

Crystallography News

British Crystallographic Association



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**Dorothy Hodgkin,
Structural Biology and Drug Discovery**

Beautiful Crystals
Beautiful People
Beautiful Structures
& Beautiful Applications

Beautiful Crystals

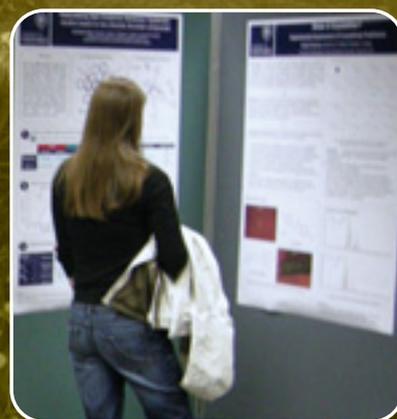
Beautiful People:
Dorothy Hodgkin

Beautiful Structures:
Insulin

Chemical Tool
or Drug?

Dorothy Hodgkin Lecture
BCA York March 2015

Tom Blundell
Cambridge



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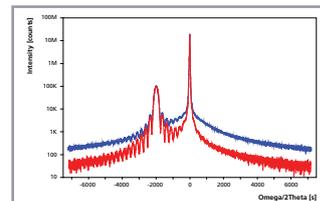
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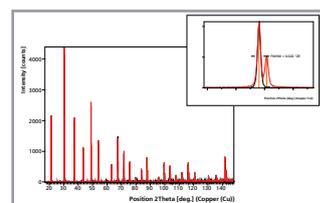
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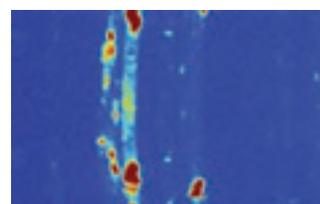
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This month's cover:

*New YC Committee,
outdoor & indoor scenes,
Dorothy Hodgkin slide
(courtesy of Tom Blundell)*



From the President



THIS is my first column for *CN* since taking on the position of President of the BCA at the Spring meeting in York. I look forward to working with the crystallography community in the UK and to representing that community. This first column presents an opportunity to introduce myself and to look ahead to what I would like to see the BCA achieve and represent.

An appropriate point to start is in thanking the outgoing BCA Council members, notably my predecessor **Dave Keen**, who I'm pleased will be remaining on Council in an advisory role as BCA Past President, **Simon Parsons**, who completes his term as Ordinary member, **Sam Callear**, as Education and Outreach Officer and **John McGeehan** as representative of the Biological Structures group. Incoming Council members (other than me) are **Mark Senn** (Oxford) as Ordinary member, **Simon Coles** (So'ton) as Education and Outreach Officer and **Mark Roe** (Sussex) representing Biological Structures. I look forward to working with them and with the continuing Council members.

Taking on this position made me reflect a little on my own career and the central role crystallography has played, and also read more about the founding of the BCA. The BCA was founded in 1982, following a sequence of meetings over two years by members of a working party established to bring together the interests of the different crystallographic constituencies, and held its inaugural meeting in Durham in April 1982. The events that led up to the founding of the BCA were later documented in an article by the chair, **David Blow**, and secretary, **Stephen Wallwork**, of that working party, entitled "The Prehistory of the BCA" (*Notes Rec. R. Soc. Lond.* **58** (2), 177–186 (2004), doi 10.1098/rsnr.2004.0054) and can be found at <http://rsnr.royalsocietypublishing.org/content/58/2/177>.

Notably, Stephen Wallwork (Nottingham) celebrates his 90th birthday in early May (around the time of my writing this column) and I sincerely hope that we will be able to welcome him to the 2016 BCA meeting, which will be held in Nottingham.

Coincidentally, I began my first research in crystallography in 1982, as an undergraduate working in **Guy Orpen's** lab at Bristol, where we shared lab space with **Judith Howard** and **Peter Woodward's** groups. The first scientific meeting I attended and at which I presented a poster was in fact a BCA meeting, in 1984 in Nottingham. Following my PhD, I spent almost 15 years in the USA, first as a postdoc, and then in an academic position at University of Missouri-St. Louis, before returning to the UK to my position at Sheffield. Although I had no involvement in the BCA during my time away, I was involved with the ACA, as Secretary and as a member of the USNCCr, and with the IUCr as a member of the Structural Chemistry Commission for 9 years and co-editor of *Acta Cryst B* for 12. So, there are many people who know much more about the BCA than I do, and I will seek their advice and help, but I hope my prior experience with other crystallographic organisations will provide me with some valuable experience that I can bring to my new role at the BCA. Scientifically the last three decades has seen an evolution in my own interests from beginnings as a small molecule crystallographer to engaging in research that involves a combination of synthesis and various methods of characterisation of molecular materials with emphasis on understanding intermolecular interactions, studies of porous

materials (notably metal-organic frameworks) and dynamic processes, such as chemical reactions in crystals.

The path of my own career and research interests reflects the fact that I am a chemist as well as a crystallographer, but is also tied to the advances in software and hardware that have propelled crystallography as a discipline. Crystallography has always been at the heart of what I have been involved in, but the nature of that work has changed almost beyond recognition since I was a student.‡ I've also come to value the pivotal role played by large facilities in crystallography, having relied upon neutron diffraction in the early part of my career and on synchrotrons for both single crystal and powder diffraction in the past decade. With the past two years having been a period of celebration of the centenary of the crystallography, and a chance to reflect on where we have come from, I think it is also important to realise that future looks very bright, not least from advances in new synchrotron and spallation neutron facilities and the advent of free-electron lasers. I strongly feel that there are also real opportunities in the future for combining crystallography with other means of characterisation. To some extent this is already evident from work combining diffraction with spectroscopy, electron microscopy and computational studies, but we are at a very early stage. I hope to encourage links between crystallographers and other communities through which common interests might be pursued and would encourage such links to be developed within the BCA Spring meeting and the Subject group meetings.

One Spring meeting has not long finished, and I am grateful to Programme Chair **John Helliwell** and his committee, and to members of BCA Council, particularly **Richard Cooper**, for their efforts in making it an excellent meeting in York. Planning for the next meeting (Nottingham, 2016) is already underway, and will be led by Programme Chair **Phillip Lightfoot** (St. Andrews). For those unfamiliar with the planning cycle, the main planning meeting will occur in late June at which the symposia for next year are expected to be agreed, and discussions will take place regarding plenary speakers and some invited speakers for the symposia. Announcements of the outline programme should appear in the September issue of *CN*.

The BCA represents the entire UK crystallographic community and I am keen to see high levels of engagement and input into the Spring meeting and the Subject group meetings (see the BCA website to contact your Subject group representatives). I was very pleased to see such engagement in the discussion that took place at the AGM, attended by about 150 people, during the Spring meeting in York, and I hope that many went away better informed about the BCA, both its history and its current status and challenges. The past two years of crystallography centenary celebrations have provided an opportunity to enhance and develop the outreach and education activities of the BCA, and I am grateful to my predecessor Dave Keen for encouraging this, and to Sam Callear and her colleagues for leading the efforts in this area. I have already spoken to incoming O&E Officer Simon Coles, who has lots of ideas for further outreach activities and I want to encourage those of you with ideas or a willingness to get involved to contact Simon and get involved. I hope that the BCA will be able to build upon the many excellent activities of the recent years.

Lee Brammer

‡. Although this sounds like an opportunity to launch into the crystallography version of the Monty Python "Four Yorkshiremen", I will refrain.

BCA Council 2015

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

From the Editor



AS I write this column, memories linger of a very successful and enjoyable BCA Spring Meeting in York. I thought that the high number of joint sessions, where relevant insights from one branch of crystallography informed practitioners of another branch, clearly demonstrated the benefits of getting the entire BCA together for a meeting. Next year's meeting

will take place in Nottingham from 4-7 April.

Of course, we won't have to wait that long for more good meetings. First up, our own Industrial Group will hold its XRF meeting on 17 June at the University of Leicester. An impressive set of presentations has already been arranged, with more to come. Details are available on the IG website. If you want an additional application of XRF, read on...

Next comes the meeting of the American Crystallographic Association from 25-29 July in Philadelphia. Conveniently for participants from the UK, the eastern location means a time difference of only 5 hours. Therefore we should still be able to enjoy social events in the evening but wake up bright and early for the next day's first lecture (at 8 AM!). Take a look at the conference logo, which cleverly integrates crystallographic notation with Philadelphia's most iconic artefact, the Liberty Bell. Philadelphia has a distinguished association with crystallography: although **Arthur Lindo Patterson** was peripatetic in his early years, including the time when he developed his famous function, for most of his scientific career he worked in the Philadelphia area.

As for the Liberty Bell, it was ordered from the renowned Whitechapel Bell Foundry in England by the Pennsylvania Provincial Assembly in 1751. As an inscription it carried the Biblical text "Proclaim LIBERTY throughout all the Land unto all the Inhabitants thereof". Tested in Philadelphia after a rough sea crossing, it cracked with the first stroke of the clapper. Astonishingly, two local craftsmen, the iron founder **John Pass** and the brass founder **John Stow**, were entrusted with recasting the precious 945 kg bell. After carefully taking a mould of the bell and its inscription, Pass and Stow broke it up with sledgehammers and remelted the pieces. The standard recipe of the time called for a bronze with about 77% copper and 23 % tin. A higher concentration of copper made the metal too soft, while more tin made it too brittle. Guessing that the original bell cracked because it had too much tin, Pass and Stow added copper. Their recast bell was stable enough and had an imposing appearance, but an observer recounted that "it sounded like two coal scuttles banged together". Embarrassed, Pass and Stow cast the bell once again after raising the tin content. Lacking pure tin, they did this by adding scrap pewter which also contained lead. The new version of the bell sounded better and gave good service for a few decades, but then it developed the crack that in some ways has made it even more famous. There are several legends about the occasion when it cracked, but all that is known for certain is that it happened sometime between 1817 and 1846. Since a set of church bells in Ipswich dating

from as early as the 1450s can still be safely rung, the failure of the Liberty Bell after less than a century of use suggests metallurgical problems. Chemical analysis of a small sample of shavings drilled from near the crack showed 73.1% Cu, 24.0% Sn, 1.3% Pb, 0.28% Ni, 0.25% Ag, 0.25% Zn and 0.05% Fe. Thus there was a bit too much tin. However, removing samples from different parts of such a hallowed object to check its uniformity was out of the question. A non-destructive alternative was provided by energy-dispersive X-ray fluorescence carried out *in situ* with radioactive Cd^{109} and Am^{241} as the sources of primary radiation. Reported by Victor F. Hanson, Janice H. Carlson, Karen M. Papouchado and Norman A. Nielsen in *American Scientist*, **64**, 614-619 (1976), such analyses at 10 points around the bell yielded a range of Cu from 64.95 to 69.12%, Sn from 25.20 to 30.16%, Pb from 2.20 to 5.47%, and smaller amounts of 6 other elements. Such non-uniformity is understandable, given that Pass and Stow probably lacked a crucible large enough to hold the full mass of their alloy and had to divide it among several smaller ones. Surprisingly, the lowest concentration of tin was found adjacent to the crack; but perhaps, if the area of impact was the least brittle, this could explain why the bell lasted as long as it did. In 1976, members of the Procrastinators' Club of America picketed the Whitechapel Bell Foundry with signs "We got a lemon" and "What about the warranty?" The foundry replied that they would be glad to supply a replacement bell, provided that the defective one was returned in its original packaging!

In August we can look forward to ECM29, the European Crystallographic Meeting in Croatia. Croatia is well known for beautiful scenery and historic towns, but Croatians also are very crystallography-minded people. The Hrvatska Udruga Kristalografata (Croatian Association of Crystallographers) has approximately 100 members. Proportional to population, that figure means the BCA should have 1500. Let that be an inspiration to us! In 1966 the Yugoslav Centre of Crystallography was established in Zagreb under the auspices of the Yugoslav Academy of Sciences and Arts (notice the order!). After independence Croatia inherited this pre-eminence. Not resting on their laurels, the Croatians have done their utmost to work with distinguished crystallographers from all over Europe to create a really interesting programme.

A satellite meeting for ECM29 looks interesting. Between 20-22 August 2015, ECACOMSIG is organising a two day Computing Workshop on Advanced Software Development for Crystallographers, in Duga Uvala, about 40 km from Rovinj, Croatia. The Workshop will provide an opportunity for younger developers to meet and engage with senior developers and also with their peers in Crystallographic Methods development. Further satellite meetings are listed in this issue.

In conclusion, I wish all our readers an enjoyable and relaxing summer. I hope that you will get some time in the garden or on a beach where you can think about crystallography with no worries about marking exams or writing reports.

Carl Schwalbe

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Puzzle Corner



FILL the grid with four-letter words that match the crystallographic clues. Spell them from left to right in the top row and all odd-numbered rows, but from right to left in even-numbered rows. The last letter of each word forms the first letter of the next word. The final letter of the last word should match the initial letter of the first word. After all this effort, boxes 2, 4, 8, 10, 14, 16, 18 will tell you what time it is.

1	2	
	4	3
5		
		6
7	8	
	10	9
11		
		12
13	14	
	16	15
17	18	
XXXX	XXXX	

1. Smallest unit of an element
3. Prefix for a million
5. Main direction in a unit cell
6. Turns real into reciprocal
7. PDB entry 4HIL comes from these animals
9. School subjects, good background for crystallography
11. Type of spectrometer that distinguishes isotopes
12. Salt of a fatty acid
13. (Clue 3)⁻²
15. Type of map based on a model with part of it left out
17. (Clue 3)²

Answer to March puzzle on page 18

2015 BCA Spring Meeting at the University of York

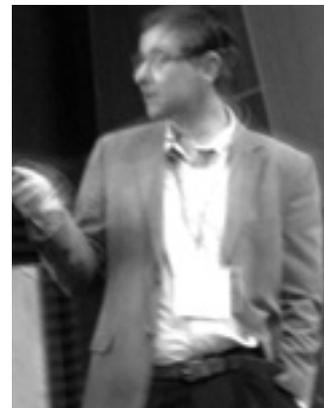
THE full programme featured so many exciting highlights that no one person could adequately summarise them. Therefore I shall confine myself to describing the plenary and prize lectures and allow our bursary recipients to present their (sometimes edited) individual perspectives on the proceedings. I took a lot of pictures of the main speakers, but I must warn you that many of them are blurred because of ADP (the speakers are Always Dynamic Persons).

Plenary Lectures

Tom Blundell started the main meeting by giving the prestigious Dorothy Hodgkin Lecture. Fittingly, he began by paying tribute to the great contributions Dorothy Hodgkin (née Crowfoot) made, both as a scientist and as a person. Proteins were thought incapable of diffracting X-rays until, in 1934, Bernal and Crowfoot showed that pepsin crystals kept wet yielded beautiful diffraction. Her triumphant work on vitamin B12 and insulin followed. When Tom joined the laboratory under Dorothy's versatile leadership, work on insulin was continuing, both at the fundamental level of monitoring its evolution and at the applied level of working with industry to optimise the treatment of diabetes. Turning to the research area where he has made such an impact, Tom described the use of information to design drugs. Structure-guided drug discovery draws on two spaces: biological (new targets found from genomics) and chemical (one's compound library). Targets in biological space include multi-protein assemblies; but these can be difficult because many protein-protein contacts have small but deep pockets, thought to be undruggable. Chemical space can be exploited by rapid structural screening against a crystallisable putative target to identify the mode of binding. Utilising the power of the Diamond synchrotron, 240 compounds have been screened in just a few hours. In the future, we need to acquire more understanding of drug resistance.



In the CCG plenary lecture **Colin Groom** praised the collaborative attitude of crystallographers, who have shared over 750,000 small-molecule crystal structures with the wider community via the Cambridge Structural Database (CSD). He regaled us with fascinating facts and figures that were frequently amusing as well. The first 3-D organic structure in the database was the



phthalocyanine PHTHCY01 in 1936. New structures are currently being supplied by over 10,000 different depositors each year. Usually there are 5-6 authors per structure, but one has 46. Depositors should not be shy about submitting unpublished structures, which are welcome. Unit cell volumes range from 52 Å³ for SACBAA to 702,000 Å³ for OCUNAC. Trends over time show a rapid increase in average formula weight per asymmetric unit for metal-organic compounds but a flat line for organics. Most, but not all, elements are now covered, including He (trapped) and Cf. A significant odd-even disparity in organic structures persists, structures with an even number of carbon atoms being more common. In 2001 the number of low-temperature structures submitted per year first outstripped room-temperature structures. A puzzle is the number of structures submitted at a reported temperature above their melting point – probably due to a mix-up between °C and K. The lowest R factor is 0.7 % for OHEREZ01. The maximum Z' is 24 for IDOSID. For the amusement of people who look for shapes in clouds, Colin showed us structures that look like something else.



That same evening **Gideon Davies** gave the BSG plenary lecture. In fact, his survey of knowledge about reaction pathways of enzymes gained through crystallography was just as fascinating to chemists. In the reaction between enzyme E and substrate S to yield product P, $E + S = ES = E + P$, he concentrated on carbohydrates as substrates. In the 1990s clever choices of S made it

possible to slow the reaction sufficiently that the Michaelis complex ES was trapped. Chair conformations with large distortions were seen. In the specific case of mannose derivatives, chemists have trouble with syntheses because of 1,2-axial steric clashes. The enzyme mannanase manages it with a Michaelis complex in skew-boat conformation, whereby one clashing OH group is equatorial and out of the way.



Conformational analysis of ES facilitates inhibitor design: for instance, Tamiflu has a double bond that imposes the same conformation as the natural substrate in the transition state. Gideon finished by giving the example of linked *N*-acetylglucosamine, O-GlcNAc. Compared to the bewildering variety of kinases and phosphatases, there is only one O-GlcNAc transferase and one hydrolase. Structural analysis of reaction mechanisms has led to mechanism-based inhibitors that are useful probes for the cellular roles of O-GlcNAc. A major cause of Alzheimer's disease is tauopathy, the over-phosphorylation of tau protein leading to tangles. In animal models inhibition of O-GlcNAc hydrolase increases O-GlcNAc and decreases phosphate, also decreasing tangles.

In the PGC plenary lecture **Anthony Cheetham** took a subject dear to chemists, namely MOFs, and showed the valuable information about physical properties that can be extracted. Unusual properties occur such as very high anisotropy or negative thermal expansion. MOFs tend to be much less robust than zeolites, but this very flexibility permits a wide variety of phase transitions.



These include pressure-induced ring-opening in the zeolitic imidazolate framework ZIF-8, which increases the pore volume by $\approx 4\%$, and the transition at 160K in ZIF-4 which leads to a decrease in volume by $\approx 23\%$. A reversible, pressure-induced phase transformation in a dense rare-earth formate proceeds with bond rearrangement. Magnetic phase transitions can be studied by low temperature neutron diffraction; most systems have very low ordering temperatures. Perovskites ABX_3 are solid-state workhorses. With $(CH_3)_2NH_2Zn(HCOO)_3$ hydrogen bond ordering occurs at one temperature, CH_3 rotation ceases at another, and there are magnetic effects besides. $[CH_3NH_3]PbI_3$ is a semiconductor with photovoltaic applications.

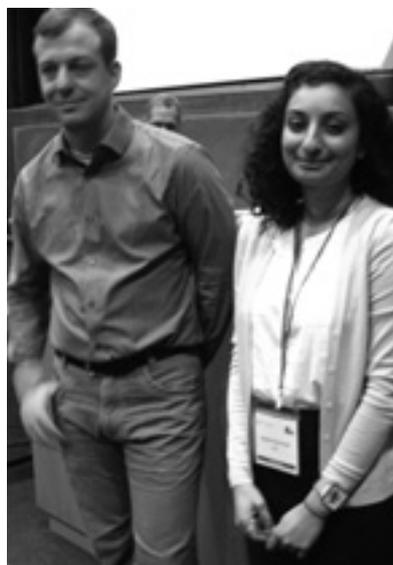
The other named lecture, the Lonsdale lecture, was given by **Simon Parsons**. Simon too discussed the effect of high pressure on the crystalline state, but with regard to molecular crystals. He began with a summary of the impressive career of **Kathleen Lonsdale**. Her analysis of space group symmetry and derivation of structure factor equations led to the International Tables. Remarkably, applying logic to the pattern of strong



Simon Parsons (left) together with speakers from the Complementary Calculations session

reflections without the aid of Fourier synthesis, already in 1929 she published the structure of hexamethylbenzene, showing that it is hexagonal and flat. She made numerous innovations in methodology and coined the term "error dustbin" for misapplied anisotropic displacement parameters. Simon continued with an analysis of the effect of pressure p on the Gibbs free energy G : $\Delta G = \Delta U + p \Delta V - T \Delta S$. Entropy S comes from vibration, and vibrational frequencies can be calculated by DFT, while p and ΔV can be measured. One way to obtain U is Gavezzotti's PIXEL method. Under pressures up to 10 GPa no super-short intermolecular contacts have been observed; phase transitions enable them to be avoided. The aforementioned free energy calculations show that simplistic analysis of distances alone, e.g. in hydrogen bonds, can lead to misleading conclusions.

The final plenary lecture was given by **Peter Chupas** for the IG. Society badly needs materials for energy storage and conversion. With use, existing batteries suffer from undesirable changes in chemical composition and crystallinity leading to dendrite formation and swelling. Nanomaterials enhance Li-ion battery performance, but understanding why physical properties change upon reduction of particle size to the nano-scale remains a challenge. For instance, the reaction $Fe_2O_3 + 6 Li^+ + 6 e^- = ? = 3 Li_2O + 2 Fe$ provides an energy dense storage medium, but the mechanism was uncertain and the broad XRD peaks were little help. Synchrotron data measured with a wavelength of 0.2 Å enabled PDFs to be calculated. Partial fluorine substitution improves the properties. While F^- and O^{2-} are difficult to distinguish with X-rays and neutrons, the different bond lengths are distinctive. Further applications of PDFs measured *in situ* are to understand the formation of nanomaterials and to chase the dynamic structure of working catalysts, e.g. Pt on Al_2O_3 in a catalytic converter.



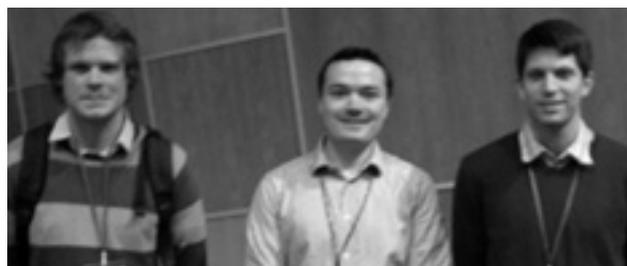
Peter Chupas together with Spoorthi Dharmayat (chair)



Prize Lectures

IN the CCG prize lecture **Nick Funnell** from Oxford presented results obtained from a combination of experimental and theoretical techniques to solve the difficult problem of structure determination on single-layer phases. For the experimental measurements of X-ray total scattering data, high-angle values are essential; and they can be obtained with a laboratory Ag source. The computational approach involves reverse Monte Carlo (RMC) calculations, developed to be applicable to two-dimensional nanosheets. These methods were applied to $[\text{Zn}_2\text{Al}(\text{OH})_2]$ -borate layered double hydroxide nanosheets to find a model that matched the X-ray data. More details can be found in the paper by N. R. Funnell et al. (2014), *Nanoscale*, 6, 8032.

Simon Newstead from Oxford gave the BSG prize lecture on the structural basis for transport and regulation in the POT family of peptide/nitrate transporters. Peptide transporters are very important for nitrogen absorption. Transport of di- and tripeptides across the brush border membrane is faster than that of single amino acids. The transporter can handle ≈ 8000 different oligopeptides and can also transport drugs. With a molar mass of 74 kDa it has 12 transmembrane helices. Simon attempted to elucidate the structural basis of its promiscuity. The peptide binds near the middle of this highly dynamic protein with multiple conformational states; once the peptide and H^+ have bound, access to the interior is opened. The inward-open structure has been solved, and the outward-open structure has been modelled.



L-R: Jonathan Skelton, Simon Newstead, Nick Funnell.

The IG/YC prizewinner, **Jonathan Skelton** from Bath, talked about temperature-dependent material structure and properties from *ab initio* lattice dynamics, to give an atomistic view of thermal motion and information about thermodynamics along with structure and properties. The basic assumption is the harmonic approximation, and the key requirement is to know force-constant matrices. Phonons and the density of states can be compared with results of IR and Raman spectroscopy. From phonon frequencies, thermal displacement matrices for a given temperature can be calculated. These techniques were applied to sulfamerazine polymorphs. Analogous work on lead chalcogenides has been published in J. M. Skelton et al. (2014) *Phys. Rev. B*, 89, 205203.

Having heard these excellent lectures, I would be not at all surprised to see these Prize Lecturers come back as Plenary Lecturers some years hence.

Carl Schwalbe

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Bursary Reports

AFTER a four and a half hour long journey from Oxford I arrived at the University of York for the BCA Spring Meeting. Immediately I was immersed in the YCG Satellite Meeting. **Chick Wilson** gave a very dynamic and engaging plenary lecture about his decades of research on developing crystal engineering methods that allow his group to make predictions on molecular associations. I was also particularly drawn to talks by **Will Fletcher** and **Briony Yorke** in the second YCG session since they both presented mathematically orientated method developments within their respective areas of research.

At the YCG AGM I stood unopposed for the position of Vice Chair, a position which I hope to fulfil to the best of my ability and further integrate myself into the crystallographic community. The meal and drinks afterwards gave me a chance to network with other young crystallographers and a chance to get to know the other committee members better.

The next day saw the end of the YCG portion of the meeting and the beginning of the main meeting, where I could see some of the people I wanted to meet with regards to helping me with my own research progress. In particular I managed to meet **Graeme Winter** for the first time. I had been in contact with him about how the DIALS project could be used to help me with my own work. Coincidentally the first workshop was given by **David Waterman** who presented progress on the DIALS project.

The very next session was the BSG Data Acquisition session which was chaired by **Elsbeth Garman**. In this session I gave a talk on how the data collection experiment is modelled with RADDOSE-3D and also gave preliminary results on my reflection intensity correction model. The talk achieved its purpose; in particular **Gerard Bricogne** of Global Phasing was very interested and has expressed interest in collaborating with me on improving the intensity correction model.

The next two days covered a variety of topics in the BSG sessions including sessions on ligand chemistry, data mining, simultaneous use of EM and MX data and low resolution refinement. **Alan Brown** gave a fantastic and clear presentation on the structure solution of the ribosome from cryo-EM maps and **Eleanor Dodson** delivered a very engaging talk about the considerations that need to be taken into account during the refinement of low resolution structures.

The BCA AGM was a lively meeting with much discussion that lasted for 90 minutes, 30 more than scheduled.



Speakers and chairs for 'Ligand Chemistry' symposium

Afterwards, we headed straight to the delightful conference dinner. The evening entertainment consisted of a ceilidh which lasted until the early hours of the morning.

Overall it was a brilliant conference. I gained valuable experience through delivering an oral presentation, became a member of the YCG committee and started a new collaboration. This was definitely worthwhile and I am grateful to Rigaku for the bursary which gave me the opportunity to attend the conference and take another step in my development as a researcher.

Jonathan Brooks-Bartlett
University of Oxford

DIALS Workshop Summary

David Waterman gave a presentation on the DIALS (Diffraction Integration for Advanced Light Sources) software that is currently being developed between two groups: DIALS West and DIALS East. DIALS West is represented by Nick Sauter's group in Berkeley USA and DIALS East is represented by groups in the UK headed by Gwyndaf Evans and Graeme Winter at Diamond Light Source. DIALS aims to be a single software distribution that can be used to process diffraction images that are and will be generated by a series of detectors at various advanced light sources including XFELs and synchrotron sources. It is open source and is available for use by the crystallographic community. It also aims to be flexible and fast. The algorithms in the software are still being extended and improved and much discussion in the session was centred on profile fitting of reflection intensities and the global parameterisation of the diffraction experiment.

Jonathan Brooks-Bartlett
University of Oxford

THE YCG meeting started out with an unexpected cancellation, leaving **Jerome Wicker** (Oxford) to take the place of our plenary speaker, a job he performed admirably. Talks ranged from predicting crystallinity, asthma drugs, and frustrated magnets. **Sam Horrell** (Liverpool) showed us – in disgusting detail – the importance of biofilms in everyday life, and the session was closed with the best use of props of the day which lead very nicely onto the poster reception, and wine...

For me, the highlight of the YCG was **Anna Warren** (Diamond) discussing how to get the most of your single crystals. As a



Speakers and chairs for 'Automation' symposium

powder neutron diffraction user, I had never appreciated how difficult it can be to grow and collect single crystal X-ray data or how much X-ray crystallographers brutalise their samples. Particularly jarring was the shooting gallery of damaged crystals after the experiment. The truly impressive thing to me was the level of automation that the scientists and support staff at I24 have set up. I guess it's needed when you can take a diffraction pattern in one second.

The YCG was particularly well organised,; even the last minute cancellation didn't seem to ruffle the organisers' feathers. I think they all deserve a pat on the back and several stiff drinks.

This was my first BCA meeting, and the most pleasant surprise was provided by the named lectures. It's very easy to get caught up in the accomplishments of prominent scientists and forget that they had (in these cases very interesting) private lives. The Dorothy Hodgkin and (Kathleen) Lonsdale lectures managed to mix personal anecdote and history of scientific discovery with the continuing relevance of the work. For me the mix of personal and scientific history was a refreshing change to see.

Of the sessions I attended, the one that caused the greatest rush of questions was **Claire Murray's** (Diamond) introduction of long duration experiments at I11. The ability to look at materials over weeks, months and even years seems to have piqued many people's interest, as did the range of sample environments that could potentially be available. This seems to be a project that will be guided by the individual user's needs; and the level of care that has been put into redundancies, contingencies for power cuts and avoiding cross contamination seems to have satisfied the crowd. The lecture was held on the 31st of March. With the application deadline of the 1st of April, I wonder how many panicked applications were written that night.

Milen Gateshki's (PANalytical) discussion on x-ray studies on nanocrystalline materials using lab based sources showed how (given enough time) local x-ray diffractometers can give results comparable to synchrotron sources. And, with the interest in long duration experiments at I11 high, that there is the option of carrying out long-term diffraction studies at your home institution.

The BCA meeting gave me a greater appreciation of the complexity and flexibility of X-ray diffraction, and a better understanding of how it complements (and is complemented by) neutron diffraction.

I would like to thank the YCG and the EPSRC Directed Assembly Grand Challenge Network for the financial support, and for the chance to present my work.

Helen Duncan
Queen Mary, University of London

THE first speaker on Monday, 30th March, was Jerome Wicker at the Young Crystallographers' satellite meeting. His great talk presented his recent work using a machine learning approach to predict crystallinity of small molecules. It gave a good taste of what we had to look forward to for the rest of the conference.

The main meeting started the next day with the Dorothy Hodgkin Lecture in which Professor Sir **Tom Blundell** gave an incredibly interesting talk on his work with Dorothy Hodgkin on structural biology and drug discovery. The first session then started after lunch with several thought-provoking talks on the problems caused by the recent dramatic decrease in read out times of detectors and the consequential overload of data.

The delicious buffet dinner in the evening provided everyone with the opportunity to catch-up and discuss the first day's talks. There were also several posters on display and it was great to be able to wander around and see what other students were working on.

The conference carried on in the same format for the next two days with talks ranging from automation in chemical crystallography to drug discovery. I particularly enjoyed the CCG discussion session 'Would you publish this?' on Thursday morning as it was great to hear all the different opinions on current research.

The conference dinner marked the end of this year's Spring Meeting and several awards and poster prizes were presented to students before a ceilidh got underway. Overall it was a really stimulating conference. It was fascinating to learn about so many different areas of crystallography during the week, and it provided me with some new ideas for my own project.

Sophie Gearing
University of Oxford

ARRIVING in York, as a number of us did, off the back of a pretty gruelling eight days in Durham, it could have been hard to get excited about another jam-packed week of crystallography... However, thanks to a busy and surprisingly varied conference programme, this happily was not the case!

The meeting theme of "Data" necessarily lent itself to an even wider variety of contributions than normal, with a significant number of talks focussing on advances in software, hardware and the growing importance of computational methods and complementary calculations.

As usual, the week got off to a great start on Monday at the Young Crystallographers satellite. With a total of 14 speakers and several posters over the two days, many younger scientists took the chance to showcase their work. On Tuesday morning the Parkin Lecture was awarded to **Anna Warren**, whose presentation took the form a tutorial introducing the current state-of-the-art techniques now available for MX experiments at Diamond. Anna highlighted the growing challenge we now face to streamline data analysis routes, in light of the ultra-fast data collections that are now routine on many beamlines. The challenge of dealing with this growing volume of data was a topic set to recur many times during the course of this Spring Meeting.

Tuesday afternoon saw two sessions focussed on this same issue: while the first CCG symposium was devoted to finding ways to organise and compare this "avalanche" of data once we have it, the second discussed the growing need to automate many of the steps in our crystallographic experiment, to help us keep pace with the speed of data collection. While promising throughout his Keynote that automation wasn't



Speakers and chairs for 'Data Avalanche' symposium

always something to fear(!), **Graeme Winter** joined Anna in outlining what the chemical community might learn from the automatic procedures that are already routine in the MX world.

The CCDC had caused quite a stir in the exhibition hall with their new 3-D printing module and, on Wednesday morning, **Nick Funnell** (winner of the CCDC-CCG award) made a number of people jealous by being the first to receive a 3-D printed molecule as his prize during the Early Career Award Symposium! In the same session, **Simon Newstead** and **Jonathan Skelton** also presented their exciting work as recipients of the BSG and IG-YCG prizes respectively.

After some spirited debate at the AGM followed by some even more spirited ceilidh-ing at the conference dinner, the final morning was a quieter affair! In spite of this, the introduction of "Would You Publish This", inspired by similar sessions held at the ACA, proved popular during the last session and all of the contributions sparked animated discussion.

Finally, the excellent food and hospitality from the conference team at the University of York were undoubtedly major contributing factors to what was a very enjoyable meeting, and I look forward to the chance of visiting again at some point in the future!

Lauren E. Hatcher
University of Bath

THE BCA Spring Meeting was once again a fantastic meeting, exhibiting in both the symposia and the evening poster sessions, the wide variety of research being undertaken within the UK crystallographic community.

The 2015 programme commenced with the YCG satellite meeting, which began with an insightful talk from **Jerome Wicker**. On the topic of 'Will it crystallise?' he showed that an accuracy of 94% can be achieved in predicting compounds' crystallinity through the use of just 2 descriptors. Subsequent talks throughout the afternoon covered a wide variety of topics affording very dynamic sessions. Highlights included the 'wine rack' continuous breathing behaviour in a MOF from **Elliot Carrington** and the applications of computational modelling and theoretical studies as demonstrated by **Will Fletcher** revealing crystallography without crystals; pair distribution functions were used to model protein crystal structures and he achieved some impressive structures.

Between these sessions **Chick Wilson** gave an excellent plenary lecture discussing the journey through crystallisation including the use of predictions for molecular self-assembly, the necessity to assess potential competing interactions as well as the difficulties faced when more and more variables are introduced into a system.

The Parkin Lecture, given by **Anna Warren**, kicked off the second day and provided an insight into the future with advances in the field. Merely seconds are required for full data collections and hence continuous crystal rotation, open shutters and continuous readouts are required; much more data and on many more samples can be obtained within a given time. **Bill Clegg** and **Mike Glazer** closed the satellite meeting 'voyaging into orbit', entering 'into deeper space' with a highly interesting teaching-focussed session revolving around space groups.

The main meeting, too, provided a plethora of interesting topics ranging from the highly scientific prize lectures of **Nick Funnell**, **Simon Newstead** and **Jonathon Skelton**, and **Richard Cooper's** take on 'squeeze harder'. Further information and current developments of the CSD were given by **Suzanna Ward** and **Colin Groom** in two highly informative talks. The recommendation emerged that to get your structure viewed more you need an interesting refcode or one which starts with the letters A to D; beyond D, the commitment to the search tails off dramatically.

Another interesting talk was that by **Juliette Pradon** discussing the trials and tribulations faced when taking the CSD and crystallography out to the Democratic Republic of Congo. Many things that would seem normal or assumed here, such as electricity and internet supply, computer and software access, students turning up on time and transport, had to be accounted for and worked around before even considering the delivery of the material.

Simon Parsons gave an engaging Lonsdale Lecture, including details on Kathleen's life, work and activities before developing the theme to his studies using high pressure crystallography in amino acids investigating the interactions and their nature. This was followed by the conference dinner, an evening of excellent food, wine and the crystallographers' ceilidh.

The final day of the BCA meeting focussed around data, in particular problem data, and the final session allowed anyone to present problem structures to the floor to ask for advice as to what to do to progress. I felt this was a fantastic idea for a session, allowing others' problems to be realised, which may



Speakers and chairs for 'Problem Data' symposium

be applicable to your data too, whilst the presenters obtained useful comments on what they can do to progress their structure(s).

I would like to thank the ICDD for the bursary helping me to attend this meeting, from which I gained a deeper appreciation for crystallography and the future, as well as some ideas and thoughts for progressing my work.

Lucy Mapp
University of Southampton

ARRIVING at York after the quick journey down from Durham where I had been attending the 15th BCA/CCG Durham School the previous week, I immediately sensed that this was going to be a lot of fun. Straight off the train I was recognising faces from the previous week and this continued for the rest of the meeting.

It was straight into the first YCG session and despite Professor **Susan Lea** being unable to attend, the session was lively and everyone was well received. This continued in the second session, and it was great to see other young crystallographers speaking so clearly about their work. The YCG AGM followed quickly. Despite some initial concerns, all matters arising were painlessly dealt with in a timely manner. Next it was on to the poster sessions and perhaps more importantly, dinner. After a week of Collingwood College's finest, York had a lot to live up to and they did not disappoint.

Tuesday kicked off with a great talk from Dr **Anna Warren** about recent developments on the MX beamlines at Diamond Light Source and where the current capabilities lie, along with how to make the most of these from a user's perspective. Many of these techniques I had not come across, but they were very interesting as they could be applied to I19, the small molecule beamline that provides half my funding.

It was time to start the main meeting, opened by Professor Sir **Tom Blundell** reminiscing on a rather extraordinary career followed by Dr **Colin Groom's** tour of extraordinary statistics available from the CSD. The afternoon brought with it many interesting talks in the CCG section, but I thought Dr **Graeme Winter's** keynote lecture on automation stood out. Seeing the level of automation now considered standard with MX data processing was almost frightening, and with the suggestion of bringing this to small molecule crystallography you could sense the eyebrows in the room being raised. I'm sure this was the response from the macromolecular world a few years ago but with an open call to the floor for volunteers several willing participants spoke up. Professor **Gideon Davies** rounded out a long day with good humour and a fascinating insight into carbohydrate chemistry and its potential applications.

Wednesday was another busy day and for the afternoon I attended the physical group talks starting off with keynote speaker Professor **Pam Thomas**. The talk centred on lead free piezoelectrics and the extent to which new technologies can rival the industry leader lead zirconate titanate (PZT). On to the next session focusing on complementary calculations and the insights well thought out computer models can give. Professor **Keith Refson** opened the session and, as one of the authors of CASTEP, who better to describe the ever-increasing power of DFT methods. In a great example of

experiment complementing calculations and vice versa to explain and ask more questions of what we thought we already knew, **Claire Hobday** showed how by combining novel high pressure gas experiments with simulations, new phases of even extensively studied systems can still be found. The last talk of the day was the Lonsdale lecture given by Professor **Simon Parsons** in which he challenged us to re-evaluate the importance of geometry on phase stability and instead look at the system as a whole. High pressure studies have emphasised the importance of mapping out the full interactions of one molecule with another using the PIXEL method to gain a more accurate understanding of phase stability. Straight on the back of this was the annual general meeting in which a lot of time was spent on the prickly question of the BCA's membership level to the IUCR. I don't think this reflected the general mood from the rest of the meeting. After a quick change it was time for the conference dinner and the prizes! This was a really fun evening and time really flew by. The official evening might have ended quickly but the party certainly did not.

The last day of my first BCA spring meeting started with problem data and then on to a fun open discussion session of "would you publish this". After all of this it was then on the train back up to Edinburgh. I would like to thank the organising committee for putting together a great program and also Rigaku for sponsoring me to attend; it was really inspiring to be there and I hope it is the first of many spring meetings.

Charlie McMonagle
University of Edinburgh

THE main meeting started with the Dorothy Hodgkin Lecture given by Prof Sir **Tom Blundell**, who gave a stimulating talk on how X-ray crystallography has had a tremendous impact on drug discovery and development. He talked about "beautiful crystals, beautiful structures and beautiful people", and also his experience of working with Dorothy Hodgkin. **Gideon Davies**, who was undoubtedly intrigued by this talk, spoke about "ugly crystals, ugly structures and ugly people" during his BSG Plenary talk. His group's work on carbohydrate processing by enzymes shows promising results for drug discovery in some neurodegenerative diseases. During the session entitled 'Exploring the limits of synchrotron radiation in macromolecular crystallography', chaired by **Elsbeth Garman**, **Gwyndaf Evans** from Diamond Light Source presented new developments of advanced X-ray sources that will allow measurement of data from submicron-size crystals in a sample-efficient manner. **Matthew Bowler** from the European Synchrotron Facility in Grenoble gave a talk on high-throughput data collection using MASSIF1 and described new developments in sample visualization and software that will allow for time-efficient routine data collection.

The development of X-ray sources that allow for medium and high-throughput data collection facilitates structure-based drug design, and has pushed forward new methods and software to analyse ligand chemistry. To that end, **Martin Noble** gave a talk on targeting a protein-protein interaction by exploiting new approaches and tools that enabled structure-based drug design. **Paul Emsley** presented an informative comparison of two programs available through the CCP4

Suite and Coot, AceDRG and Pyrogen respectively, for small-molecule descriptions and ligand restraint generation. During the 'Data Mining' session, **Ted Baker** highlighted the importance of crystal packing in understanding the biological function of macromolecules. A detailed presentation of small molecule validation and the generation of new ligands through AceDRG were also given by **Garib Murshudov** during the same session.

Although tired from Ceilidh dancing at the Conference dinner on Wednesday night, I had a great learning experience during the 'Data Acquisition Tools' workshop. **Liz Potterton** and **Jon Agirre** introduced the new CCP4 Suite interface (CCP4I2). **Stuart McNicholas** gave a hands-on tutorial on CCP4MG software for visualizing macromolecular structures. **Phil Evans** and **Johan Turkenburg** gave useful tips on processing X-ray data and assessing its quality.

The BCA 2015 was a unique experience. I was grateful for the invitation to give an oral presentation on my work entitled 'Exploration of target recognition by a therapeutic antibody' to such an enthusiastic audience. To that end, I would like to acknowledge the BCA and King's College London for their financial support to enable me to attend this meeting.

Alkistis Mitropoulou
Kings College London

SET in the scenic city of York, the week started with the Young Crystallographers' Meeting, which showcased interesting work from various fields ranging from crystal-structure prediction to high-pressure crystallography and therapeutic antibodies. **Briony Yorke**, from University of Hamburg, gave an excellent presentation on the use of Hadamard transformations for noise reduction, and how the technique can not only be implemented in crystallography, but also applied to other kinds of spectroscopies. **Elliot Carrington**, from the University of Sheffield, gave a very interesting presentation involving the use of a prop wine rack to explain the structural changes observed in metal-organic frameworks in the presence and absence of gases or solvent molecules. The 30s presentation challenge, where each poster presenter had to explain their work in a nutshell, was another definite highlight.

The teaching session on space groups, organised by the YCG, proved very useful, with Profs. **Bill Clegg** and **Mike Glazer** unravelling the mysteries of crystallographic space groups through simple illustrative examples. If you had been to the Durham School of Crystallography, this talk served as a good sequel, and if you hadn't, it still gave a pretty good overview of the concepts involved.

It was fascinating to hear about the advances happening at the UK central facilities, and how the beamline scientists are very willing to help their users make the most of them. Talks by **Anna Warren** and **Claire Murray** were prime examples. Automation has taken X-ray structural analysis to new heights, and Anna's talk showed how it has been implemented in the I24 beamline at Diamond Light Source, e.g. by allowing multiple crystals to be loaded simultaneously to obtain better data. Anna also gave a good overview of the general "do's and don'ts" of crystallographic studies carried out at the

central facilities. **Claire**, who works at the powder diffraction beamline I11 at Diamond, introduced their newly-built EH2 hutch for carrying out long-term studies (between 2 months and 2 years), aimed at fields such as battery research, corrosion studies and pharmaceuticals.

Computational work goes a long way towards providing better understanding of the physical phenomena observed during experimental studies, as showcased during the **Complementary Calculations** session. **Keith Refson**, along with **Jonathan Skelton** and **Nick Funnell** in another session, showed during their talks us how they were pushing the boundaries of state-of-the-art computational facilities to carry out calculations that previously were impossible owing to resource limitations. Another emerging field showcased at the meeting was the study of nanocrystalline materials that appear X-ray amorphous. The **Amorphous Materials, Nanomaterials and Liquids** session highlighted the use of pair-distribution function (PDF) analysis to aid the characterisation of these challenging materials.

This year's BCA main meeting also heard exceptional plenary talks from Prof. Sir **Tom Blundell**, Prof. **Antony Cheetham** and Prof. **Simon Parsons**, who through their talks not only showcased a wealth of knowledge, but also experience, which would serve as an inspiration to many a young crystallographer. Celebrating the CCDC's 50th anniversary, Dr **Colin Groom** talked about the inception and growth of the well-known Cambridge Structural Database, highlighting some interesting trends drawn from a vast repository of crystal structures, and some of the common mistakes people make when reporting structures. He also gave an insight into the latest developments in the software, which enable its users to perform statistical analyses to make the most of the wealth of information deposited in the database.

A new addition to the BCA meeting, the **workshops** given by industrial partners helped users get the best from their instrument and data-processing software, which most crystallographers would use on a daily basis.

Another great success, also a new addition to the BCA for 2015, was the "**Would you publish this?**" session, which showcased typical examples of the obstacles that crystallographers encounter when trying to attain a publication-quality crystal structure solution. Set up as a guided interactive discussion, the session was aimed at allowing beginners to get the approval of, and valuable opinion from, experts in the field.

All in all this year's BCA Spring Meeting was an excellent platform for meeting researchers from various areas of crystallography, exchanging ideas, and, of course, forming new collaborations. The University of York provided an excellent venue, not to mention the delicious food, which drew plentiful compliments from the delegates.

Anuradha Pallipurath
National University of Ireland

THE YCG satellite meeting is always a highlight of the BCA spring meeting as it is an opportunity to see work presented by up-and-coming researchers in a multidisciplinary session. Where the main meeting enables you to select micro symposia relating to a specific field, here we are offered snapshots of current research across the field. With that in mind, it is always useful to consider how developments in one area of crystallography may enhance our own research and vice versa. This year the University of York was chosen as host and provided a relaxed setting with good facilities, especially in the lecture theatres.

Jerome Wicker gave an engaging presentation about utilising the wealth of structural data available online regarding the crystallization of small molecules. Data in the Cambridge Structural Database (CSD) and the ZINC database are used to train algorithms designed to predict crystallinity. This machine learning process has been used to indicate which small molecules should crystallise and to predict functional group changes that increase the likelihood of crystallisation. The results of this research will be of particular use to the pharmaceutical industry; however, the processes involved in machine learning and data mining large structural databases, are bound to have a positive impact on the crystallization of notoriously difficult proteins and macromolecules. This theme was also explored in **William Fletcher's** presentation "A Bayesian route to protein structures without crystals", where data from the PDB is used to provide parameters for Monte Carlo modelling of protein structures using SAXS data.

The development and characterization of metal-organic frameworks was discussed in more than one presentation, highlighting the breadth of diffraction based and complementary techniques applied to these systems. **Alice O'Connor's** work combined crystallographic structure with spectroscopic studies at high pressure to understand phase transitions in platinum complexes. The effect of high pressure on guest uptake and magnetic properties of MOFs was discussed by **Scott McKellar**, and **Elliot Carrington** discussed the effect of solvent on breathing modes. **Helen Duncan** presented her investigation into the nature of hydrogen bonds during phase transitions of MOFs using neutron scattering with reverse Monte Carlo refinement, while **Lucy Saunders** presented the development of a method enabling the evolution of hydrogen bonds to be imaged using synchrotron X-ray diffraction. This research area was beautifully summarized during the energetic plenary lecture by Professor **Chick Wilson**, which included his amazing colour changing car.

I found that all of the talks contributed to the conclusion that multidisciplinary approaches to structural studies are essential to provide a full story of the system in question. The gap between simulation and experiment is being bridged by combining multiple types of data and utilizing the various databases for algorithm design.

Briony Yorke
DESY, Hamburg, Germany



BCA Spring Meeting 2015 EXHIBITORS



The Young Crystallographers' Satellite Meeting

THE first session of the 2015 Young Crystallographer's Satellite Meeting kicked off with Jerome Wicker, who described his big data approach to predicting crystallisability of small organic molecules using machine learning algorithms and descriptors derived from 3D conformations of molecules. He showed that incorporation of more relevant descriptors and use of a diverse training dataset improves the predictive accuracy of the model.

Lucy Saunders spoke next, describing how she has designed short hydrogen bonds in urea-based molecular complexes that can be used to investigate proton migration or design extended arrays.

Alkistis Mitropoulou was up next and presented structures of asthma treatment drugs, examining the effect of packing on the structure, which is useful in the understanding of the drug-immunoglobin interactions.

Helen Duncan went on to talk about her use of Reverse Monte Carlo methods to elucidate the short range ordering of atoms during phase transitions in a multiferroic metal-organic framework.

Jonathan Skelton gave an outline of the application of lattice dynamics as a complementary technique for understanding systems, including their use in the elucidation of properties.

Alice O'Connor then discussed her high pressure crystallographic and spectroscopic approaches to the investigation of a Pt(II) complex, which revealed interesting structural and colour changes.

Prof **Chick Wilson** then delivered an entertaining YCG Plenary lecture where he gave an overview of the use of hydrogen bonding in the design of multicomponent crystalline systems, and how it has evolved over the last couple of decades. He then went on to discuss his work on applying these crystal engineering methodologies in new continuous manufacturing approaches.

Anuradha Pallipurath described the polymorphism of Sulfamerazine, an anti-microbial agent, to understand the thermodynamic stabilities and, in turn, why form I has different milling properties than form II.

William Fletcher presented a 'Bayesian reverse Monte Carlo method', which is able to accurately reproduce a model of the folding of small proteins from their PDFs and additional prior knowledge, including the Ramachandran distributions of the amino acid residues.

In the second high-pressure talk of the day, **Scott McKellar** then discussed his work on porous formate frameworks, where the structure and corresponding magnetic behaviour can be tuned via the application of pressure in a variety of pressure-transmitting liquids.

Briony Yorke gave a presentation on the initial results from HATRX, a novel approach to time-resolved crystallography, utilising the Hadamard transform. This method allows time-resolved crystallography to be performed at a standard synchrotron beamline.

Sam Horrell spoke about his work on the biofilm regulating metallo-protein PA3825-EAL, and the insight gained into the catalytic mechanism through structural analysis. Structures from each step of the reaction were presented with the final

product bound structure presenting a novel third metal binding site involved in hydrolysis of cyclic-di-GMP.

Elliot Carrington concluded the second session by describing the unprecedented change in pore size and shape of a wine-rack MOF in response to a change in the guest content.

On the second day of the meeting, the session kicked off with the Parkin Prize Lecture, which is awarded to a young crystallographer who has made an outstanding contribution to crystallographic outreach. This year it was delivered by **Anna Warren**, who gave a great overview of tips and tricks to make the most of recent technological innovations at synchrotron sources which has allowed data collection and structure solution on crystals that would have been impossible just a few years ago.

Anna was followed by **Philip Adler**, who talked about applying statistical tools to crystal structure prediction, whereby we can use the wealth of knowledge already available to us in the CCDC and the PDB to better understand the formation of novel structures. By applying "descriptors" to crystal engineering techniques, he discussed the key factors governing crystal formation.

Thomas Roseveare delivered the final contributed talk of the meeting by discussing gas uptake in molecular clusters, which provide one route to interesting host-guest behaviour in discrete rather than classically porous extended structures.

To end the YCG Satellite meeting, Prof **Mike Glazer** and Prof **Bill Clegg** delivered an inspiring two part Space Groups teaching session describing how to use Volume A of the International Tables of Crystallography with some interesting examples. They then delved a little deeper, and cleared up some possible areas of confusion, such as the hexagonal crystal system.

Many thanks to all the speakers and meeting attendees who made this another great YCG Satellite meeting!

The YCG Committee



Speakers at session 1 of the YCG Satellite Meeting



Speakers at session 2 of the YCG Satellite Meeting

Biological Structures Group

The data acquisition session was chaired by **Elsbeth Garman** and the first talk was given by **Gwyndaf Evans** on 'Exploring the limits of synchrotron radiation in macromolecular crystallography'. The current developments and excitement surrounding the potential of XFELs has encouraged beamline scientists to tackle the current challenges faced at synchrotron sources. These challenges include collecting data with smaller crystals, reducing the background, sample visualisation and sample stability during the experiment. He mentioned that a paper published in 2010 by **James Holton** and **Kenneth Frankel** regarding the theoretical limit to the size of a crystal that is suitable for successful data collection at a synchrotron source has been a significant factor in the aspirations for a new beamline at Diamond. The new beamline is being designed with a cryostage to assist preservation of samples and high stability goniometry. It will also be able to perform serial data collection and as a result it will take advantage of multi crystal data analysis.

Matthew Bowler delivered the second talk on 'Fully automatic data acquisition: MASSIF1 at the ESRF'. He began by highlighting that when he started in 2007 a dataset took between 20 minutes to several hours to collect. He noted that several steps unnecessarily required manual input which were time consuming and detracted from the important step of designing the data collection strategy. The MASSIF1 facility at the ESRF has been designed to perform automatic data collection and sample evaluation. The beam is of high quality and very stable. The optics have reduced in complexity allowing for flexibility in manipulating the beam profile. He mentioned that the robots for sample changing have been designed to improve the sample mounting with much more reliable positioning and the workflow has been modified to allow automatic sample screening to automatically find the best diffracting volumes of a crystal. This automated pipeline has improved the time taken to collect a dataset to around 6 minutes on average, without any input from the user.

The final talk of the session was given by **Jonathan Brooks-Bartlett** on 'Simulating the data collection process'. He split the talk into two sections. First was about how the data collection experiments were modelled with the dose calculation software RADDPOSE-3D. Significant extensions to RADDPOSE-3D include the capability for the software to use arbitrary crystal shapes, read experimental beam profiles and use PDB files and sequence files for user input. Additionally RADDPOSE-3D can now simulate SAXS experiments to provide reliable dose estimates for assessing radiation damage to SAXS samples. The second part of his talk focussed on how the information from RADDPOSE-3D is used for correcting damaged reflection intensities. He presented a model for reflection intensity decay with increasing radiation damage and presented preliminary results of the correction method on a subset of reflections in data collected from insulin crystals.

Gideon Davies provided the BSG plenary lecture 'Probing the reaction pathways of enzymes through crystallography'. He highlighted that enzymes work in various conformational spaces and it is via conformational pathways that they can perform their functions efficiently. Serine and threonine-linked N-acetylglucosamine (O-GlcNAc) plays a significant role in modification of intracellular proteins; the O-GlcNAc modification. Using the structures determined by X-ray analysis of the reaction mechanism, the group have been able to investigate the function in more detail. By mutating the

carbohydrate at several places they were able to change the enzyme kinetics. The rate constants were switched for the different stages of the reaction pathway, which allowed them to exploit the cavity in the structure to improve enzyme inhibition. It is hoped that further research into the reaction mechanisms can improve the treatment of tauopathy-based neurodegenerative diseases.

The joint BSG/IG session on ligand chemistry chaired by **Ehmke Pohl** and co-chaired by **Jason Cole** was opened with a talk by **Martin Noble**. His talk titled 'Chemical and Computational Tools for Drug Discovery: Targeting the Mdm2/X-p53 Interaction' discussed the difficulty of identifying suitable drug targets which stressed the importance of streamlining the downstream stages as much as possible. Mdm2 is a negative regulator of p53 which is implicated in cancer formation, making mdm2 a sensible choice of drug targets to suppress its activity. Molecular dynamics simulations were used to aid the design of ligands as chemical probes. However, comparison of the structure to the computer models show that the models are not adequate to completely base ligand design on. He also showed work in which mutation of certain residues led to reduced surface entropy which increased crystal contacts, thereby increasing the chance of crystallisation. Finally he presented the capabilities of the new CCP4i2 interface, in particular its ability to efficiently run and store hundreds of jobs therefore supporting the shift towards high throughput structural biology in support of medicinal chemistry.

Paul Emsley gave the next talk where he presented two new programs for generating ligand restraints: AceDRG and PYROGEN. The fact that the REFMAC monomer library hasn't been updated since 2012 largely motivated the creation of these programs to fill the gaps. It was shown that these programs improved the refinement of ligands in the electron density maps. Conversely it was also demonstrated that incorrect ligand dictionaries led to incorrect refinement results. Examples of both good and bad refinements were shown with COOT. He ended by showing the correlations between various ligand libraries and showed that AceDRG and PYROGEN gave consistent results.

Jon Agirre closed the session with a talk on 'Deriving a chemical context from public data sources: a carbohydrate-centric case study'. Modelling carbohydrates is very difficult and various nomenclature errors exist in structures deposited in the PDB. This is a huge problem due to the fact that carbohydrates are largely implicated in a high number of pathological processes. Issues with carbohydrate ring conformation has arisen recently and is likely to be due to under-parameterised refinement. He presented Privateer-validate, an additional validation tool for assessing cyclic carbohydrate models, which is part of the Privateer program. Privateer-validate analyses monosaccharide moieties from a PDB file, using a database of three-letter codes, stereochemistry and conformations derived from the wwPDB database and outputs linear descriptions of any glycans found.

The next session was chaired by **Kevin Cowtan** on Data Mining – wealth and pitfalls. **Robbie Joosten** gave the first talk of the session titled 'Share and enjoy: data mining macromolecular crystal structures through PDB_REDO'. The PDB is an important resource for structural analysis and many tools already exist for data-mining its contents. However none of the existing tools address the actual data. The structures deposited over the last 40 years vary in quality due to the developments in the analytical techniques over that time span, but the PDB doesn't update the old models. PDB_REDO tries

to overcome this problem by automatically refining, rebuilding and validating these models via a consistent pipeline for all structures. It can determine whether anisotropic B factors will improve statistics over isotropic B factors and generally lowers the crystallographic R factor values.

Ted Baker delivered the second talk of the session on 'Discovering novel covalent crosslinks in bacterial cell-surface proteins'. These proteins are common drug targets since they are involved in functions such as adhesion, infection and communication. A recently solved structure within his group of a pilus protein subunit Spy0128 exhibited unusual electron density which turned out to be isopeptide bonds. Intramolecular isopeptide bonds of this kind had previously not been observed. The bond was verified to exist by mass spectrometry. This finding prompted the question: Do other proteins contain intramolecular peptide bonds? A subsequent search of the PDB showed that other structures also contained similar isopeptide bonds. This exemplifies the need to look carefully at the electron density. He makes the point that structural analysis using both X-ray methods and mass spectrometry are essential for model interpretation and that prior knowledge can sometimes be detrimental to model building.

Garib Murshudov presented a talk on 'AceDRG – a tool for generating small molecule descriptions' to close the session. He highlighted the fact that chemical knowledge is a form of prior knowledge during model refinement. However the table from which the information is used is limited in its number of atom types. AceDRG is a program that uses data mined from the Crystallographic Open Database (COD) to derive atom types. This characterises the atoms' local environment and generates better restraints for refinement.

The first BSG session on Thursday was chaired by Garib Murshudov on 'Simultaneous use of Electron microscopy (EM) and Macromolecular crystallography (MX) data'. The first talk was given by **Alan Brown** titled 'Tools for macromolecular model building and refinement into cryo-EM maps'. EM has seen a recent 'resolution revolution' now structures are being solved to beyond 3Å resolution and the molecules on which successful structure solution is possible are becoming smaller. This revolution is due to better software, microscopes and grid technology. The detectors, in particular, have much improved signal to noise and are much faster. The solution of yeast mitochondrial ribosome to 3.2Å presented many new challenges and required collaboration with the computational crystallography group at the MRC LMB. Software pipelines to locate proteins in the EM map were created. Jiggle fits and methods of generating external restraints were incorporated into refinement. A new metric was created to monitor the model fit to the density and careful validation was required to prevent overfitting of the data.

Arun Pandurangan followed this up with a talk on 'Simultaneous fitting of multiple subunits into low-resolution cryo electron microscopy maps of macromolecular assemblies'. Fitting huge macromolecular assemblies into low-to-intermediate resolution EM maps presents many challenges. The factors that affect the complexity include the size and shape information from the map, the intermolecular interactions and the resolution of the map. This means that an efficient global optimisation routine is necessary to fit the subunits into the map. A genetic algorithm that uses a K-means clustering procedure of the electron density information is then used to reduce the sampling space. Optimisation is then guided by a combination of goodness-of-fit scores and overlap penalties. This method showed that in most of the tested cases the algorithm matched the native placement of the molecules.

Martyn Winn gave the last talk of the session on 'Collaborative Computational Project for Electron cryo-Microscopy'. The CCP-EM project started in 2012 in response to EM becoming an increasingly important structural technique. The project's initial focus is on single particle reconstruction supporting the image processing pipeline. He stressed the importance of building a cryoEM community as part of the collaborative nature of the project. It will take years before it reaches the footing of CCP4 and so it is crucial to manage expectations. An alpha release of the software is due for release for Mac and Linux distributions in mid-2015. This release hopes to include easy installation and a modern GUI.

The final BSG session of the conference chaired by Keith Wilson was on low resolution refinement. This session began with a talk by **Steven Johnson** titled 'Through the distorted looking glass: tales of low resolution refinement'. He gave a very accessible introduction to the definitions of resolution and refinement in the context of crystallographic data and what problems they can lead to in interpreting the electron density. Solutions to tackle the low resolution problem were: collect better data, use up-to-date software, use appropriate cross validation, use appropriate constraints and restraints and familiarise yourself with what details are appropriate at the given resolution. He then proceeded to give a series of case studies of low resolution structures that provided obstacles during the refinement and model building process. A particular case study was given in which one program failed to give interpretable electron density where the other program succeeded. This suggested that exploration of all possible factors that affect refinement of low resolution is necessary to get the most information possible.

The penultimate talk was given by **Huw Jenkins** on 'Determination of the structure of the capsid protein from bacteriophage SPP1'. The focus in particular was on the model building and the refinement of the structure. Two mutations were introduced to produce a monomeric form of the capsid protein (gp13). The phases were experimentally determined by Se-SAD and the 5-fold NCS enabled production of a high quality map. The local NCS highlighted differences in the side-chain rotamers, although sometimes refinement didn't always converge to the correct one. He also demonstrated how NCS weighting can influence the R free and R work values, and decrease clash and MolProbity scores.

Eleanor Dodson closed the session with her talk 'Special interpretation issues for low resolution refinement: Why do it?' The talk was centred on the four factors that need to be considered during refinement with a focus on the additional considerations for low resolution refinement. First was the objective function which is a maximum posteriori construction. With this formulation it is necessary to take into consideration how we deal with our data; in particular, how we model the scale factors and sigma values. Secondly the optimisation needs to be considered. If the initial guess starts too far away from the true value then the solution is likely to converge to the incorrect local minimum. Good models make refinement easier. Thirdly prior knowledge needs to be accounted for which usually arises in the form of restraints. Low resolution data coupled with bad priors consequently leads to bad refinement. Finally it is necessary to deal with the parameterisation of the model. With low resolution data we want to minimise the number of parameters which may mean using isotropic B factors and rigid body refinement.

Jonathan Brooks-Bartlett
University of Oxford

Exhibitor company names, pictured on page 14 and alongside, are as follows:

- ① Agilent
- ② Douglas Instruments
- ③ Cambridge Reactor Design
- ④ Bio-Rad Laboratories
- ⑤ BioSylta
- ⑥ Genevac
- ⑦ Expedeon
- ⑧ CCDC
- ⑨ BioMEX Solutions
- ⑩ Bruker
- ⑪ Hiltonbrooks
- ⑫ Incoatec
- ⑬ Stoe
- ⑭ Olympus
- ⑮ Taylor & Francis
- ⑯ IUCr
- ⑰ PANalytical
- ⑱ Rigaku Europe
- ⑲ Oxford Cryosystems

The Exhibition Passport winner of a mini iPad was **Semën Gorfman** (University of Siegen).

Answer to March Puzzle Corner

WITH the International Year of Crystallography still fresh in our minds, this and other “years” can be combined according to the operations shown below, giving the digits of a 4-digit number that should set your pulses racing.

Chemistry + Physics – Crystallography – Thanksgiving
 = 2011 + 2005 – 2014 – 2000 = 2

Forests – Biodiversity + Planet Earth – Astronomy
 = 2011 – 2010 + 2008 – 2009 = 0

Freshwater – Deserts + Mountains – Ocean
 = 2003 – 2006 + 2002 – 1998 = 1

Soils – Family Farming + Quinoa – Potato
 = 2015 – 2014 + 2013 – 2008 = 6

The UN has resolved that the year 2016 will be designated as the International Year of Pulses (peas, beans, lentils, etc., not heartbeats).

BCA Spring Meeting 2015 EXHIBITORS



Prize Winners

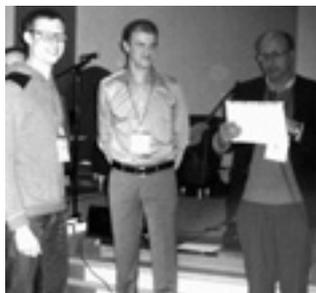


President Lee Brammer presents a thank-you gift to **John Helliwell** for his hard work as Programme Chair.

BCA Prize Winners



Vilmos Fulop presenting the Rigaku poster prize to **Hayley Owen** (Sheffield)



John Helliwell presenting the ACA Structural Dynamics poster prize to **Christoph Zehe** (University of Bayreuth)



Matt Tucker presenting the IoP Physical Crystallography Poster Prize to **James Cumby** (University of Edinburgh)



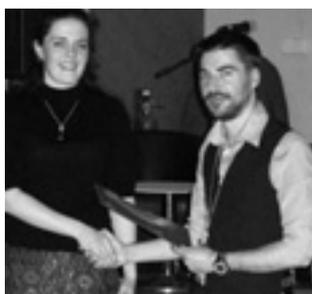
Matt Tucker presenting Solid State Chemistry Group Poster Prize to **Joshua Hill** (Oxford)



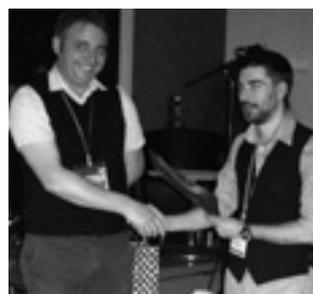
Paul O'Meara and Matt Tucker giving the PANalytical Thesis Prize to **Joshua Makepeace** (Oxford)



Pete Wood presenting the IUCr poster prize to **Christoph Zehe** (University of Bayreuth)



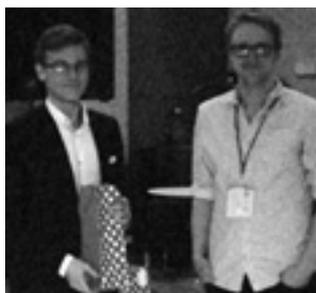
Pete Wood presenting a CrystEngComm poster prize to **Sophie Gearing** (University of Oxford)



Pete Wood presenting a CrystEngComm poster prize to **Tony Keene** (University of Southampton)



Pete Wood presenting a CrystEngComm poster prize to **Jorge Sotelo** (University of Edinburgh)



Scott McKellar presenting the YCG poster prize to **Lewis Owen** (ISIS)



Scott McKellar presenting the Durward Cruickshank Young Crystallographers' Prize to **Jorge Sotelo** (University of Edinburgh)



Pierre Rizkallah presenting the BSG Poster Prize to **Gustavo Mercaldi** (Sao Paolo University)

Eighth ECA Max Perutz Prize

THE 8th Max Perutz Prize of the European Crystallographic Association has been awarded to Professor **John R. Helliwell**, Emeritus Professor of Chemistry, University of Manchester, United Kingdom for his long, generous and fruitful dedication to developing all aspects of the use of synchrotron radiation for crystallography and for his boosting support to global development of synchrotron and neutron facilities. In addition to his pioneering achievements and to the key role that he played in the development of experimental beamlines for structural biology worldwide, he also has been constantly engaged in outreach and dissemination of crystallography to the scientific community.

John Helliwell led the development of the world's first dedicated protein crystallography beamlines; he pioneered the collection of the first broad-band Laue diffraction patterns for protein and virus crystals using synchrotron radiation; he combined biochemistry, spectroscopy, microscopy, protein crystallography and small-angle scattering to study the crustacyanins. He contributed to some of the first developments of synchrotron radiation for phasing based on optimised anomalous scattering and began the investigations of the effects of radiation damage and its potential use for phasing, demonstrating the use of MAD phasing for *ab initio* structure determination from powder diffraction data. John Helliwell has also served the global crystallographic community through numerous Advisory Committee responsibilities to ensure a speedy and effective growth at as many synchrotrons and



neutron facilities as possible; he was the first Chair of the IUCr's Commission on Synchrotron Radiation. He was president of the European Crystallographic Association (2006–2009) and served as Editor-in-Chief of the IUCr journals (1996–2005).

John Helliwell will receive the award at the 29th European Crystallographic Meeting in Rovinj (Croatia), 23–28 August 2015.

(Editor's note: the crystallographic significance of Cloughton is that, while spending a summer holiday there, W H Bragg and W L Bragg first learned about and started to interpret Laue's reports on X-ray diffraction.)

EPSRC recognises the requirement for a National Crystallography Service

IN late January, the 11 members of the Statement of need prioritisation panel, coming from academia and industry, published the recommendations outlined below:

"EPSRC supports a range of mid-range facilities which provide resources of limited availability to the UK Engineering and Physical Sciences research community. In July 2014, communities were invited to submit statements of need for new facilities and currently supported facilities with contracts expiring in the near future.

Following the prioritisation panel for these statements of need on 28 January, EPSRC is exploring the possibilities of supporting the following types of facilities:

- X-ray crystallography
- Aberration corrected scanning transmission electron microscopy
- Engineering instrument pool
- Ion beam and gamma ray facility
- Electron paramagnetic resonance
- Semiconductor epitaxy
- Subscription to the European Magnetic Field Laboratory
- IR/THz FEL

The next call for statements of need will open in early summer 2015."

The 15th BCA/CCG Intensive Teaching School in X-ray Structure Analysis

Trevelyan College, University of Durham
21-29 March 2015



THE 15th BCA/CCG Intensive Teaching School in X-ray Structure Analysis was held in Durham from 21-29 March 2015. The course runs on a biennial basis and its successful format has evolved as a result of feedback and suggestions from students and staff since the first course in 1987. As the name suggests the course is intensive and consists of a mixture of lectures interspersed with tutorials in which the students get chance to apply concepts they have just learnt to sets of problems. The lectures and tutorials were held in the Sir James Knott Hall at Trevelyan College again which provides an ideal space to switch into and out of group work and lectures. Each tutor group consists of ~8 students and has a tutor who stays with them throughout the week to act as their first port of call for help throughout the course. The accommodation and meals were provided in Collingwood College which is less than a 5 minute walk from the Sir James Knott Hall, the food was of a very high standard and there was plenty to keep everyone going.

This 15th course was attended by 80 students studying in 15 different countries: the UK, Canada, Finland, Denmark, Slovenia, India, Poland, USA, Germany, Ireland, United Arab Emirates, Brazil, Australia, Japan and Italy. The academic backgrounds of the participants vary and they arrive with a range of crystallographic experience. The majority of the participants that attend the course are PhD students with a small number of PDRA's and academic/industrial researchers.

The school has a national and international reputation and the benefits of attending the school are well recognised and we were again heavily oversubscribed.

The school's lecturing staff were largely unchanged from previous years although Dr **Stephen Moggach** stepped out of his role as a tutor to deliver one section of lectures. We did however have a number of new tutors Dr **Katharina Fucke**, Dr **Lauren Hatcher**, Dr **Mark Senn** and Dr **Helena Shepherd**, all of these new tutors had previously attended the course as a student so knew what to expect!

The main lecture topics tackled during the 7 day course in the following order were Introduction (Professor **William Clegg**), Maths (Dr **Devinder Sivia**), Symmetry (Professor **William Clegg**), Data Collection from Instrumentation through to Data Collection Strategies (Dr **Roy Copley**), Fourier/Paterson Methods (Professor **William Clegg**/Dr **Stephen Moggach**), Charge Flipping and Direct methods (Dr **Lukas Palatinus**), Uncertainty and Inference (Dr **Devinder Sivia**), Refinement (Professor **Richard Cooper**), Derivation of Results and Twinning (Professor **Simon Parsons**), Validation (Dr **Roy Copley**) and a Disorder Workshop (Dr **Amber Thompson**). In addition to the main lectures and tutorials there were two optional lectures, one on 'Incommensurate Structures' (Dr **Lukas Palatinus**) and one on 'Synchrotrons and Neutrons' (Dr **Mark Warren** and Dr **Katharina Fucke**) both of which were essentially fully attended and appreciated by the students.

Alongside the lectures and tutorials during the days, the evening activities were generally more relaxed and designed to enable the students to mix with each other for both fun and educational activities. These activities included an introductory mathematics lecture (Dr **Devinder Sivia**), a bar quiz (Professor **Richard Cooper**), a talk on databases (Dr **Peter Wood**) and student group presentations (Dr **Michael Probert** and Dr **Katharina Fucke**). For their group presentation each tutor group was assigned a different crystallographic topic which they had to present in as entertaining a way as possible whilst still being educational. The presentations were judged by an elite panel of the lecturers and as with previous years the standard of the presentations was very high and amusing. On the final evening we had the course dinner which was a chance to thank all of the contributors to the school, the local staff, organisers, lecturers, tutors and students all of whom led to another very successful school.

For the first time on Sunday 29 March, we held an optional hands-on Olex2 workshop that was run by Dr **Horst Puschmann** and Dr **Oleg Dolomanov** (OlexSys). This workshop was attended by ~40 students, some had previously used Olex2 while for others it was a new software, but for all of the participants it was a chance to apply concepts they had learnt to structure solution and refinement in Olex2. This kind of hands on session following the school had been requested by previous participants of the school and the workshop was very well received and found to be useful by the participants.

The school was heavily oversubscribed and we believe that the high demand is probably related to the growing use of crystallography by a wider range of users as a result of the development of easy to use software for data collection as well as structure solution and refinement much of which does not require a large amount of crystallographic expertise to obtain a result. Consequently schools such as this are essential to provide users of crystallography with a solid understanding of the underlying theory so that they can identify and treat any problems they may run into as well as checking the validity of their results prior to publication. As with previous years the feedback from the students has been carefully analysed to look for any areas of improvement which will be fed into the planning meeting for the next school. Overall the feedback from the students was very positive having enjoyed the course and learnt a lot which they will take back to their home institutes and apply to their own science, as appropriate.

We would particularly like to thank all of the organisations who provided financial support for the 15th course and without whom we would not have been able to run the school so successfully. These are **Diamond, IUCr, ECA, CCG, ICG, Oxford Cryosystems, Agilent Technologies, CCDC, Rigaku, Bruker** and **Incoatec**.

Professor Judith A. K. Howard, CBE, FRS
(University of Durham) and **Dr Hazel A. Sparkes**
(University of Bristol) (Local Organisers)

Student Report

THE 15th BCA/CCG Intensive Teaching School in X-Ray Structure Analysis organized in Durham University was indeed a very exceptional course. Starting with basic mathematics, they eased us into “hardcore” topics which form the core of X-ray crystal structure determinations.

Understanding symmetry is a key part not only of designing data-collection strategies, but also in the final structure determination itself. Prof. **Bill Clegg** helped us understand various concepts in symmetry, with a little help from his favourite M. C. Escher drawings. Dr **Devinder Sivia** explained the phase problem associated with structure determination by applying the same concept to two photographic images, giving us a visual explanation of the underlying problem. The course also went into great depth about data collection, instrumentation, and various methods of structure solution. Listening to the best practices of using the various methods from the people who developed them, including Prof. **Simon Parsons**, Prof. **Richard Cooper** and **Lukas Palatinus**, was a definite highlight. **Royston Copley** went into great detail about the dos and don'ts of data collection. **Stephen Moggach** helped us construct vector tables to tackle Patterson syntheses, and also warned us about getting multiple possible solutions in the case of pseudosymmetry.

Apart from the main lectures, the optional sessions also saw a full house. Lukas beautifully explained the application of the superspace method to understanding incommensurate structures, and to help arrive at a structure solution for these challenging systems. **Mark Warren** and **Katherine Fucke** illustrated the various applications of central facilities such as synchrotron and neutron sources, and explained how we can go about enhancing our research by making use of them, and how to put in a successful beamtime application. **Peter Wood** told us about how to make the best use of the CCDC packages, and how they have now an inbuilt module to 3D print structures for teaching purposes, etc. Finally, before the close of the school, **Amber Thompson** carried out a workshop on tackling difficult disordered structures.

Being an intensive course, it required hard work, but we were well rewarded with excellent food at Collingwood College, and interesting sessions in the evenings. Knowing that the attention span for a human is only about 20 mins, the organisers cleverly mixed in tutorials between every lecture, allowing us to practice problems to better understand the concepts being taught, with the aid of simple computer programs or props. The lectures were themselves also very entertaining, and the course included some fun exercises such as “celebrity CIF files” and fun presentations where groups had to present quite complicated crystallography topics in the style of various television programmes. In all, the course was highly successful, and we not only got to understand the techniques which software employs while solving structures, but we also got to meet some excellent crystallographers from all over the world.

For those of you who want to know more about crystallography, I would definitely recommend you get a place on the course in 2017!

Anuradha Pallipurath, University of Ireland

Outreach Report

THE Big Bang Fair is the UK's largest Science and Engineering fair with over 75,000 visitors. The BCA stand returned this year to Birmingham for four days, resplendent with enough marshmallows and cocktail sticks to build the Eiffel Tower! 2015 is the International Year of Light and so our fantastic volunteers were out in full force promoting the importance of crystallography and the use of X-rays and neutrons. The activities include unit cell construction with marshmallows, lysozyme crystal growing, Mike Glazer's fantastic marbles, demonstrating the ISIS Beamline and molecular model building, as well as diffraction with a laser. The activities were well received with many happy punters getting the opportunity to build their own crystal and to speak to our enthusiastic volunteers about crystallography and their research.

We would like to thank **Sam Callear** for her herculean effort in organising this, as well as the **BCA**, **STFC**, **ISIS** and **Diamond** for all their support. We could not have done this without them and are very grateful for their ongoing support.

We would also like to thank our brilliant volunteers **Claudine Bisson**, **Pat Bryant**, **Irene Munao**, **Jonny Brooks-Bartlett**, **Craig Bull**, **Steve Hull**, **Philip Bradfield**, **Claire Murray**, **Adam Crawshaw**, **Helen Playford**, **Lata Govada**, **Naomi Chayen**, **Lucy Saunders**, **Mike Glazer**, **Matt Tucker**, **Genevieve Baker**, **Ron Smith**, **Pascal Manuel**, **Giles Flowitt-Hill**, **Nicholas Harmer**, **David Price**, **Laura Holland**, **Lewis Owen**, **Marek Jura**, **Gavin Stenning**, **Luke Daniels**, **Moritz Machelett**, **Matt Rodrigues**, **Peter Canning**, **Nick Funnell**, and **Elliot Carrington**. A few photos of these volunteers in action are presented alongside.

Simon Coles (University of Southampton) is the new Education and Outreach Officer, so expect to hear a lot from him over the coming months. The BCA will be returning to the Cheltenham Science Fair with Warwick University, STFC and Diamond so if you would like to get involved and volunteer let Simon know on education@crystallography.org.uk

If you're interested in getting involved, or have an idea for an Outreach event you would like to make a reality, check out the website (learn.crystallography.org.uk), Facebook ([British Crystallographic Association Education and Outreach](https://www.facebook.com/BritishCrystallographicAssociationEducationandOutreach)) or Twitter ([@Whatsinacrystal](https://twitter.com/Whatsinacrystal)) accounts and get in contact with us on education@crystallography.org.uk.

Claire Murray



Crystallography on “In Our Time” ... Again

THAT remarkable polymath **Melvyn Bragg** always leads an interesting discussion on Radio 4, whether it is about science, history or art. On April 30 the topic was “The Earth’s Core” with congenial and articulate guest experts **Stephen Blundell** from the University of Oxford, **Arwen Deuss** from Utrecht University and **Simon Redfern** from the University of Cambridge. It is well known that the core contains liquid metal, largely iron mixed with nickel, and its motion generates the magnetic field that protects us from harmful cosmic rays. However, careful analysis of weak seismic waves has modified this model: the innermost part of the core is believed to be crystalline solid iron or iron alloy. This solid inner core is growing at approximately 0.5 mm per year. As crystallographers we have a natural tendency to regard crystal growth as a good thing. However, according to Wikipedia, the thickness of the liquid outer core is about 2300 km. My back-of-the-envelope calculation, assuming the inner core continues to grow at the same rate, suggests that in another 4.6×10^9 years the core should have solidified entirely, putting an end to the generation of our protective magnetic field. Another thing to worry about in the ultra-long term!

What’s more, the slightly faster transmission of seismic waves along the Earth’s rotation axis compared to between two diametrically opposed positions on the Equator suggests that the crystals in the solid core may have a preferred orientation. But what phase of iron could be present at a temperature of

5700 K and a pressure of 330–360 GPa (according to Wikipedia)? To answer this question the panellists invoked crystallography. With recent advances in diamond anvil cell technology it is possible to generate pressures approaching or matching this value. Heating a thin sample to the required temperature is tricky, but it can be done with intense irradiation from a laser. During its fleeting existence the structure can be probed with X-rays from a synchrotron. Research conducted in Japan [S. Tateno, K. Hirose, Y. Ohishi & Y. Tatsumi (2010) *Science*, **330**, 359–361] showed that the hexagonal close-packed (hcp) structure of Fe is stable up to the relevant conditions of 377 GPa and 5700 K. The temperature dependence of the c/a axial ratio was found to be small, suggesting that hcp Fe is elastically anisotropic at core temperatures. Other important work has been done at our own Diamond synchrotron.

A recording of the broadcast is accessible at <http://www.bbc.co.uk/programmes/b05s3gyv>. For a specifically crystallographic perspective, an open-access article by **Thomas Duffy** from *Nature* a year ago presenting advances in crystallography of minerals under conditions resembling the deep mantle and inner core can be downloaded from <http://www.nature.com/news/earth-science-crystallography-s-journey-to-the-deep-earth-1.14755>.

Carl Schwalbe



Arwen Deuss, Simon Redfern and Stephen Blundell with Melvyn Bragg in the studio.

Open letter to “A Crystallographic Dinosaur”

Open letter to “A Crystallographic Dinosaur” from his erstwhile student, **Howard D. Flack**

See *Crystallography News*, December 2014, pp 22-23.

Dear Steve,

I studied chemistry at the University of Nottingham in 1962-65. I even managed to obtain a B.Sc. degree. I recognized you immediately from the photograph. You seem to have matured very nicely indeed. I append a copy of my graduation photograph to jog your memory of my physical appearance at that time.
[Available at <http://nottchem65.flack.ch/HDF6501.jpg>]

I am no longer quite sure but you may well have been one of the pair of chemistry staff who interviewed me for admission. Things were a little difficult for me during the interview because the headmaster of the school I attended had written that I was very keen on shooting (rifles). In fact I detested that sport. One of the staff members started to ask questions about my interest in shooting.

I listened to the second-year lectures that you presented on IR, Raman and NMR spectroscopy. As part of this venture, you had to explain about normal modes of vibration. You had a very personalized way of demonstrating them which made us absolutely roar with laughter. The example you chose was that of a triatomic molecule and you invited us to imagine that your clenched fists were two of the atoms and your head was the other one. You then proceeded to vibrate in the appropriate way for each mode. It looked very much like a series of physical exercises or some of the ways of dancing in vogue in the early 1960s.

Of course, you also gave a series of lectures on crystallography and had arranged a series of practical exercises to back up the lectures. As the subject sparked my interest, I did all of the exercises. In spite of the quality of your lectures, I am still trying to understand crystallography. As part of this effort I now try to explain parts of this science to other people. The most recent excursion in this direction is a new chapter “Methods of space-group determination” for the sixth edition of *International Tables for Crystallography – Volume A Space-group symmetry*. The chapter is co-authored with **U. Shmueli** and **J. Spence** and replaces section 3 of the fifth edition written by **A. Vooijenga-Vos** and **M. J. Buerger**.

The membership of the British Crystallographic Association needs to be aware that you are in a very real way the founding father of the association. In the early 1970s there were two separate groups with differing interests: the “X-ray analysis group” of the Physical Society and a group interested in chemical crystallography attached to the Chemical Society. It was at your suggestion and initiative, that these two groups could become joint groups of their parent society and also of a fledgling crystallographic society.

I received a letter the other day from the Alumni Relations of the University of Nottingham. They explain that in 2015 I graduated 50 years ago and there is a 1965 Golden Reunion to be held on Saturday 10 October 2015. I shall try and shake up some of my fellow chemistry graduates to attend and maybe we can meet you again on that occasion.

H.



Stephen Wallwork

Satellite Meetings for ECM29

(Register for all meetings through the ECM29 registration system)



Advanced Software Development for Crystallographers

August 20th (Thursday) to August 22nd (Saturday), 2015, Duga Uvala (Hotel Croatia)

Registration fee: EUR 100 including lunches and refreshments.
Website: <http://sig9.ecanews.org/rovinj.html>

Metadata for raw data from X-ray diffraction and other structural techniques

August 22nd 2015 (Saturday), 10:00 AM to 5:00 PM & August 23rd, 2015 (Sunday), 9:00 AM to 4:00 PM, Rovinj, Hotel Park (Arupinum Hall)

Registration fee: EUR 60 including lunch boxes and refreshments.

Website: <http://www.iucr.org/resources/data/dddwg/rovinj-workshop>, see also discussion forum at: <http://forums.iucr.org/viewforum.php?f=21>

Making the most of PDB and EMDB data

Saturday, August 22nd, 2015 10:00 AM – 5:00 PM, Rovinj, Hotel Park, (Congress hall CISSA)

Registration fee: EUR 20 including lunch box and refreshments.

Website: pdbe.org

OLEX2 Satellite Meeting

Sunday, August 23rd, 2015, 9:00 AM – 4:00 PM, Rovinj, Hotel Park, (Congress hall CISSA)

Registration fee: EUR 75 (limited to 40 participants)

CCDC workshop

Registration fee: No registration fee, but limited to 40 participants.

Website: www.ccdc.cam.ac.uk

Session 1 CSD deposition and access services

Sunday, August 23rd, 2015, 9:00 AM – 12:00 AM, Rovinj, Hotel Lone, Meeting room 4 (ground floor)

Session 2 Crystal engineering applications using the CSD Solid Form Suite

Sunday, August 23rd, 2015, 1:00 PM – 4:00 PM, Rovinj, Hotel Lone, Meeting room 4 (ground floor)

DIALS workshop

August 23rd, 2015 (Sunday), 10:00 AM – 3:30 PM, Rovinj (Red Island), Hotel "Istra", Huetterot congress hall

Registration fee: EUR 20 including lunch box and refreshments.

Website: <http://dials.sourceforge.net>

Automating and Simplifying Reduction of 2D powder diffraction data with DAWN

August 23rd, 2015 (Sunday), 10:00 AM – 4:30 PM, Rovinj, Hotel Park, Grisia Hall

Registration fee: EUR 20 including lunch box and refreshments (limited to 30 participants).

Fundamentals of Materials Analysis Using Powder Diffraction

August 23rd, 2015 (Sunday), 10:00 AM to 5:00 PM, Rovinj, Hotel Eden (Conference Hall)

Registration Fee: Free. Box lunch will be provided.

Website: **General info:** www.icdd.com, Database product capabilities: <http://www.icdd.com/products/2014/index.htm>

Young crystallographers' satellite meeting

Sunday, August 23rd, 2015, 9:00 AM – 3:00 PM, Rovinj, ADRIS Exhibition & Convention Centre (AECC), Lecture Hall 8

Registration fee: EUR 20

Electron Crystallography School – ECS2015

August 28th (Friday) – August 31st (Monday), 2015, Duga Uvala (Hotel Croatia)

Registration fee: EUR 180 (A number of IUCr supported student bursaries will be available. Detailed information can be found at the school webpage.)

Website: <http://www.blogs.uni-mainz.de/ecs2015/>

EosFit Workshop

August 28th, 8:30 AM – 5:00 PM, Rovinj, Hotel Lone, Meeting room 4 (ground floor)

Registration fee: EUR 30

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.

17 June 2015

BCA Industrial Group – XRF meeting, University of Leicester.

<https://sites.google.com/site/bcaxrf/meetings/17-june-2015>

21-23 June 2015

46th BACG Annual Conference, London.

www.bacg.co.uk

22-24 June 2015

Mesosopic & Condensed Matter Physics, Boston, MA, USA.

<http://condensedmatterphysics.conferenceseries.com/>

22-25 June 2015

UXSS2015. Ultrafast X-ray Summer School 2015, Hamburg, Germany.

http://conferences.cfel.de/uxss_2015/

24-26 June 2015

57th Electronic Materials Conference, Columbus, OH, USA.

www.mrs.org/57th-emc/

28 June – 2 July 2015

ZMPC 2015. International Symposium on Zeolites and MicroPorous Crystals, Sapporo, Japan.

www.zmpc.org/

28 June – 3 July 2015

Crystal Growth & Assembly. Gordon Research Conference. Biddeford, ME, USA.

www.grc.org/programs.aspx?id=12673

29 June – 3 July 2015

AFM2015. International Conference on Advances in Functional Materials, Long Island, NY, USA.

<http://functionalmaterials.org/afm-2015/>

29 June – 8 July 2015

EMBO Practical Course on High Throughput methods for protein production and crystallization, Marseille, France.

<http://events.embo.org/15-htp-protein/>

30 June – 3 July 2015

2nd International Conference on Nanomagnetism and Spintronics (RTNSA) & 7th International Workshop on Magnetic Wires (IWMW), Ordizia, Spain.

www.ehu.es/en/web/rtnsa-iwmw2015/home

4-9 July 2015

40th FEBS Congress, Berlin, Germany.

www.febs.org/

5-10 July 2015

Euroclay 2015, Edinburgh.

www.euroclay2015.org/

6-10 July 2015

SRI2015. 12th International Conference on Synchrotron Radiation Instrumentation, New York, NY, USA.

www.bnl.gov/sri2015/

12-17 July 2015

22nd International Conference on the Chemistry of the Organic Solid State (ICCOSS XXII), Niigata, Japan.

www.iccoss2015.org

13-19 July 2015

ISBIO 2015. Second edition.

<http://eventos.fct.unl.pt/isbio/home>

18-22 July 2015

ESBA2015. 10th European Biophysics Congress, Dresden, Germany.

www.ebsa2015.com

19-26 July 2015

Electron Diffraction for Quantitative Surface Structure Determination. ICSSOS workshop-3 on surface structures, Lodz, Poland.

www.wfis.uni.lodz.pl/ICSSOSworkshop2015/

20-22 July 2015

ANM2015, Aveiro, Portugal.

www.anm2015.com/

20-23 July 2015

12th International Conference on Materials Chemistry (MC12), York.

www.rsc.org/ConferencesAndEvents/RSCConferences/MC12/index.asp

25-29 July 2015

ACA2015. American Crystallographic Association Annual Meeting, Philadelphia, PA, USA.

www.amercrystalassn.org/

2-7 August 2015

20th American Conference on Crystal Growth and Epitaxy (ACCGE-20), Big Sky, MT, USA.

www.crystalgrowth.org/ACCGE-20---OMVPE-17-Conference.html

3-7 August 2015

64th Annual Denver X-ray Conference (DXC2015), Westminster, CO, USA.

www.dxcicdd.com/

6-14 August 2015

IUPAC-2015: 48th General Assembly and 45th World Chemistry Congress, Busan, Korea.

www.iupac2015.org

16-20 August 2015

250th ACS National Meeting, Boston, MA, USA.

www.acs.org/content/acs/en/meetings/nationalmeetings/meetings.html

20-22 August 2015

Advanced Software Development for Crystallographers, Duga Uvala, Croatia.

<http://sig9.ecanews.org/rovinj.html>

23-28 August 2015

ECM29. The 29th European Crystallographic Meeting, Rovinj, Croatia.

<http://ecm29.ecanews.org/>

24-27 August 2015

Structural Biology on the Move, Copenhagen, Denmark.

www.benzon-foundation.dk

24 August – 4 September 2015

European School on Magnetism (ESM), Cluj-Napoca, Romania.

<http://magnetism.eu/esm/2015/index.html>

26-28 August 2015

Dynamic Behaviour of Structures and Materials, Interaction and Friction across the Strain - PETER 2015, London.

<http://peter2015/iopconfs.org/>

30 August – 1 September 2015

2nd ICSU/IUPAC Workshop on Crystal Engineering, Como, Italy.

<http://convinceproject.eu/>

30 August – 3 September 2015

ESB2015 European Conference on Biomaterials, Krakow, Poland.

www.esb2015.org/

30 August – 4 September 2015

VI European Conference on Neutron Scattering, Zaragoza, Spain.

<http://ecns2015.unizar.es/index.php/home>

30 August – 4 September 2015

Aperiodic 2015, Prague, Czech Republic.

<http://crysa.fzu.cz/aperiodic2015/>

30 August – 4 September 2015

Joint AIRAPT-25th & EHPRG-53rd International Conference on High Pressure Science and Technology, Madrid, Spain.

<http://airapt-ehprg-madrid2015.com>

31 August – 5 September 2015

ECS2. Second European Crystallography School, Mieres (Asturias), Spain.

<http://ecs2.ecanews.org/>

5-8 September 2015

ESCG. European School on Crystal Growth, Bologna, Italy.

<http://escg2015.eccg5.eu/>

6-10 September 2015

European Conference on Molecular Magnetism (ECMM2015), Zaragoza, Spain.

<http://ecmm2015.unizar.es/>

6-18 September 2015

14th Oxford School on Neutron Scattering, Oxford.

www.oxfordneutronschool.org/

7-9 September 2015

Design and Engineering of Neutron Instruments, Budapest, Hungary.

www.bnc.hu/denim2015/

7-10 September 2015

VI International Conference of Synchrotron Radiation in Polymer Science, Madrid, Spain.

<http://srps6.com/>

8-11 September 2015

3rd International GISAS Conference, Nice, France.

<http://gisas2015.univ-lemans.fr/fr/index.html>

9-11 September 2015

Fifth European Conference on Crystal Growth, Bologna, Italy.

<http://www.eccg5.eu/>

13-17 September 2015

35th Symposium on Dynamical Properties of Solids, Munich, Germany.

<https://webapps.frm2.tum.de/indico/conferenceDisplay.py?confId=18>

13-18 September 2015

SAS2015. 16th International conference on Small-Angle Scattering, Berlin, Germany.

www.helmholtz-berlin.de/events/sas/

14-16 September 2015

FMC2015. Frontiers in Medicinal Chemistry 2015, Antwerp, Belgium.

www.ldorganisation.com/v2/produits.php?langue=english&cle_menu=1238915914&cle_data=1360153416

14-18 September 2015

23rd International Congress on X-ray Optics and Microanalysis (ICXOM23), BNL, Upton, NY, USA.

www.bnl.gov/icxom23/

14-18 September 2015

Neutrons and Synchrotron Radiation for Magnetism - Hercules Specialized Course 18, Grenoble, France.

<http://www.esrf.fr/events/conferences/HSC/HSC18>

14-18 September 2015

PULSE summer school, Porquerolles, France.

<http://pulse-school.sciencesconf.org>

14-25 September 2015

13th School on Synchrotron Radiation, Grado, Italy.

www.synchrotron-radiation.it

15-18 September 2015

2015 E-MRS Fall Conference & Exhibit, Warsaw, Poland.

www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=13&Itemid=1651

16-19 September 2015

XIIIth International Symposium on Biomineralization, Granada, Spain.

<http://granada-en.congresoseci.com/biominXIII>

16-23 September 2015

5th International Conference Nanomaterials: Applications & Properties, Lviv, Ukraine.

<http://nap.sumdu.edu.ua>

20-24 September 2015

XXIII Conference on Applied Crystallography, Krynica Górska, Poland.

www.cac.us.edu.pl/

21-24 September 2015

Size-Strain VII. Diffraction Analysis of the Microstructure of Materials, Oxford.

<http://www.size-strain2015.org/>

28-30 September 2015

Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.

www.icdd.com/education/rietveld-workshop.htm

28-30 September 2015

4th International Workshop on Neutron Delivery Systems, ILL, Grenoble, France.

www.ill.eu/nds2015

28 September – 2 October 2015

ICESSE-15. International Conference on Electron Spectroscopy and Structure, Stony Brook, NY, USA.

www.stonybrook.edu/commcms/icesse/index.html

28 September – 3 October 2015

International Rietveld School, Sofia, Bulgaria.

www.bgcryst.com/RS2015/

1-2 October 2015

Basic & Advanced Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.

www.icdd.com/education/rietveld-workshop.htm

12-16 October 2015

8th International Conference on Electromagnetic Processing of Materials, Cannes, France.

<http://epm2015.sciencesconf.org/>

19-20 October 2015

BCA Physical Crystallography Group Autumn Meeting, Cosener's House, Abingdon.

21 October 2015

International Workshop on Liquid-Liquid Interfaces, Grenoble, France.

www.ill.eu/liq2015

18 November 2015

BCA Chemical Crystallography Group Autumn Meeting, Glasgow.

29 November – 4 December 2015

Materials Research Society 2015 Fall Meeting, Boston, MA, USA.

www.mrs.org/fall2015/

5-8 December 2015

AsCA2015. The 13th Conference of the Asian Crystallographic Association, Science City, Kolkata, India.

<http://www.asca2015.org/>

6-10 December 2015

4th Nano Today Conference (Nano Today 2015), Dubai, United Arab Emirates.

www.nanotoday-conference.com/

14 December 2015

NMR Crystallography, Institute of Physics, London.

www.iop.org/activity/groups/subject/brsg

16 December 2015

BCA Biological Structures Group Winter Meeting, Manchester.



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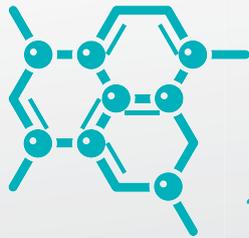


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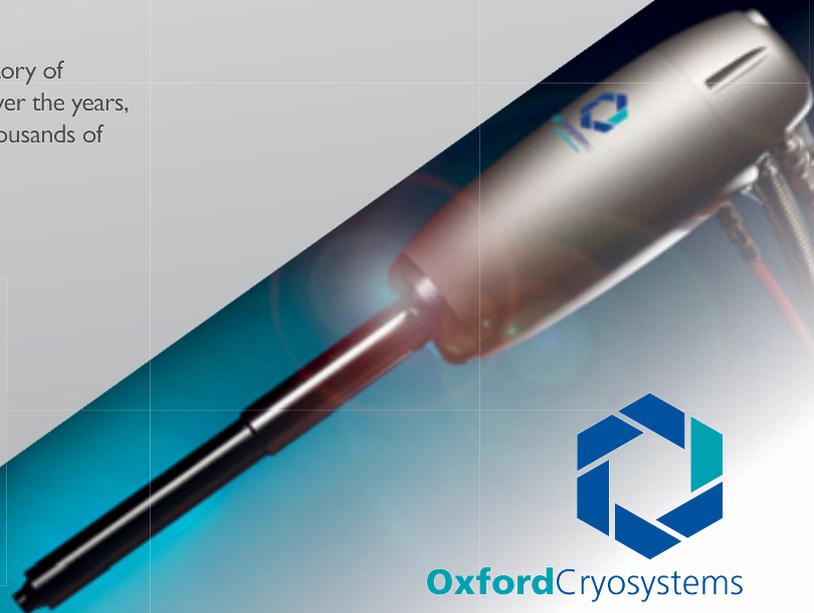
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