016
14th International Conference on Surface X-ray and Neutron Scattering (SXNS14), Stony Brook, NY, USA.
https://www.bnl.gov/sxns14/

10-15 July 2016
Ion Channels. Gordon Research Conference, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?id=11436

10-15 July 2016
18th International Conference on Metal Organic Vapor Phase Epitaxy (ICMOVPE-XVIII), San Diego, CA, USA.
http://www.mrs.org/icmovpe-xviii/

10-15 July 2016
FASEB Summer Research Conference on Post-transcripitonal control of gene expression: Mechanisms of RNA decay. EMBO Keynote Lecture, Lisbon, Portugal.
http://www.faseb.org/SRC-Microsite/mRNA/Home.aspx

11-13 July 2016
Circular and Linear Dichroism Summer School 2016, Coventry.
http://www.rsc.org/events/detail/20611/circular-and-linear-dichroism-summer-school-2016

14-15 July 2016
Frontiers in BioImaging, London.
http://www.rms.org.uk/discover-engage/event-calendar/frontiers-in-bioimaging.html

16-17July 2016
High Pressure, Research at (GRS), Holderness, NH, USA.
http://www.grc.org/programs.aspx?id=15297

16-17July 2016
Solid State Chemistry. Gordon-Kenan Research Seminar, New London, NH, USA.
http://www.grc.org/programs.aspx?id=17232

17-22 July 2016
Diffraction Methods in Structural Biology. Gordon Research Seminar, Lewiston, ME, USA.
http://www.grc.org/programs.aspx?id=16486

16-19 July 2016
The Protein Society Conference. The 30th Anniversary Symposium of The Protein Society, Baltimore, MD, USA.
http://www.proteinsociety.org/meetings/symposium/

17-21 July 2016
16th IUBMB Conference, Vancouver, Canada.
http://www.iubmb2016.org/

17-22 July 2016
High Pressure, Research at. Gordon Research Conference, Holderness, NH, USA.
http://www.grc.org/programs.aspx?id=12110

17-22 July 2016
Solid State Chemistry. Gordon-Kenan Research Seminar, New London, NH, USA.
http://www.grc.org/programs.aspx?id=14318

17-22 July 2016
Diffraction Methods in Structural Biology. Gordon Research Conference, Lewiston, ME, USA.
http://www.grc.org/programs.aspx?id=11655

18-22 July 2016
SymFest'16. Symmetry Festival, Vienna, Austria.
http://festival.symmetry.hu/

21-25 July 2016
12th International Congress of Cell Biology, Prague, Czech Republic.
http://iccb2016.org/

22-26 July 2016
American Crystallographic Association Annual Meeting, Denver, CO, USA.
http://www.amercrystalassn.org/content/pages/main-annual-meetings

23-24 July 2016
Enzymes, Coenzymes & Metabolic Pathways. Gordon Research Seminar, Waterville Valley, NH, USA.
http://www.grc.org/programs.aspx?id=17008

23-24 July 2016
Polymer Physics. Gordon Research Seminar, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?id=15409

23-24 July 2016
Thin Film & Small Scale Mechanical Behavior. Gordon Research Seminar, Lewiston, ME, USA.
http://www.grc.org/programs.aspx?id=15458

24-28 July 2016
Microscopy & Microanalysis (M&M2016), Columbus, OH, USA.
http://www.microscopy.org/MandM/2016/

24-29 July 2016
Enzymes, Coenzymes & Metabolic Pathways. Gordon Research Conference, Waterville Valley, NH, USA.
http://www.grc.org/programs.aspx?id=11265

24-29 July 2016
Polymer Physics. Gordon Research Conference, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?id=11989

24-29 July 2016
Stereochemistry. Gordon Research Conference, Newport, RI, USA.
http://www.grc.org/programs.aspx?id=12168

24-29 July 2016
Thin Film & Small Scale Mechanical Behavior. Gordon Research Conference, Lewiston, ME, USA.
http://www.grc.org/programs.aspx?id=12750

24-29 July 2016
Virus Structure and Assembly, Steamboat Springs, CO, USA.
http://www.faseb.org/SRC-Microsite/VStruc/Home.aspx

25-27 July 2016
7th International Conference on Advanced Nanomaterials (ANM2016), Aveiro, Portugal.
http://www.anm2016.com/

25-27 July 2016
Neutrons in Chemistry. Bunsen Discussion Meeting, Bielefeld, Germany.
http://www.uni-bielefeld.de/chemie/neutrons_in_chemistry/

25-29 July 2016
19th International Conference on Non-Contact Atomic Force Microscopy (NC-AFM), Nottingham.
http://ncafm2016.iopconfs.org/Home

30-31 July 2016
Ceramics, Solid State Studies in. Gordon Research Seminar, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?id=17147

30-31 July 2016
Colloidal Semiconductor Nanocrystals. Gordon Research Seminar, West Dover, VT, USA.
http://www.grc.org/programs.aspx?id=17152

30-31 July 2016
Scientific Methods in Cultural Heritage Research. Gordon Research Seminar, Newry, ME, USA.
http://www.grc.org/programs.aspx?id=16648

30-31 July 2016
Molecular Basis of Microbial One-Carbon Metabolism. Gordon Research Seminar Waterville Valley, NH, USA.
http://www.grc.org/programs.aspx?id=15360

31 July – 5 August 2016
Ceramics, Solid State Studies in. Gordon Research Conference, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?id=11083

31 July – 5 August 2016
Colloidal Semiconductor Nanocrystals. Gordon Research Conference, West Dover, VT, USA.
http://www.grc.org/programs.aspx?id=16726

31 July – 5 August 2016
Scientific Methods in Cultural Heritage Research. Gordon Research Conference, Newry, ME, USA.
http://www.grc.org/programs.aspx?id=15101

31 July – 5 August 2016
Molecular Basis of Microbial One-Carbon Metabolism. Gordon Research Conference, Waterville Valley, NH, USA.
http://www.grc.org/programs.aspx?id=12764

31 July – 5 August 2016
Machines on Genes IV. 80th Harden Conference, Macclesfield, Cheshire.
http://www. biochemistry.org/Events/tabid/379/Page/2/MeetingNo/80HDN/view/Conference/Default.aspx

1-4 August 2016
Summer School on nanoscience@Surfaces, Cambridge.
http://nanoscience2016.iopconfs.org/home

1-5 August 2016
Denver X-ray Conference. 65th Annual Conference on Applications of X-ray Analysis, Rosemont. IL, USA.
http://www.dxcicdd.com/

7-10 August 2016
5th International Symposium on Diffraction Structural Biology (ISDSB2016), Knoxville, TN, USA.
https://conference.sns.gov/event/2/

7-12 August 2016
Multiferroic & Magnetoelectric Materials. Gordon Research Conference, Lewiston, ME, USA.
http://www.grc.org/programs.aspx?id=16774

7-12 August 2016
18th International Conference on Crystal Growth and Epitaxy ICCGE-18, Nagoya, Japan.
http://www.iccge18.jp/

7-12 August 2016
15th International Symposium on Metal-Hydrogen Systems, Interlaken, Switzerland.
https://mh2016.ch/

8-10 August 2016
Structural Aspects of Infectious Disease, Cambridge.
https://www.biochemistry.org/Events/tabid/379/MeetingNo/SA182/view/Conference/Default.aspx

13-14 August 2016
Biomineralization. Gordon Research Seminar, Girona, Spain.
http://www.grc.org/programs.aspx?id=15199

13-14 August 2016
Conductivity & Magnetism in Molecular Materials. Gordon Research Seminar, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?id=17157

13-14 August 2016
Defects in Semiconductors. Gordon Research Seminar, New London, NH, USA.
http://www.grc.org/programs.aspx?id=16480

13-14 August 2016
Synaptic Transmission. Gordon Research Seminar, Waterville Valley, NH, USA.
http://www.grc.org/programs.aspx?id=16672

14-19 August 2016
Biomineralization. Gordon Research Conference, Girona, Spain.
http://www.grc.org/programs.aspx?id=11012

14-19 August 2016
Conductivity & Magnetism in Molecular Materials. Gordon Research Conference. South Hadley, MA, USA.
http://www.grc.org/programs.aspx?id=16768

14-19 August 2016
Defects in Semiconductors. Gordon Research Cpnference, New London, NH, USA.
http://www.grc.org/programs.aspx?id=11966

14-19 August 2016
Synaptic Transmission. Gordon Research Conference, Waterville Valley, NH, USA.
http://www.grc.org/programs.aspx?id=12757

14-19 August 2016
Molecular Structure Elucidation. Gordon Research Conference, West Dover, VT, USA.
http://www.grc.org/programs.aspx?id=17262

14-19 August 2016
Advances and Challenges in Multimodal
Characterizations of Functional Materials, Cancun, Mexico.
https://www.mrs-mexico.org.mx/imrc2016/index.php

15-19 August 2016
X-Ray Microscopy Conference 2016 (XRM2016), Oxford.
http://www.xrm2016.com/

21-24 August 2016
12th International Conference on Biology and Synchrotron Radiation (BSR), SLAC National Accelerator Laboratory, CA, USA.
https://conf-slac.stanford.edu/bsr-2016/

21-26 August 2016
BCA/CCP4 Summer School in Protein Crystallography, Didcot.
http://www.diamond.ac.uk/Home/Events/2016/BCA-Summer-School.html

21-26 August 2016
Joint European Magnetic Symposia (JEMS), Glasgow.
http://jems2016.iopconfs.org/home

22-23 August 2016
International Conference on Structural Biology, New Orleans, LA, USA.
http://structuralbiology.conferenceseries.com/events-list/hybrid-approches-for-structure-prediction

22-26 August 2016
Joint European Magnetic Symposia (JEMS), Glasgow.
http://jems2016.iopconfs.org

22-26 August 2016
Powder Diffraction School. Modern Synchrotron Methods, Villigen, Switzerland.
https://indico.psi.ch/conferenceDisplay.py?confId=2592

23-26 August 2016
International School on Charge and Spin Density: From Experimental Determination to Interpretation, Nancy, France.
http://crm2.univ-lorraine.fr/lab/education/congres/ecm30-congress-satellite-school/

28 August – 1 September 2016
European Crystallographic Association Meeting, Basel, Switzerland.
http://ecm30.ecanews.org/ecm2016/home.html

31 August – 3 September 2016
Chemical Biology 2016, Heidelberg, Germany.
http://www.embl.de/training/events/2016/CHB16-01/speakers_gallery/index.html

3-8 September 2016
FEBS2016. 41st FEBS Congress, Ephesus, Turkey.
https://www.febs2016.org/

4-8 September 2016
SMARTER 5. Fifth Structure elucidation by combining Magnetic Resonance, Computational Modelling and Diffraction, Bayreuth, Germany.
http://www.smarter5.uni-bayreuth.de/de/index.html

4-8 September 2016
XTOP 2016 – 13th Biennial Conference on High-Resolution X-Ray Diffraction and Imaging, Brno, Czech Republic.
http://xtop2016.sci.muni.cz/

4-9 September 2016
The 54th European High Pressure Research Group (EHPRG) International Meeting on High Pressure Science and Technology, Bayreuth, Germany.
http://www.ehprg2016.org/

4-9 September 2016
The 16th International Conference on Liquid and Amorphous Metals (LAM-16), Bonn – Bad Godesberg, Germany.
https://dlr-mp.meetingmasters.de/LAM16

5-7 September 2016
Science@FELs, Trieste, Italy.
http://www.elettra.eu/Conferences/2016/Science_at_FELs/

5-8 September 2016
Quasielastic neutron scattering QENS 2016, Berlin, Germany.
http://www.helmholtz-berlin.de/events/qens-2016/index_de.html

7-10 September 2016
Actin in action: From molecules to cellular functions. EMBO | EMBL Symposium, Heidelberg, Germany.
http://www.embo-embl-symposia.org/symposia/2016/EES16-06/index.html

7-11 September 2016
Polymorphism, stability and phase transitions in crystals. AIC International Crystallography School 2016, Rimini, Italy.
http://www.cristallografia.org/aicschool2016/eng/detail.asp?idn=1854

8-9 September 2016
WINS2016: Workshop on Inelastic Neutron Spectrometers, Berlin, Germany.
http://www.helmholtz-berlin.de/events/qens-2016/wins-2016/index_de.html

11-15 September 2016
5th International Conference on Metal-Organic Frameworks & Open Framework Compounds (MOF 2016), Long Beach, CA, USA.
http://www.mrs.org/mof-2016/

11-15 September 2016
International Beam Instrumentation Conference IBIC 2016
http://www.ibic2016.org/

11-16 September 2016
MEDSI2016. Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation, Barcelona, Spain.
https://indico.cells.es/indico/event/42/

12-14 September 2016
AEM2016, Guildford.
http://www.aem2016.com/

12-20 September 2016
Protein expression, purification, and characterization (PEPC10), Hamburg, Germany.
http://events.embo.org/coming-soon/index.php?EventID=pc16-22

14-16 September 2016
Murnau Conference 2016, Murnau, Germany.
http://www.murnauconference.de

14-17 September 2016
5th Joint Workshop on High Pressure, Planetary and Plasma Physics (HP4), Hamburg, Germany.
https://indico.desy.de/conferenceDisplay.py?confId=14266

19-24 September 2016
Diamond Synchrotron Radiation School, Oxford.
http://www.diamond.ac.uk/Home/Events/2016/SR-Summer-School.html

22 September 2016
Debye-Rietveld Symposium, Amsterdam, The Netherlands.
https://debye-rietveld.nl/?page_id=16

25 September – 2 October 2016
3rd European Crystallography School (ECS3), Bol, Croatia.
http://3rdeuropeancrystallographyschool.weebly.com/

29 September – 1 October 2016
19th Heart of Europe Biocrystallography Meeting, Warberg, Germany.
http://www.helmholtz-hzi.de/de/aktuelles/veranstaltungen/hec_19_meeting/overview/

2-7 October 2016
International Workshop on Nitride Semiconductors (IWN 2016), Orlando, FL, USA.
http://www.mrs.org/iwn-2016

2-7 October 2016
Retinal proteins. EMBO Conference, Potsdam, Germany.
http://events.embo.org/16-retinal-proteins/

3-4 October 2016
Current Challenges in Integrated Structural Biology, Strasbourg, France.

3-7 October 2016
International Workshops on Accelerator Alignment (IWAA2016), Grenoble, France.
http://www.esrf.eu/home/events/conferences/area-events/esrf-events-list/iwaa-2016.html

3-7 October 2016
The 4th International Conference on Competitive Materials and Technology Processes, Miskolc-Lillafured, Hungary.
http://www.ic-cmtp4.eu/

5-8 October 2016
Methods and Techniques in structural biology: beyond black boxes. Season 2, Strasbourg, France.
https://isb-bbb2016.sciencesconf.org/

9-14 October 2016
Autumn School on Microstructural Characterization and Modelling of Thin-Film Solar Cells, Akademie Schmöckwitz (southeast Berlin).
http://www.helmholtz-berlin.de/events/autumn-school/index_de.html

17-19 October 2016
International Conference on Applied Crystallography, Houston, TX, USA.
http://crystallography.conferenceseries.com/

17-24 October 2016
Solution scattering from biological macromolecules. EMBO Practical Course, Hamburg, Germany.
http://events.embo.org/coming-soon/index.php?EventID=pc16-20

21-22 October 2016
International Research Conference on Structure and Thermodynamics of Oxides at High Temperature, Davis, CA, USA.
http://thermo.ucdavis.edu/stoht16/

7-11 November 2016
Biomolecular interaction analysis 2016: From molecules to cells. EMBO Practical Course, Porto, Portugal.
http://events.embo.org/coming-soon/index.php?EventID=pc16-18

14-15 November 2016
De-Mystifying X-ray Data Processing in Macromolecular Crystallography, London.
https://www.biochemistry.org/Events/tabid/379/Page/1/MeetingNo/TD008/view/Conference/Default.asp

16-18 November 2016
GISAXS2016, Hamburg, Germany.
https://indico.desy.de/conferenceDisplay.py?confId=14264

25 March – 2 April 2017
16th BCA/CCG Intensive Teaching School in X-Ray Structure Analysis, Durham.
http://community.dur.ac.uk/durham.x-ray-school/staff.htm

10-13 November 2017
BCA Spring Meeting, Lancaster.
http://www.crystallography.org.uk/bca-spring-meeting-2017-programme-committee/

Thank you to all exhibitors at

BCA Spring Meeting 2016

1. AlphaBiotech
2. Bruker
3. Cambridge Crystallographic Data Centre
4. Douglas Instruments
5. Excillum
6. Formulatrix
7. Incoatec
8. MiTeGen
9. Molecular Dimensions
10. Oxford Cryosystems
11. PANalytical
12. Rigaku Oxford Diffraction
13. SciMed
14. STOE
15. Taylor and Francis
16. Thermo Fisher

30th Meeting of the European Crystallographic Association

28 August – 1 September 2016
Congress Center Basel, Switzerland

COME TO BASEL

ABSTRACT SUBMISSION DEADLINE: April 6th 2016

50 MICROSYMPOSIA

in 5-6 parallel sessions of Biology • Chemistry • Materials • Mineralogy • Physics

Focus Area 1 (SIG 1)

- SAXS in structural biology
- Development of new types of sample preparation
- Data collection and processing software
- New developments in phasing and refinement
- Structural information in drug design
- Molecular machines and big complexes
- Protein & glycobiology structure determination
- Membranes and membrane interacting proteins
- Enzyme reactions and dynamics in crystals
- H-bonding & weak interactions in crystals
- Hybrid approaches and validation
- Biophysical characterization and crystallization
- Hot structures in biology

Focus Area 2 (SIG 5, 11, 12)

- Biomineralogical crystallography & bioinspired inorganic materials
- Minerals and materials
- Structure-property relationships in high pressure crystallography
- Crystal chemistry of C-bearing materials & minerals at extreme conditions
- Structural studies of meteoritic, extra-terrestrial, & planetary materials
- Solid state oxygen fuel cell, hydrogen storage & battery materials
- Materials for energy conversion and harvesting
- Structural disorder & materials' properties at ambient & non-ambient conditions

Focus Area 3 (SIG 2, 3, 4)

- Beyond multipolar refinement
- Charge and spin density of materials at extreme conditions
- Inorganic and metal-organic magnetic structures
- Quasicrystal and approximant: structure and properties
- Incommensurate modulated and composite phases
- Dynamical refinement of electron diffraction data
- New approaches in electron crystallography

Focus Area 4 (SIG 7, 13)

- Molecular interactions in crystal packing and molecular assemblies
- Hydrogen bonding from theory to applications
- Crystal energy landscapes: computation and uses
- Polymorphs, cocrystals, solvates, salts: a jungle for scientists & industries
- Hot structures of small molecules
- Molecular recognition, supramolecular chemistry & crystal engineering
- Simulation of dynamics in molecular compounds
- Crystallography in solid state reactions and catalysis
- Molecular compounds & MOFs at ambient conditions & under high pressure
- Nanomaterials & graphene

Focus Area 5 (SIG 6, 8, 9)

- X-Ray diffraction on the µs to ps time scale
- New detectors for high energy x-ray applications
- The use of X-ray, electron and neutron scattering in nanoscience
- Advances in neutron scattering under non-ambient conditions
- Combining x-ray diffraction and other techniques for *in situ* and *in operando* studies
- Total scattering: pdf analysis & diffuse scattering
- Measuring data quality
- Computational tools for theoretical chemistry in crystallography

General Microsymposia

- Contributions to and of crystallography
- Teaching & education: Linkedin, Google scholar, etc.
- Crystallography in art and cultural heritage
- How to…: crystallization for small and large molecules
- History of ECA, history of crystallography

Plenary Speakers


Ada Yonath


Jean-Marie Lehn

Keynote Speakers

Jan Pieter Abraham, Basel University, Switzerland
Bob Cernik, University of Manchester, UK
Birger Dittrich, Georg-August-University Göttingen, Germany
Robert von Dreele, Argonne National Laboratory, USA
Francesca Fabbiani, Göttingen, Germany
Petra Fromme, Arizona State University, USA
Makoto Fujita, University of Tokyo, Japan
Sandra W. Jacob, Novartis Pharma AG, Basel, Switzerland
Sven Lidin, Lund University, Sweden
Marcus Neumann, Avant-garde Materials Simulation, Freiburg, Germany
Gabor Oszlanyi, Academy of Sciences, Budapest, Hungary
Simon Parsons, University of Edinburgh, UK
Werner Paulus, Montpellier, France
Martin U. Schmidt, University of Frankfurt, Germany
Peter Schurtenberger, Lund University, Sweden
Olivier Thomas, Aix-Marseille University, France

Responsibles Focus Areas 1 – 5:
Michael Hennig (Basel), Piero Macchi (Bern), Jürg Schefer (PSI), Katharina M. Fromm (Fribourg), Radovan Cerny (Geneva)

Basel 2016 ECM-30

http://ecm30.ecanews.org/ecm2016/home.html

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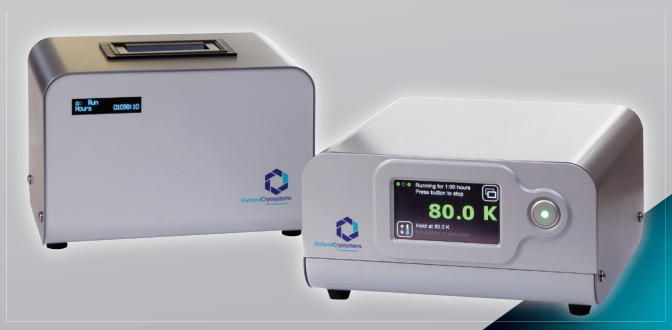

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