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British Crystallographic Association

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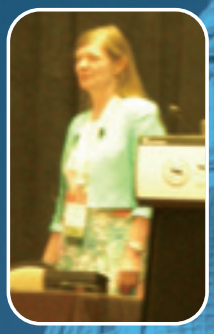

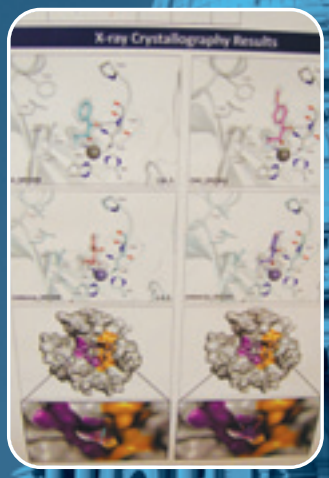

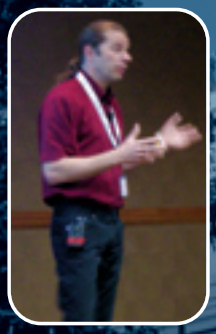

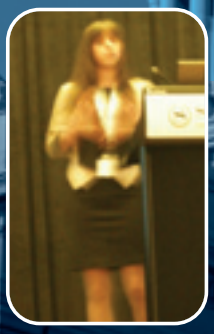

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by Bowmans, Leeds. Text should preferably be sent electronically as MSword documents (any version - .doc, .rtf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

ACA scenes: Fankuchen Lecture, poster art, BCA/CCDC speakers

From the President

SINCE my last *CN* column, planning has been in full swing for the 2017 BCA meeting, which will be held on the campus of University of Lancaster at the gateway to the Lake District. The programme committee, chaired by Andrew Bond, held the planning meeting on June 2nd at the conference venue. This allowed everyone the opportunity to look round the site, which looks well suited for the meeting. Lecture theatres are ample in size and there is plenty of meeting room space to accommodate the conference. The exhibition, posters and refreshments area is spacious and should allow space to linger and hold discussions, check email, etc. outside of the formal sessions, which I know is appreciated by attendees.

The programme is also taking shape. An outline can be found elsewhere in this issue and will also be available via the BCA website, which will be updated as the programme develops. In 2017 we are pleased to host the Bragg Lecture, which will be given by Prof. **Mike Glazer** (University of Oxford) and the Lonsdale Lecture given by Prof. **Kay Diederichs** (Universität Konstanz), which will mark the opening of the main meeting.

The four BCA Officers held our summer teleconference meeting on 30th June. These meetings are held midsummer and midwinter to enable discussion of BCA matters in between the biannual full BCA Council Meetings that are held in September and during the BCA Spring Meeting. Among a number of matters that we discussed were the process for identifying and selecting award winners and the election process for BCA Council. These matters will be further discussed and decisions taken at the September Meeting of the BCA Council, which will take place in Sheffield on 15th September. We propose to establish a formal nomination and selection process for the BCA Prize Lecture and Hodgkin Lecture. The Bragg Lecture, which is determined by the Bragg Committee, and is independent of the BCA, will also accept nominations via the BCA in future. These three lectures will be placed on a triennial schedule, with one per year being held at the BCA Spring Meeting. The Lonsdale Lecture has now been established as an annual lecture at the Spring Meeting. We have also responded to the fact that many BCA Council elections have had unopposed candidates in recent years. The Council had previously taken the approach that it has a duty to ensure that at least one individual stands for election for each available post since there is no limit to nominations from BCA members. Unfortunately, as other candidates have often not come forward, this has led to uncontested elections, which is not desirable. We are currently exploring options that will provide a mechanism to ensure two candidates to be nominated for elected posts and welcome input from the membership on improvements that we might implement.

Elections to BCA Council in 2017 will be for Treasurer and for one of the three Ordinary Member positions. Our current Treasurer, **Pamela Williams**, will be stepping down in 2017 after 5 years of service to the BCA in that post. **Amber Thompson** will complete a 3-year term as Ordinary Member. I would like to encourage nominations for these positions from the many able candidates among the BCA membership and to do so, as noted in the by-laws, with a view to ensuring a balanced representation of fields of interest and geographical areas. Details about the election process and the duties of those elected can be found in the BCA statutes (section E.4) and by-laws (sections D & E) on the BCA website at **http://www.crystallography.org.uk/about/statutes/**. Current membership of BCA Council can be found on page 5 of this magazine.

I would like to thank **Scott McKellar** for his involvement in the BCA as its webmaster, a position he will be stepping down from in September. We are seeking someone to take over this important position and encourage those interested in taking on this role either to contact me or Richard Cooper, who as former webmaster, will take on the role again in the interim until the position is filled.

One of my other roles outside my regular university position is as one of the 'Champions' of the Directed Assembly Grand Challenge Network, one of the EPSRC Grand Challenges in Chemistry, which has been operating since 2010 and now has over 1000 members. Its goals of understanding and harnessing self-assembly for the development of new materials across the physical and biological sciences and engineering align well with the interests of many BCA members. The network is actively engaged in enabling collaborations and support of early career researchers, through regular small conferences and workshops, summer schools and even modest seed-corn funding for collaborations. See **http://www.directedassembly.co.uk/index.html**.

In mid-July I enjoyed participating again as a lecturer in the Directed Assembly Summer School held in Cambridge. On this occasion I also had the opportunity to spend a little time looking around Cambridge and I was very pleased to discover the Whipple Museum of the History of Science, which has many fascinating artefacts from all areas of science. Of course it was hard for me not to be drawn to some items relating to crystallography or chemistry. There is a tremendous large-scale model of myoglobin, built by John Kendrew and Herman Watson in 1963. Another cabinet houses some old wooden molecular models of very simple molecules such as acetylene, fluorine (F_2), formaldehyde and water. Each has its original sticky label with the chemical formula handwritten on it. Most surprising, however, is that the model of water has on its label the structural formula H–O–O–H (even drawn with sensible O-O-H bond angles). I did query this remarkable error with the museum staff and was told that this could not be changed as the model is being displayed as it was received. I had hoped to include pictures of some items in this column, but discovered that the museum does not permit photos taken by visitors to be used in any publication. I would certainly recommend visiting the museum if you have a spare

half-hour or more in central Cambridge. The molecular models are shown on the museum website at http://www.hps.cam.ac.uk/whipple/explore/models/modellingchemistry/spacefillingmodels/ but sadly the label on the water molecule is not visible.

My final discovery at the Whipple was among the collection of slide rules. I am just old enough to have been required to use a slide rule for the first year of secondary school, before we then were allowed to use calculators. At the Whipple Museum I came across what was labelled as a Crystallographic Slide Rule. It compises two (movable) scales one with ratios from 1/10 to 10/1 and the other with angles from 0 to 90°. By the time I began crystallography as an undergraduate, desktop computers, which seem ancient today, were in use, so I never came across a crystallographic slide rule. After a little bit of investigation (using a well-known search engine) I realise that there were many specialist slide rules developed for specific calculations in different scientific disciplines and professions (finance, brewing, chemistry), but I didn't find anything to enlighten me beyond my own guesses on using a crystallographic slide rule. Perhaps there are some BCA members who once used one.

Lee Brammer

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From the Editor

AS I write this column, I am still in the United States relaxing after a very stimulating and enjoyable meeting of the American Crystallographic Association that was held in Denver, Colorado, from Friday 22 July to Tuesday 26 July. Once again, BCA members had a high profile at the meeting. Elspeth Garman gave the prestigious Fankuchen Lecture, "awarded to recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography". It honours the memory of Professor Isidore Fankuchen, who combined exactly these achievements. Some early work by Fankuchen features in another article in this issue. The Fankuchen award is only given every three years; and six years ago we had another BCA winner, David Watkin. Although Elspeth's lecture was scheduled for 8 AM on the final day of the conference, she still attracted a large, wide-awake and attentive audience. As well as giving a presentation in a different session, Pete Wood co-chaired the symposium on "Structure-Property Relationships" where I gave the first of my two talks. In that same session impressive talks were given by Lauren Hatcher and Laszlo Fabian. On the final busy Tuesday there was a 9-to-5 session on "Standard Practices in Structure Refinement and Validation" which was recorded for educational purposes. I had the first lecture in a final block of three, followed by Ton Spek and George Sheldrick – so no pressure there!

The venue for the conference was the downtown Sheraton hotel. A walk of less than two blocks yielded a clear view of the Colorado State Capitol Building, its shining dome clad in Colorado gold. Like many American cities, most of Denver is laid out on a north-south-east-west grid that is intuitively appealing to crystallographers. However, this particular crystal has a large defect. The downtown streets run at 45° to those in the rest of town. The reason is historical: Denver arose out of mining camps along the Platte River and Cherry Creek, which just happen to run diagonally to the cardinal compass points.

As always, it is impossible for one person to provide balanced coverage of a conference that runs in parallel sessions. It is even more difficult for someone who spends a certain amount of time in quiet corners mumbling through his own talks to make sure that they finish within the allotted time (mine did). In hopes of providing at least a flavour of the meeting, I include my summary in this issue.

It was interesting to attend the ACA business meeting (yes, it really was). The ACA is facing many of the same problems as the BCA. By common consent, and I would certainly agree, the programme for this year's meeting was one of the most interesting ever; yet the attendance was down by about 100 compared with last year. Dwindling travel grants were suspected as a cause, and holding joint sessions with a related scientific society and/or dovetailing the ACA meeting in the same place immediately before or after theirs were suggested as possible remedies. On the positive side, the ACA's new journal *Structural Dynamics* has continued to receive an abundance of good papers. It has now been in existence long enough to receive an impact factor, which is a commendable 3.667.

I am glad once again to print a report from our Industrial Group on their recent X-Ray Fluorescence meeting, held jointly with the Royal Society of Chemistry and written up in their usual speedy and comprehensive fashion. Also included in this issue is my report on the CCDC Research Day, which took place last May. This meeting provided a refreshing change from the usual conference fare. The presenters, mostly students, spoke candidly about the approaches that failed as well as those that were successful. I'm sure that by doing so, they saved their colleagues a lot of wasted effort trying to reinvent a broken wheel! For the future, I draw readers' attention to an important forthcoming event, the 16th Intensive Teaching School in X-Ray Structure Analysis, which will take place in Durham next March. That school has become the inspiration and model for a variety of courses elsewhere in the world.

PANalytical are continuing their generous support for early-career researchers. The winner of the latest round is introduced in this issue along with an invitation for applications in the next round.

Our friends in the ICDD have announced the latest call for applications for Ludo Frevel Scholarships. Since 1991 the ICDD has awarded 181 scholarships with a total value over $429,750. Applicants should be graduate students during calendar year 2017 with a major interest in crystallography. Applications must be submitted online to the website **www.icdd.com/resources/awards/frevel.htm** with a deadline of 16 October 2016.

A standard tactic of a disreputable editor seeking to boost circulation figures is to write something about sex. I shall do just that. We have another 80th anniversary to celebrate: in 1936 **Dorothy Crowfoot** (later Hodgkin) submitted her PhD thesis, entitled *X-ray crystallography and the chemistry of the sterols*, under the supervision of **J. D. Bernal**; and this work included crystallographic research on oestrone and androsterone. An article appears later in this issue covering the development of our structural understanding of sex hormones and their mode of action, from inferences about size and shape of steroid molecules derived from unit cell dimensions to full 3D structures of such molecules to structural studies on receptors and receptor binding.

Just about every British publication has given its opinion on Brexit. I intend to maintain this column as a Brexit-free zone; but for a crystallographic variant, take a look at the Puzzle Corner.

I hope that when this issue reaches you, many of you will have enjoyed the European Crystallographic Meeting in Basel. I hope that you also will have had the opportunity for some summer relaxation and are now ready for successful and productive crystallographic work.

Carl Schwalbe

BCA Council 2016

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

Full committee details on the BCA website

www.crystallography.org.uk

BCA Spring Meeting 10 - 13th April 2017

THE 2017 BCA Spring Meeting will take place at the University of Lancaster, following the format that has operated successfully for the last few years. The Young Crystallographers meeting starts at 13:00 on Monday 10th April and runs through to the morning of Tuesday 11th April. The main meeting starts formally with lunch and the first exhibitor's session at 12:15 on Tuesday 11th, and ends at 13:30 on Thursday 13th April.

We are pleased to announce the following prize and group plenary lectures:

Bragg Lecture:

Prof. **Mike Glaze**r (University of Oxford).

Lonsdale Lecture:

Prof. **Kay Diederichs** (Universität Konstanz).
Towards a better understanding of (non-)isomorphism in macromolecular crystallography.

BSG Plenary:

Prof. **James Naismith** (University of St. Andrews).

CCG Plenary:

Prof. **Santiago Alvarez** (Universitat de Barcelona).
Transition metal coordination polyhedra: shape, spin and secondary bonding.

IG Plenary:

Prof. **David Rugg** (Rolls Royce).
Crystallography for aerospace and nuclear sectors: an industrial perspective of the next decade.

PCG Plenary:

Prof. **Sharon Ashbrook** (University of St. Andrews).

The traditional early-career prize session will be held on the afternoon of Wednesday 12th April. The remainder of the program comprises three parallel sessions, with a selection of workshops also to be included. Planned sessions are outlined below, with some practical information concerning deadlines and abstract submission. Further details and updates are available at the new permanent base for the BCA Spring Meetings: http://www.bcaspringmeetings.org.uk/

We look forward to seeing you in Lancaster.

Andrew Bond
Programme Committee Chair

Biological Structures Group (BSG)

BSG Session (1): Antimicrobial Targets
*Chair: Dr **Lydia Tabernero*** (University of Manchester).

Keynote: Prof. **Bill Hunter** (University of Dundee).

Infectious diseases are still a major health burden worldwide and the increase of antimicrobial resistance to current therapies poses a serious threat for their eradication. The session will focus on new targets and new approaches to tackle these important challenges.

BSG Session (2): Extracellular Matrix and Cell Adhesion
*Chair: Dr **Jordi Bella*** (University of Manchester).

Keynote: Dr **David Hulmes** (CNRS, Lyon).

This session will focus on recent developments on the structural biology of extracellular matrix proteins and cell adhesion molecules including crystallographic analysis of their biosynthesis and molecular assembly mechanisms, processing, secretion and extracellular matrix deposition, and cell-extracellular matrix interactions.

BSG Session (3): Multidisciplinary Protein Structural Analysis
*Chair: Prof. **Clair Baldock*** (University of Manchester).

Keynote: TBC

Understanding the structure-function relationships of complex biological systems usually requires data obtained from several structural techniques that provide complementary insight into the biological problem. This session will look at recent developments on the combination of crystallographic analysis with techniques such as small angle X-ray scattering, NMR, electron microscopy or electron paramagnetic resonance, amongst others.

BSG Session (4): Advances and Challenges in Drug Discovery
Chair: TBC

Keynote: Prof. **Rod Hubbard** (University of York).

Recent years have brought the development of different approaches in drug development leading to more specific and sophisticated targeted therapies. Structure-based fragment methodologies together with protein-protein interaction inhibitors are now generating new opportunities for drug development. The session will focus on new advances and challenges in drug discovery and how structural analyses support their development.

BSG Session (5): Tackling Cancer: New Approaches to Therapy
Chair: TBC

Keynote: Prof. **Jane Endicott** (University of Newcastle).

Cancer is a multifactorial complex set of diseases that respond to a number of environmental and intrinsic factors. Understanding the molecular basis of different types of cancer is essential to progress towards better treatments.

The session will focus on new potential targets for cancer therapy as well as recent advances on the development of protein inhibitors of known targets.

BSG Session (6): Multiprotein Complexes
Chair: Dr ***Steve Prince*** (University of Manchester)

Keynote: Prof. **Mark Banfield** (John Innes Centre).

Multiprotein complex formation is at the centre of critical biological processes such as macromolecular assembly, receptor-ligand recognition, or host-pathogen interactions. Crystallographic analysis of these complexes remains a challenging problem due to technical complexity that starts at the molecular biology level and extends all the way to the structure determination. This session will look at recent representative examples of crystallographic analyses of multiprotein complexes, the difficulties encountered, and the approaches taken to overcome them.

Chemical Crystallography Group (CCG)

CCG Session (1): Computational Approaches
Chairs: Dr ***Anthony Reilly*** (CCDC), *Dr* ***Krešo Bučar*** (UCL)

Keynote: Dr **Colin Seaton** (University of Bradford).

The session will highlight computational methods in crystallography, crystal chemistry, materials science and crystal engineering. Emphasis will be on computational approaches aiding crystal-structure prediction and elucidation, structure-property correlations and predictions of physicochemical properties of organic, metal-organic and inorganic materials.

CCG Session (2): Chemical Insights from Charge Density
Chairs: Dr ***Hazel Sparkes*** (University of Bristol),
Dr ***Graham Tizzard*** (University of Southampton).

Keynote: Prof. **Simon Parsons** (University of Edinburgh).

The session will examine approaches to obtain insights into chemical processes and properties through analysis of the electron density. The aim is to include results obtained using both experimental X-ray diffraction data and theoretical methods such as charge density analyses, Hirshfeld surfaces or *PIXEL* calculations to obtain a more detailed understanding of the charge distribution in the crystal structure.

CCG Session (3) (joint with PCG): Complementary Techniques
Chairs: Dr ***Elliot Carrington*** (University of Sheffield; CCG),
Dr ***Emma McCabe*** (University of Kent; PCG).

Keynote: Dr **Paul Hodgkinson** (University of Durham).

Significant developments have recently been made to characterise crystalline and non-crystalline materials using techniques other than diffraction. Such methods are often especially valuable for materials whose behaviour is affected by local structure or disorder. The session will focus on complementary characterisation methods such as spectroscopy, and insights from theory and physical properties, including work from both chemical and physical crystallography backgrounds.

CCG Session (4): Multi-Component Crystals
Chairs: Dr ***Gareth Lloyd*** and ***Hayley Green***
(both Heriot-Watt University).

Keynote: Dr **Krešo Bučar** (UCL).

The session aims to highlight research on multi-component crystalline systems including co-crystals, solvates, hydrates, and inclusion compounds. Of particular interest is understanding structure-property relationships in such materials through their design and characterisation.

CCG Session (5): Extended Materials
Chairs: Dr ***Helena Shepherd*** (University of Kent),
Dr ***Jonathan Foster*** (University of Sheffield).

Keynote: Prof. **Neil Champness** (University of Nottingham).

Designing and synthesising extended materials with a desired topology remains an outstanding challenge in crystal engineering. Understanding how to control the assembly, and ultimately the properties, of such materials requires insights from a wide range of techniques alongside crystallography. The session welcomes contributions from speakers working with a diverse range of materials.

CCG Session (6) (joint with YCG): Would You Publish This?
Chairs: *Dr* ***William Lewis*** (University of Nottingham; CCG),
Claire Hobday (University of Edinburgh; YCG).

Keynote: Dr **Iñigo J. Vitórica-Yrezábal** (University of Manchester).

Following last year's success, this interactive session will discuss problematic crystal structures that can be hard to interpret and publish. After the opening keynote talk, the session is open for anyone to describe structural results that raise the session title question. The audience will discuss, with the aim to provide constructive advice. Problems might include charge imbalance or other chemical issues, poor resolution or data completeness, complicated disorder, highly restrained models, unexplained residual electron density, etc. A formal abstract is not required, but please contact the session organisers in advance of the meeting (as soon as possible!) if you wish to contribute; 1-3 slides will be requested for concatenation into a single session presentation. Contributions from YCG members are particularly encouraged.

Industrial Group (IG)

IG Session (joint with CCG): Phase Transitions
Chair: Dr ***Tony Bell*** (Sheffield Hallam University; IG),
Dr ***Katharina Edkins*** (University of Durham; CCG).

Keynote: **Dr Quanshun Luo** (Sheffield Hallam University).

The session will discuss phase transformations, including characterisation techniques and associated modelling. The aim is to discuss a broad range of chemical and materials systems under a variety of environmental conditions. Relevant abstracts are invited from all areas of the community.

Physical Crystallography Group (PCG)

PCG Session (1): Extreme Conditions
*Chair: Dr **Alex Gibbs*** (ISIS).

Keynote: Prof. **Stephen Blundell** (University of Oxford).

Working at extreme conditions can often provide critical access to particular areas of phase space and therefore deep insight into the behaviour of materials, along with surprises not predicted by current theory. The session will cover scientific and technological developments across a wide range of extreme experimental conditions such as high magnetic field, high temperature, low temperature and high pressure.

PCG Session (2): New Insights into Old Problems
*Chair: Dr **Mark Senn*** (University of Oxford).

Keynote: Dr **Abbie McLaughlin** (University of Aberdeen).

The session aims to present work that brings new structural insights into long-standing problems, where new methodology or unconventional techniques have been used to tackle problems which have conventionally been viewed as insoluble or, where the study of new materials has led to old problems being re-evaluated. Abstract submission is encouraged from a broad range of scientific areas.

PCG Session (3): Order/Disorder
*Chair: Dr **Helen Playford*** (ISIS).

Keynote: TBC

Structural disorder can be a material's defining feature. It can influence properties and applications, and change our understanding of fundamental physics. This session celebrates the order within disorder, with potential topics including (but not limited to): the structure of nanomaterials, single crystal diffuse scattering, pair distribution function analysis, self-assembly, low-dimensional materials, disordered magnetism, materials with anomalous physical properties, and so on. Studies that illustrate the challenges of dealing with complex materials are particularly welcome in this session.

PCG Session (4): Crystallography of Minerals and Planets
*Chair: Dr **Anthony Phillips*** (Queen Mary).

Keynote: TBC

Crystals are ubiquitous throughout our world and beyond it; we will focus in this session on the many applications of crystallography to Earth and planetary science. This might include experimental and computational studies of structure under geological conditions, at extremes of temperature and pressure; analysis of minerals with terrestrial or extra-terrestrial origins; and even remote crystallography from space missions.

PCG Session (5): Ad-hoc Session

This session is set aside to encourage presentation of the latest results that may not fit within the other session topics. Abstracts are invited from any area of physical crystallography.

Young Crystallographers Group (YCG)

YCG Session (1): YCG Presentations
*Chair: **Claire Hobday*** (University of Edinburgh).

Plenary: Prof. **Stefan Kaskel** (Technische Universität Dresden).

YCG Session (2): YCG Presentations
Chair: TBC

Plenary: Dr **Simon Coles** (University of Southampton).

YCG Session (3): Flash Poster Presentations
*Chairs: **Natalie Johnson*** (Univeristy of Newcastle), ***Alex Cousen*** (University of Bath).

YCG Session (4): How The Other Half Live
*Chair: Dr **Sam Horrell*** (University of Essex), ***Charlie McMonagle*** (University of Edinburgh).

Keynotes: Dr **Matthias Gutmann** (ISIS), Dr **Helen Playford** (ISIS), Prof. **Jane Endicott** (University of Newcastle).

This educational session aims to unite the fields of chemical, physical and biological crystallography. Three invited speakers will discuss their scientific approaches and point the way towards a brave new world of enlightenment and mutual understanding.

Registration and Abstracts

Registration and abstract submission open in October 2016. The deadline for early-bird registration is Friday 10th March 2017, and the final registration deadline is Tuesday 4th April. The deadline for abstract submission is Friday 20th January 2017.

Programme Committtee

Chair: **Andrew Bond** (University of Cambridge).

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

BSG: **Lydia Tabernero** (University of Manchester), **Jordi Bella** (University of Manchester).

CCG: **Gareth Lloyd** (Heriot-Watt University), **William Lewis** (University of Nottingham).

IG: **Ghazala Sadiq** (CCDC), **Helen Blade** (AstraZeneca)

PCG: **Nick Funnell** (ISIS), **Jan-Willem Bos** (Heriot-Watt University).

YCG: **Sam Horrell** (University of Essex), **Claire Hobday** (University of Edinburgh).

Workshops: **Horst Puschmann** (OlexSYS).

Organisers: **Steph Bryant**, **Nicola Peel** (HG3 Conferences).

BCA 2017

American Crystallographic Association 66th Annual Meeting

THIS year's Transactions Symposium was on a topic that has received a lot of attention from the ACA: Structural Dynamics. Since the Transactions eventually appear online, I shall not include a summary here. Instead, I shall summarise some of the other lectures that I found particularly interesting.

Innovative ways to teach crystallography provided a recurrent theme, not just in the session explicitly devoted to education. In the General Interest session **Shao-Liang Zheng** described the case study method adopted at Harvard. After students have learned the basic theory and practice of structure determination and refinement, groups of 3-4 students are given 2 weeks to prepare a critique of a crystallographic publication. The goal is to impart a clear understanding of the uncertainties which can arise in the measurement of experimental data and in the fitting of a structural model to these data. A detailed description is provided in J. Chem. Educ. 2016, DOI: 10.1021/acs.jchemed.5b00629.

Next, **Simon Coles** described the innovative 1-year MSc course, "Instrumental Analytical Chemistry" that has been established in Southampton (http://www.southampton.ac.uk/chemistry/postgraduate/taught_courses/instrumental_analytical_chemistry.page). While it provides the expected instruction in the theory and practice of crystallography, mass spectroscopy, NMR, other spectroscopies and separation science, its emphasis on role play distinguishes it from a conventional course. Students are given a patent with its dry and highly technical language, to use as the basis for a more popular article in the style of *Chemistry World*. After learning about laboratory management, they have to present a convincing business plan for their analytical laboratory to a "Dragons' Den" style panel. They are also given samples of a patented drug supposedly seized from "Soton Pharmaceuticals", a generics manufacturer of dubious reputation. This sample may comprise a novel polymorphic form of the drug as claimed by Soton, the established form, leading to a lawsuit for patent infringement, or a counterfeit drug, leading to criminal prosecution. Students appear as expert witnesses in a mock court.

Two other "General Interest" presentations were particularly noteworthy. **Carolyn Brock** continues to find highly interesting features in her chosen field of high-Z' molecular crystals. Out of more than 280 structures in the CSD with $Z' \geq 4$ and $R \leq 0.075$, 25-30% have layers: strongly (hydrogen) bonded slabs separated by two-dimensional regions of van der Waals contacts. Frequently each layer has higher approximate local symmetry than does the crystal as a whole, and successive layers may be related by rotation. It seems likely that such layers may suggest mechanisms for crystal nucleation and growth.

Erin Davis from the American branch of CCDC reminded us that, far from maintaining as an exclusive closed system the wealth of structural data in the CSD and the powerful software associated with it, CCDC is keen to make integration with third party software as easy as possible. While the details of CSD interfaces can be highly technical, the API (Application Programming Interface), which is roughly equivalent to a scripting language, makes it straightforward. Erin gave examples of popular software that has been successfully integrated with the CSD.

A session following this one had the explicit title "High Impact Crystallographic Education". **Gervais Chapuis** began by telling us about "Innovative Tools". Because most institutions are cutting the time devoted to lectures on crystallography, students need to use modern communication technology. MOOCS (massive open on-line courses) are beginning to cover crystallographic topics. Shorter applets have been written by, among others, **Kevin Cowtan**, **Dean Johnson** and **Thomas Proffen**. In the future students are likely to want applets for their tablets or smartphones.

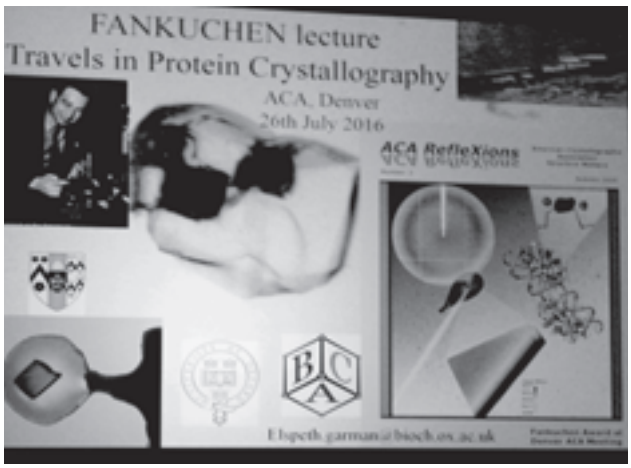
Under the intriguing title "What do you Mean "Less Than" **Louise Dawe** showed how the teaching of VSEPR (Valence Shell Electron Pair Repulsion) can be enriched by using real data from the CSD rather than the standard model kits which may give the false impression that the geometric parameters always take on ideal values. She had advanced fourth year students prepare teaching materials for use by first year students. The "clients" gave reviews of the material, mostly very favourable.

In view of my own research interests, I made sure to hear a lecture by **Susan Reutzel-Edens** entitled "Digital Design of Pharmaceutical Solids" in the session "Advances in Supramolecular Chemistry". The pharmaceutical scientist seeking improved properties, particularly higher solubility, can usually do nothing to change the active pharmaceutical ingredient (API). The choice of salts or co-formers may provide suitable alternatives. A plot of free energy versus temperature is instructive. An amorphous solid offers higher solubility but usually requires polymer to inhibit recrystallization. Susan stated that "we live in fear of the ritonavir / rotigotine scenario", i.e. the unexpected appearance of a more stable and less soluble crystal form of a drug after it has already been marketed. A survey made two years ago of about 50% parent compounds and 50% salts showed that the majority had multiple polymorphs or hydrates. No particular attribute has been shown to render a molecule liable to polymorphism. We shall still require solid form screening in the foreseeable future, but the calculation of crystal energy landscapes by **Doris Braun** and **Sally Price** has shown encouraging correlations between observed structures and favourable positions on the plot.

Then I crossed to a session with the intriguing title "Things We No Longer Need to Know". Inevitably there are a number of key concepts, now embodied in software that we can apply in routine work without any deep understanding. However, when difficulties arise, we need that understanding. The title of the first talk, by **John Rose**, contained the words that summarised the matter: "Button Pushers or Crystallographers". Under the title "Some Reflections on Symmetry" **Bill Clegg** was a

persuasive advocate for such deep understanding, particularly of pseudosymmetry. He outlined three cases. The first one was a structure in space group P-1 that resembled $P2_1/n$: the unit cell had an interaxial angle near 90°, and *h0l* reflections with *h*+*l* odd were systematically weak (about 10% as intense as other reflections). The pseudosymmetry was further complicated by twinning, the minor component amounting to 17%. Next Bill introduced an oxirane derivative with evident monoclinic symmetry. It gave a clearer structure solution in $P2_1/n$ than in $P2_1$ but a worse refinement, the oxirane ring being disordered. The explanation is that this structure is a pseudo-racemate with Z' = 2 and near-perfect inversion except for the chiral attachment of the oxirane. Bill's final example was triclinic, thought to be a Co complex, and incapable of solution by standard direct methods. However, recourse to a Patterson map (something else we thought we could forget about!) produced a model that refined to R = 0.09. The only problem was flat cyclohexane rings. Even fitting them as two overlapping rings failed to solve the problem. Refinement in P1 allowed the rings to attain the expected geometry. The lesson is that we must know about metric *versus* space group *versus* diffraction symmetry. Next, **Carla Slebodnick** renewed our acquaintance with point group diagrams. In a generous succession of diagrams starting with the transition from $P2_1/c$ to 2/m, she showed how the suppression of translations in space groups that we know and love converts them to point groups. Finally, **Amy Sarjeant** gave us a tool for visualising matrix transformations. Sometimes under circumstances like high-pressure crystallography we may collect a set of reflections indexed in a non-standard space group that we subsequently wish to convert to standard; alternatively, the standard $P2_1/c$ may have very oblique axes while $P2_1/n$ looks more reasonable. The function Change Space Group Setting in the CCDC's Mercury software provides a convenient and vendor – independent means of carrying out such transformations.

In her Fankuchen Lecture **Elspeth Garman** wove a colourful tapestry of personal anecdotes and research results. At age 18 she went to Swaziland, tasked with the demanding job of teaching not just English but the entire curriculum except for the local language. This gave her a sense of mission for teaching along with practical lessons about how to do it effectively: whether speaking to a large class of very lively young Swazi schoolgirls or to a collection of crystallographers, it is important to speak slowly and distinctly and always to hold the audience's attention. Her physics PhD at Oxford included valuable training in using the machine shop and work on using accelerator mass spectrometry for carbon 14 dating of archaeological and historical artefacts. Her postdoctoral research on parity violation in nuclei not only was cutting-edge nuclear physics but also provided discipline in being absolutely certain of one's data. With this post coming to an end and a young family to think about, Elspeth took up **Louise Johnson**'s suggestion to work in the Laboratory of Molecular Biophysics, still in Oxford. When concerns were raised about her wish to work part-time, Elspeth replied that "You will have part of my time but all of my brain". As X-ray Facilities Manager she put her workshop training to good use, and her knowledge of radiation physics led her to help develop systematic methods for cryo-cooling protein crystals, thereby reducing radiation damage rates about 70-fold. As crystal mounting loops with minimal X-ray absorption she first used hairs extracted from her wincing baby, then, more humanely, threads from Louise's mohair jumper. The maximum dose of radiation that a crystal can absorb before it loses half its diffracting power is dictated by physics and is now called the



The title slide for Elspeth's talk, featuring Isidore Fankuchen, an irradiated crystal and the ACA RefleXions cover image (provided by Jonathan Brooks-Bartlett and Charles Bury).

Garman limit. Secondary chemical reactions may speed up the degradation. Spectroscopic measurements on irradiated lysozyme show that solvated electrons appear very rapidly, followed by disulphide radical anion. Nitrate added as a scavenger steadily becomes reduced over time, protecting disulphide bonds from damage. Dose calculation in 3D enables rotation of the crystal so that the beam traces out a torus, avoiding overdosing of any one region. It may be necessary to establish which heavier elements (metals, phosphorus in DNA and RNA etc) are present in a protein. Proton induced X-ray emission (PIXE) makes this possible. Finally, Elspeth regaled us with her adventure with the press. As part of the vital work making HIV infection a treatable disease, she was part of the team that attempted to grow crystals of HIV reverse transcriptase by the hanging drop method. However, the crystal quality was poor and so the group tried crystallisation carried out in microgravity on the space shuttle (1988: STS26). While the Daily Telegraph gave an accurate summary of this work, the Daily Star trumpeted "Madness! Boffins put AIDS in space".

Carl Schwalbe

XRF Meeting Report 15th June 2016

A joint BCA/ RSC Atomic Spectroscopy Group Meeting at University of Leicester

Overview of Event

THE XRF group is a sub-committee of the British Crystallographic Association (BCA) which covers a range of instrument techniques and interest areas. Further details can be found at http://www.crystallography.org.uk/

Annual meetings are held by each sub-committee which gather together industrial users, academics and instrument vendors in one place. This year's XRF meeting was held at the University of Leicester in collaboration with the Royal Society of Chemistry and was attended by 47 delegates along with 10 vendor stands presenting their products.

Morning Sessions

Session 1

The welcome to the BCA XRF meeting of 2016 at Leicester University was given by **Nick Marsh**.

The chair of the session, **David Beveridge**, then introduced Professor **Andrew Shortland** who gave a fascinating talk on XRF analysis of historical glass and glazes. After a short introduction to Cranfield Forensic Institute, Professor Shortland described the work performed on Meissen porcelain glazes. Differentiation between visually similar items of porcelain is critically important to auction houses and collectors.

Provenance dramatically affects the value of porcelain, reducing the £100K price tag of a genuine 18thC piece to just £1000 for a fake. Later 19thC reproductions produced by the Meissen factory from original moulds and later repairs or conservation of original 18thC pieces complicate the situation further. A bench top XRF instrument was used to non-destructively analyse over 300 original objects, and 800 fragmented pieces of known origin. This created a database and cluster plots were generated to characterise early porcelain. The elemental composition of enamel and gilding also allowed for differentiation between restored and original pieces accurate to within a 10-30 year timeframe for the Meissen factory. Professor Shortland went on to describe the in-situ HH-XRF analysis of a medieval glass window at Christ Church Cathedral, Oxford. Using early fragments of 17thC glass found in a coal hole (!) for comparison and balancing precariously on a ladder (!!) to do the measurements, the entire window was mapped for 12 elements. Using compositional groupings, the results showed that much of the original window had been taken down but later restored by a contemporary artist (and an English Civil War document supported this finding) while Victorian and modern glass inclusions were also identified.

The exhibitor's forum followed with representatives giving 3 minute overviews of their latest instruments, innovations and products:

SciMed (Paul Vanden Branden)

- Introduced the Rigaku Nex-DE ED-XRF with 60kV tube and SDD high speed detector; the WD-XRF Primus and Supermini 200 bench top XRF. The Hitachi SE1000 large capacity mapping spectrometer was also mentioned.

Spectro (Graham Hibberd)

- Presented the latest Spectro XEPOS benchtop ED-XRF; this direct excitation instrument features a bandpass filter and new detector to handle high countrates.

Niton UK (Ken Granger)

- A live real-time demonstration of HH-XRF described the features and applications of the different Niton models available.

Spex Europe (Dave Speake)

- XRF sample preparation equipment (mills, grinders and cryogenic mills), pellet presses and the latest 1, 3 and 6 place Katanax electric fusion machine were shown. A fusion method development service is available in addition to binders, fluxes and ICP liquid standards. The presentation closed with a tribute to Fernand Claisse (1923-2016).

Bruker (Simon Bailey)

- A new WD-XRF crystal, the XS-400 was described. The performance of this surface-treated crystal was compared to the LiF200 and LiF220; it gives good signal-to-noise, increasing sensitivity for transition metals. A lab report on this new crystal is to be released shortly.

Specac (Allan Finlay)

- Presses and dies for XRF pressed pellet preparation were featured. Manual, electrical, auto-touch and hand press models are available; some with evacuable dies. Heated presses are also available and suitable for producing thin films from polymers.

PANalytical (Michael Brogan)

- The new Zetium WD-XRF was presented; different Zetium models feature a Theta free lime channel, small spot mapping and WD/ED core combinations. In 2014, Claisse merged with PANalytical bringing in-house fusion systems and fluxes into the PANalytical portfolio.

Shimadzu (Lee Parry)

- The product range of HPLC, GC-MS and LC-MS was described. Shimadzu offer applications, technical support and FOC training in conjunction with the RSC. The EDX-7000 and 8000 bench top instruments were featured.

Datech Scientific Limited (Adam Housley)

- An extensive range of XRF sample preparation equipment (Herzog) and automated lab solutions (Nucomat) were presented. New additions to the portfolio include LIBS and LA-ICP-MS instrumentation from Applied Spectra.

XRF Scientific (Frederic Davidts)

- Socachim fluxes, platinumware and the Phoenix II cold-cold fusion machine were featured. XRF sample preparation equipment for crushing, milling and pressing are available. The xrWeigh was presented; this carousel can weigh up to 30 vials of flux in 20 minutes with one-touch operation.

Overall, the suppliers' representatives kept to their allotted 3-minutes slots, much to relief of the chair. The presentations were very informative and welcomed by the delegates who were then encouraged to visit the stands during the lunch break.

Heather Harrison and **Racheal Ige**, British Gypsum.

Session 1 Speakers: left to right: *Simon Bailey, Frederic Davidts, Chris Calam, Allan Finley, Ken Granger, David Beveridge (Chair), Adam Housley, Lee Parry, Michael Brogan, Paul Vanden Branden, Thierry Theato and Dave Speake.*

Session 2

New super eruptions from Yellowstone hotspot: XRF fingerprinting

Leicester University's Dr **Tom Knott** told us about the super eruptions which can cover 10,000 km^2. No need to worry though, as we have only had 42 in the last 36 million years! Looking at Yellowstone in USA, he studied Snake Plain as part of an international team to understand effects and frequency. Snake Plain formed at 900 °C to 1000 °C. With multiple eruptions it can be difficult to identify one from another. XRF is used to look at trace element ratios. A 2 km borehole revealed analysis of Ti, Si, Al & Fe consistent throughout the core. However, problems arose when looking at rhyolites. When samples were analysed by two separate labs there was a 20% discrepancy; this was due to the USA lab running samples outside the calibration range.

Tom found that the biggest single continual eruption was at Castleford measuring 1900 km^3, this being the 2nd largest in Snake River. The frequency of these eruptions has tailed off. Tom assured us that Yellowstone is safe to visit and the pictures look truly amazing.

Recent ground breaking developments in ED XRF

"The more counts the better!" This was the message from Thierry from Spectro. Traditional ED XRF gives around 100,000 cps and WD systems give 1,000,000 cps. This all

leads to fewer errors for us the user. The ED XRF XEP05 offers nearly ten times more counts than their previous ED XRF and is 3 times more sensitive by using direct excitation. The new Pd/Co alloy X-ray tube can use Pd for (Na-Cl, Fe-Mo, Hf-U) with the Co for K-Mn; the advantages are like having 2 tubes in 1. This new instrument uses polarized and direct excitation, with a band pass filter with a 60 KV tube. The Co/Pd tube is difficult to manufacture so tube targets can't be changed for different elements but the Co/Pd alloy is doing a great job at delivering the magic million cps for ED XRF.

DOT 3 Update

So it's time to find out how good we are at analysing the unknown. Ros provided feedback on the results obtained for the DOT 3 sample which was a gypsum based cement that consisted of mainly calcium and sulphur. The data were variable but normalising the data to CaO gave better grouping and removal of IR combustion analysis made trending sulphur easier. With a number of fused bead results low in sulphur, these are likely to be from loss on fusion. Calibration errors may well be adding to the variability. CaO and SO_3 were good on pressed pellet, but high results arose on SiO_2 and Al_2O_3.

The best approach to analyse the sample was explained by Heather from British Gypsum. Heat sample at 45-50 ºC to remove any free water. Fusion was then carried out by pre-igniting at 1000 ºC for 1 hour, using 66 % lithium tetraborate and 34% lithium metaborate in a ratio 7:1. Raw materials and certified reference materials were used as standards. To note, because these samples contained sodium, these wouldn't make a good plaster, as these migrate to the surface causing stains. Thanks to all that carried out analysis.

Judith from Alfred H Knights gave us an insight into how to carry out the analysis of unknown samples. Start by checking if your sample is wet? Think about what the loss on ignition (LOI) will tell us with regards to carbonates, volatiles or gains. Trial a fusion at 9: 1 g (lithium tetraborate/lithium metaborate) and utilise an internal standard. Judith then invited us all to analyse a DOT4 sample. We were all given a clue about the composition being a ferromolybdenum sample that requires oxidation… but what else can we find in this? Let's get busy and send our results in for next year.

Adam Grayson, Johnson Matthey

Session 2 Speakers: left to right: *Judith Bain, Iain Howland (Chair), Tom Knott, Heather Harrison, Thierry Theato and Ros Schwarz.*

Afternoon Sessions

Session 3

Session 3 Speakers: left to right: *Paul Vanden Branden, Steve Davies and Judith Bain (Chair)*

Calibration Strategies for Quantitative XRF Analysis

Paul Vanden Branden, SciMed.

Paul started from first principles, that quantification is the conversion of measured intensity into concentration, according to:

$$W_i = f(I_j, "matrix")$$

which he expanded to

$$W_i = (aI_i^3 + bI_i^2 + cI_i + D)(1 + "Matrix") + Line\ Overlap$$

Where $(aI_i^3 + bI_i^2 + cI_i + D)$ are calibration constants x intensity

And $(1 + "Matrix")$ is the matrix correction coefficient

He began by showing a basic linear empirical calibration, equivalent to "y = mx + c",

$$W_i = (cI_i + D)(1 + "Matrix") + Line\ Overlap$$

The slope and intercept of this line form the calibration coefficients.

The effect of changing the sample matrix was discussed using PbO in glass as an example. Adding another component to the matrix gave a PbO calibration line with a different slope, because the MAC (mass absorption coefficient) of the sample had changed.

Paul described the different types of matrix effects, absorption and enhancement, and strategies for compensating for them.

Alpha Corrections.

In the general formula for quantitative calculation this is the "1 + Matrix" term:

$$W_i = (bI_i^2 + cI_i + D)(1 + \alpha) + Line\ Overlap$$

Where α is a calculated correction coefficient for the absorption / enhancement effect of other components in the sample.

Sometimes the Alpha Correction approach cannot be used, if for example, the full compositional information on our calibration standards is not known.

Paul presented some possible alternative approaches to matrix correction as follows;

Internal Standardisation

- With internal standardisation, we add a selected component to the sample
- The addition is maintained at the same concentration for all standards / samples
- Measure the analyte and internal standard peak intensity and ratio analyte to internal standard
- Calibration is concentration vs. intensity ratio

The calibration is independent of matrix effects.

Scatter Correction – Compton and Background

In the earlier example Paul explained how the intensity of a measured peak was affected by changes in the matrix absorption coefficient. We also find that other spectral lines are affected the same way, in particular, tube or secondary target lines which are scattered by the sample. Hence there is a consistent relationship between the analyte intensity and the Compton scatter peak from the X-ray source.

This method can be useful when the matrix is "unknown" e.g. waste materials.

However, if there are any major absorption edges between the analyte line and the Compton scattering, the correlation to the sample matrix is broken and the correction does not work well.

Background in XRF is also caused by scattering. Paul used an example of Zn peak intensity ratioed to its own background.

Standard Additions

This method is effective when we don't have calibration reference samples and can't generate a calibration curve.

A known amount of the element to be analyzed is added and then we estimate the concentration of the element by the increasing ratio of x-ray intensities.

We need to pay attention to the following items:

– Since it is assumed that the calibration curve is linear, this method is applicable to concentrations below 1 %.

– We have to use net intensities (with background subtraction). Any inaccuracy in background correction = error in result.

– In the case of powder sample, we need to add the element by solution; adding the solution as the whole sample is soaked, mixing well and drying it, then pressing the dried sample.
– Standard additions analysis may be prone to mineralogical errors.

Conclusion

- Many options to calibrate
- Choose carefully based on sample type and amount of CRMs available

Small Spot Mapping – The Latest 'Must Have'

Steve Davies, PANalytical.

It is becoming popular because of the following reasons: small spot analysis with element distribution mapping is an ideal tool for materials research and production process troubleshooting. No longer confined to research facilities, this technique is now available anywhere you need it.

The latest developments in XRF analysis allow bulk analysis combined with small spot analysis and elemental mapping on a single device. The added capability of small area analysis and elemental mapping on a fine scale extends the scope of possible applications for basic investigations in materials research and production control.

Wavelength dispersive (WD) XRF and energy dispersive (ED) XRF are used in combination with two detectors for light and heavy elements. This combination expands the scope of applications of the instrument. In addition to the accelerated data acquisition, using the ED core for small spot analysis provides other benefits like allowing the WD core to exclusively perform high accuracy and precision bulk analysis.

Unlike other elemental mapping techniques such as electron microprobe analysis or scanning electron microscopy which require extensive pre-treatment of samples the XRF method requires minimal sample preparation.

Applications include: Metals analysis, Geological, Small samples, Inclusions, minerals.

Steve said that he was looking to achieve several points:

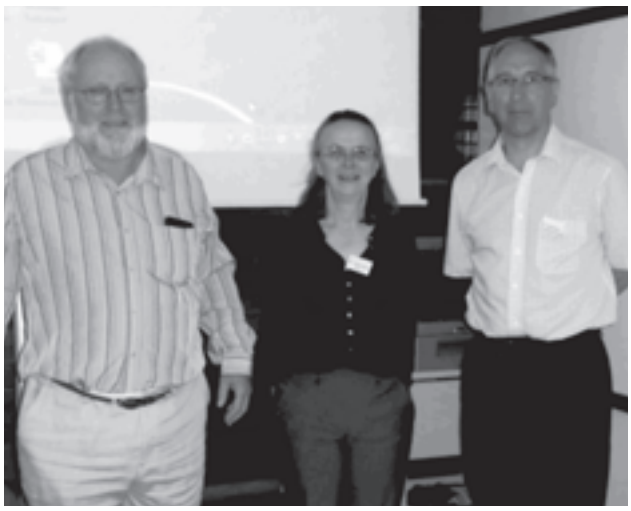
What's the precision of measurement of a small spot, homogeneity of prepared specimens? Is the sample the same at different points on the surface?

He used a bead made from DOT-3 to test for sensitivity of light elements and reproducibility over 10 measurements on one spot. To examine the homogeneity of fusion he used a pre-prepared specimen of ECRM776-1 measuring 5 separate spots down a radius of the bead.

He found that the precision values were as expected, although he was disappointed about light element results. A different flux would have been more appropriate for the fused bead. Homogeneity was good but he concluded that he should look after his beads better!

Richard Morris, Morris Analytical X-ray Ltd.

continued overleaf



Session 4 Speakers: left to right: *Jonathon Prus, Ros Schwarz (Chair) and Charles Shand.*

… and finally some scenes from the Exhibition:

Session 4

Trace element analysis of whisky by TXRF

(Dr Charles Shand)

This was an interesting topic and concept, which was to see if TXRF could be used in order to group different whiskies from different regions of Scotland, as well as be able to identify counterfeit whisky. All the elements in question (11 in total) had to tell apart the raw materials, product process equipment, storage vessel and any additives that were used in order to paint a full picture of the final product for good traceability. From the results it was clear to see that there were noticeable groups with only few overlaps. What was interesting was the major difference in the counterfeit whisky which was in a clear group by itself with considerably more Br present. These results were compared to ICP and were in good agreement. This proved that although TXRF is not commonly used for trace analyses of elements in alcohol, that it can play a role in this process.

Quantitative aspects of iron extraction in the Sussex Weald

(Dr Jonathan Prus)

The final talk of the day was based on iron minerology which was close to many people's area of work but also had a historical twist.

The efficiency of the bloomery iron smelting technique to extract iron from its oxides and slags was discussed. PXRF was used to compare the larger samples from different sites and then compared with electron microscope which fell within the tolerance and matched fairly well. From the results it found that around 44% of iron was extracted leaving behind a considerable amount which went to show that this method used was not for efficiency but more because it was a simple way to smelt.

Robert Wood, Alfred H Knight

CCDC Research Day 18th May 2016

THIS annual event provided an opportunity for young scientists, usually in research groups collaborating with the CCDC or in the CCDC itself, to give half-hour presentations on their research. Due both to the generous time allocation and to the presence of kindred spirits in the audience, there was a relaxed ambience. Presenters felt free to describe the blind alleys in their research as well as those approaches that were productive; and they divulged their plans for future research, inviting comments. In his welcome message Colin Groom aptly pointed out that we would be "seeing science as it happens". He also paid tribute to Jack Dunitz, who was a keenly interested member of the audience as he has been in every single Research Day.

With the title "Hydrogen bonding in solution and the solid state" **James McKenzie** (University of Cambridge) discussed how non-covalent interactions can be quantified. From the association constants for hydrogen bonded complexes in solution ΔG can be calculated and then related to donor strength α and acceptor strength β by the simple equation $\Delta G = \alpha\beta$. However, there is a lot of functional-group scatter, especially for β. Hydrogen bond (HB) stabilities can be evaluated from information in the CSD: HB lengths, HB linearity and propensities $P_{A/D} = N_{HB} / N_{tot}$, where N_{tot} is the total number of observations where groups A and D are present while N_{HB} is the number with HB between these groups. Due to missed HB or steric inaccessibility a plot of α against P has a fair amount of scatter. A plot of β against P has even more scatter because there are more acceptors than donors in the database, so some are out-competed. This idea of competition led to the application of Trueskill, developed by Microsoft to rank computer gamers and put together evenly matched opponents. A Bayesian ranking system is updated by the results of each new match. A plot of β against acceptor Trueskill rank shows promising linearity.

Rachel Skyner (University of St. Andrews) addressed a pharmaceutically fundamental property under "Using the CSD to probe solubility and its prediction". ΔG of solution is usually calculated via a cycle involving sublimation of the crystal followed by hydration. Structural information relevant to hydration can be derived from organic hydrates in the CSD, yielding radial distribution functions (RDF) which overlay quite well with the RDF for liquid water. These functions are to be applied to solvent accessible surfaces. Rachel's other goal was "solubility by design". She found that the General Solubility Equation cannot be significantly improved by retraining its coefficients. Instead, descriptors were assigned to a set of structures in the CSD for which melting point and solubility were known. Descriptors included such things as atom count, fragment count and molecular graphs. Sophisticated regression techniques were used to evaluate their importance.

Luca Iuzzolino (UCL) presented the "Thoughts on using the CCDC Conformer Generator for crystal structure prediction (CSP) of large flexible molecules". Luca described the progress made in the latest (6th) Blind Test of CSP. Participants were challenged with more complex structures than ever before. Reflecting the significance of polymorphism, they were invited to submit lists of 100 predicted structures rather than just the 3 they deemed the best. Encouragingly, the UCL group found the known form in its list of 100 for 6 of the test molecules. Unfortunately, despite such positive developments, the pharmaceutical industry makes little use of CSP because of the high computational cost for the flexible molecules of interest. Applying the conformational information in the CSD, Luca aimed to cut this cost by using the Conformer Generator (CG). He dispensed with *ab initio* calculations where torsion angles show clear preferences such as the central bond in amide groups. For the rotatable bonds deemed most important, particularly ring-ring or ring-chain junctions, *ab initio* calculations were carried out; but the range was restricted to values from CG and Mogul. Good correlations with full *ab initio* results were obtained for structure XXVI from the Blind Test.

In her talk "Structure determination from powder diffraction data: the power of prior conformational knowledge" **Elena Kabova** (University of Reading) showed that the power and usefulness of the CSD extend to the early stages of structure determination. Using DASH, one can routinely solve structures with up to 15 rotatable bonds from powder diffraction data. Larger structures such as verapamil with 22 degrees of freedom (DoF) require many attempts, while a structure like d-sorbitol (33 DoF) is extremely difficult. Tuning the simulated annealing parameters to the new "aggressive" set has provided some help. Prior conformational knowledge can be taken from MOGUL, the MOGUL distribution bias or the Conformation Generator and used as a constraint in simulated annealing calculations, which can be run in parallel. Allowing torsional flexibility of ±20°, this method was tried on the test structures. The calculation time for verapamil was reduced from 68 hr with the standard method to 2.5 hr. However, the method was unsuccessful for ritonavir because of its unusual torsion angle.

Mat Bryant (CCDC) reported research done at Bath on "Vapochromic platinum pincer materials". Planar four-coordinate Pt(II) complexes are formed by a conjugated 2,6-dipyridylbenzene ligand coordinating through both pyridyl N atoms and a central phenyl C atom. The fourth position on Pt is occupied by a ligand that can be chosen to tune the properties of the complex; π-donor strength affects the HOMO-LUMO gap. A substituent placed at the 4-position of the phenyl ring also affects the properties of the complex. The planar geometry facilitates the formation of stacks with close contact between successive Pt atoms, further affecting the relevant orbitals. A representative complex is red under moist air (I) but becomes yellow if dried (II). In the presence of methanol, the crystals are blue (III). Crystal structures show that in (I) water occupies helical channels and Pt atoms form a zigzag pattern. In (II) a slight scissors distortion impairs the alignment of Pt atoms. In (III) the MeOH requires wider channels.

continued overleaf

Chris Radoux (University of Cambridge and CCDC) began his talk "Identifying interactions that determine fragment binding at protein hotspots" by presenting various authors' definitions of a hotspot: a site that (1) makes a disproportionately large contribution to ΔG of binding, (2) is particularly sensitive to changes in the molecule, (3) binds a fragment or fragments, or (4) is occupied by an "unhappy" water molecule. For purposes of fragment-based drug discovery, a fragment has found a hotspot if it stays there as it is joined into a candidate drug. A site is "ligandable" if it receives multiple hits with various fragments. Methodology for identifying the important sites was successfully tested [C. J. Radoux *et al.* (2016) *J. Med. Chem.,* **59**, 4314-4325] on pantothenate synthetase. SuperStar with an aromatic CH probe for hydrophobic sites, an uncharged NH probe as a hydrogen bond donor and a carbonyl O probe as an acceptor was used to predict hotspots on the apo enzyme. To cull the plethora of possible sites, they were weighted to favour buried pockets. Thereby, scores were assigned to sites. When crystal structures with bound lead molecules were superimposed onto the apo enzyme, fragment atoms were consistently found in the highest scoring regions.

In his talk entitled "Using protein binding site information in virtual screening" **Timo Krotzky** (CCDC) continued the theme of analysing binding sites. With a target protein of unknown structure one has to adopt a ligand-based approach, aiming to define a pharmacophore. If the protein structure is known, one can do receptor-based design. Binding site comparisons are better at the structural level than if they are merely sequence-based since the latter can be misled by convergent evolution. Structural cavity comparison is implemented by using CavBase (part of Relibase) to scan the surface and detect clefts. The design of the automatic grid-based approach is important because *ca.* 30% of the structures in the PDB are of the apo form; and in the absence of a ligand, pocket volume is reduced by intrusion of protein atoms. Next, binding sites are transformed into molecular graphs, combined into product graphs and subjected to clique detection. The cliques are scored regarding overlap of surface points. This is time-consuming, and the distance-based RAPMAD approach is being investigated as a faster method.

The last talk on "Derivation and application of knowledge-based bonded interaction parameters in small-molecule simulations" was given by **Florian Roessler** (University of Cambridge). Small-molecule force fields vary from those meant to be general, such as GAFF (Generalised AMBER Force Field) down to force fields with parameters intended for just one molecule. The information held in the CSD and MOGUL is a valuable resource for parameterisation of force fields. With Python/API 10,000 structures were extracted from the CSD and grouped by CHARMM force field type. Comparison of CSD bond angles for each type with the value in CHARMM generally gives a straight line plot, albeit with some outliers in two pockets. In a similar way CSD and CHARMM torsion angles were compared. The next step was to use the CSD to generate parameters. Care had to be taken to exclude crystals influenced by other effects, and barriers may be represented less well because of a paucity of crystal structures with such geometry; but the results provide a stable parameter set.

Carl Schwalbe

Puzzle Corner

FORGET Brexit! Here we have CREXIT – either crystals from which molecules contained within them can exit, or crystals of molecules that enable cells to expel unwanted substances. From the URL for an abstract or the PDB identifier for a macromolecule determine what is being expelled and what is doing the expelling.

https://aca.confex.com/aca/2016/webprogrampreliminary/Paper1326.html

http://www.ncbi.nlm.nih.gov/pubmed/26954555

http://science.sciencemag.org/content/early/2016/05/18/science.aaf2458

PDB entry 2gfp

PDB entry 2onj

Answer to June Puzzle

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

The first of all: **H / Hyderabad**

Beginning of a series – a rare treat: **La / Lancaster**

It's inert, but the start of a lively venue: **Ne / New Orleans**

Named for a prize-giver whose fame endures, but it is very short-lived: **No / Nottingham**

It's heavy, but this one's a real getter: **Ba / Basel**

Like the first one, but heavier: **D / Denver**

Builds teeth and bones, just like cream cheese: **P / Philadelphia**

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

From Sweden, it's not a rare earth but acts like one; the English city was influenced by Vikings: **Y, Ytterby / York**

A stalwart for generating X-rays and excitement: **Mo / Montreal**

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

First and third letters this time: the last rare earth: **Lu, Lutetia (Paris) / Loughborough**

Good in filaments; it's a well-used venue: **W / Warwick**

A rare earth that's hard to isolate, but Sherlock would have identified it: **Ho / Honolulu**

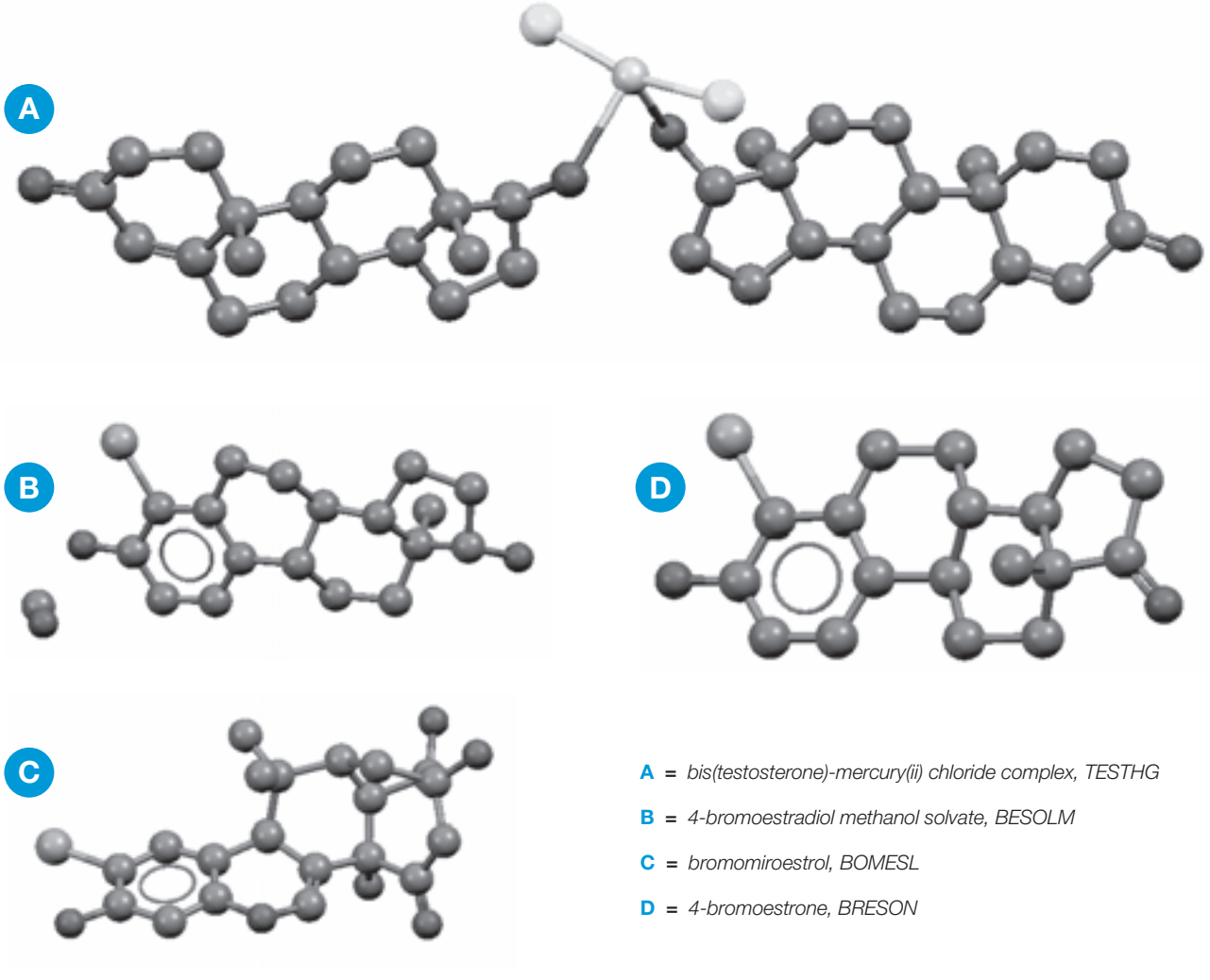
The winner is **Jim Trotter**.

Sex Hormones

THE work of Bernal and Crowfoot (Hodgkin) described in her thesis of 1936 was expanded to no less than 80 steroids in a magisterial publication in 1940 [J.D. Bernal, D. Crowfoot & I. Fankuchen, *Philos.Trans.R.Soc.London,Ser.A*, **239**, 135]. As the authors readily admitted, while plausible inferences about the size and shape of steroid molecules can be drawn from the unit cell dimensions alone, certainty about these features requires determination of three-dimensional structure, which was beyond researchers' capabilities at the time. In an important milestone, this was achieved for cholesteryl iodide in 1945 by Carlisle & Crowfoot [*Proc.R.Soc.London,Ser.A*, **184**, 64]. Structures of sex hormones followed in due course. Interestingly, three early 3-D structures of female hormones, brominated to aid structure determination, were worked on by women: bromomiroestrol (refcode BOMESL) by **Dorothy Hodgkin** [N.E.Taylor, D.C.Hodgkin, J.S.Rollett, *J.Chem.Soc.*, 3685 (1960)], 4-bromoestrone (BRESON) by **Dorita Norton**, who died tragically young (1931-1972) [D.A.Norton, G.Kartha, C.T.Lu, *Acta Crystallogr.*, **16**, 89 (1963)], and 4-bromoestradiol methanol solvate (BESOLM), again by Dorita Norton [D.A.Norton, G.Kartha, C.T.Lu, *Acta Crystallogr.*, **17**, 77 (1964)]. All of these had R factors well above 10%. Testosterone had to wait until 1968 when the structure of bis(testosterone)-mercury(ii) chloride complex (TESTHG) was determined, but this had a much more reassuring R factor of 6.4% and included the absolute configuration [A.Cooper, E.M.Gopalakrishna, D.A.Norton, *Acta Crystallogr.*, **B24**, 935 (1968)]. A torrent of steroid structures soon followed, along with speculative attempts to correlate structural features with biological activity.

We finally understood in detail how oestrogens achieve their activity, and how they can be blocked by anti-cancer drugs such as tamoxifen, when structural information about the oestrogen receptor was obtained. This macromolecule featured as the Molecule of the Month in September 2003 and is accessible under doi:10.2210/rcsb_pdb/mom_2003_9 . As usual, the article by **David Goodsell** provides a clear description in lucid prose and beautiful illustrations and still is well worth reading.

Carl Schwalbe



A = *bis(testosterone)-mercury(ii) chloride complex, TESTHG*

B = *4-bromoestradiol methanol solvate, BESOLM*

C = *bromomiroestrol, BOMESL*

D = *4-bromoestrone, BRESON*

UK Crystallographers Collaborate with Africa

AT the ceremony in Paris opening the International Year of Crystallography in 2014, along with past achievements, the potential of crystallography particularly in the developing countries received emphasis. Examples were cited: to quantify the minerals present in an ore for efficient processing, to determine the structure(s) of the active chemical(s) in traditional medicines, and to identify the materials used in art works to guide conservation procedures. UNESCO and equipment manufacturers began setting up a series of "open laboratories". The first such labs were made ready for use early in 2014 in Argentina, Ivory Coast, Morocco, South Africa and Uruguay. Scientists from these countries and their neighbours within these regions became able to work with and learn from local staff and apply crystallography to their research. At this same meeting Juliette Pradon surprised and delighted us by reporting on a successful collaboration between CCDC and the University of Kinshasa, which maintained a stable environment throughout the troubles in the Democratic Republic of Congo. CCDC provided the CSD along with software for chemistry, supported two postgraduate students and imparted training.

Even earlier, in 2011, the International Union of Crystallography designed an ambitious programme for sub-Saharan African countries. Known as the Crystallography in Africa Initiative, the program sought not only to train teaching staff and PhD students in crystallography but also to provide participating universities with diffractometers. The first faculty trained to be prepared for the arrival of a powder diffractometer (2013) came from the University of Dschang in Cameroon. In 2013 also, the Cameroon Crystallographic Association (CCrA) was founded. In August 2014 in Montreal (Canada), Cameroon was admitted as first sub-Sahara African IUCr member during the 23rd General Assembly of IUCr. Dschang will provide the venue for the First Pan African Conference on Crystallography, to be described later.

These efforts were augmented with "Building Science Capacity in Africa via Crystallography", which is an initiative of the IUCr funded by the International Council for Science (ICSU) through the ICSU Grants Programme 2015. Support was provided by ECA, UNESCO, the ICSU Regional Office for Africa, the INDABA Series of meetings and SAASTA (South African Agency for Science and Technology Advancement) Public Engagement with Nanotechnology. This project aims at further cementing the African Crystallographic Association (AfCA), whose Steering Committee was established at the Summit meeting in Bloemfontein in October 2014. The programme is being conducted as part of the IUCr Crystallography in Africa initiative.

Continuing the support of CCDC for crystallography in Africa, Juliette Pradon taught in crystallography schools in Kenya and Senegal last year. Her blog follows:

Crystallography in East and West Africa

I have been very fortunate this autumn to visit two markedly different African countries, Kenya and Senegal, on behalf of the CCDC. My first visit was to Nairobi, where Dr **Lewis Whitehead** of Novartis and I presented a week-long Kongamano: a series of lectures and workshops on crystallographic databases, featuring the Cambridge Structural Database (CSD), and in-silico visualization and modelling applications in drug discovery.

The course was repeated at two different Nairobi universities so we were able to reach nearly 90 Kenyan, Nigerian, Eritrean, Ethiopian, Ugandan and Congolese participants. For the first Kongamano, we headed to Kenyatta University (KU), just within the city limits on the north side of town and reached via the Thika road, a superhighway connecting Nairobi and Thika, used daily by more than 200,000 commuters. The first two full days of workshop flew by, with participants keen to hear about how to use the CSD-System in their research and, for the lecturers among them, how to use the tools to enhance their chemistry course with 3D visualization for the benefit of their students.

On the final day of the KU workshop, students rehearsing for a traditional dance performance invited Lewis to join in, but unfortunately our packed schedule meant that we had to leave right after lunch to continue the workshop that same afternoon at the Chiromo Campus of the University of Nairobi (UoN). Chiromo is located at the heart of the city centre but remains an oasis of calm, with buildings and food outlets dotted throughout the campus among beautiful trees and greenery. It is also where the Mitishamba database of Kenyan natural products was established for the benefit of all in Kenya, East Africa and beyond. The two and a half days at UoN were particularly productive and well received by the participants, including the only undergraduate – and, at 20, the youngest – student on the course. Friday night arrived much too early for me and it was soon time to go back to the UK. Asante sana (thank you very much) to all who made me feel so welcome in Kenya, I will be back one day!

After my experiences in Kenya, I headed to Ziguinchor, Senegal, having been invited to present and give a workshop on the CSD at the first Senegalese crystallography school and travelling laboratory. There were over 50 participants from francophone Africa: most from Senegal, but also some from Madagascar, Cameroon, Ivory Coast, Benin, Burkina-Faso and Mauritania. It was to be a very productive week for participants as most had brought with them at least one sample to be analysed, either on the powder or single crystal diffractometers which had been lent for the duration of the workshop by the Bruker company. So they left with their spectra and their structures solved. The time-constrained aspect of the course was compounded by the heat and humidity, which made the average temperature of 35 degrees feel closer to 43 degrees. Thankfully Senegal is not short of delicious fruits which can be turned into thirst quenching juices.

The school was superbly organized at the university in the town of Ziguinchor, the main city of the Casamance region, about 300 km south of Dakar across the Gambia but easily reached with an internal flight. Ziguinchor is located right on the Casamance river which slowly meanders its way to the Atlantic Ocean, and every morning fishermen were seen expertly guiding their pirogues and bringing back an array of river fishes, some of which certainly ended up on our plates during the week!

We were fortunate that, after an initial five days of hard work getting our heads immersed in crystallography, there was a planned excursion which allowed us to see more of the Casamance region. The conference gala dinner in Cap Skirring marked the end of this very successful first Senegalese crystallography school. We now look towards Dschang in Cameroon for the first pan-African crystallography conference in October 2016, which will no doubt further help shape the advancement of crystallography in Africa and contribute to recognition of the ways it and more general science can benefit the entire continent. A final Jërëjëf to everyone I was fortunate to meet through this school and more specifically to the organisers who clearly showed why Senegal is known for its unforgettable teranga (hospitality in Wolof).

Latest UK-Africa Crystallography Workshop

During the first week of August **Simon Coles** (NCS, University of Southampton) and **Suzanna Ward** (CCDC) were running a workshop at KNUST university in Kumasi, Ghana. The event was for a Royal Society / Department for International Development funded consortium led by **Nora De Leeuw** (Cardiff University) aimed at increasing capability for colleagues in universities in Ghana, Namibia and Botswana. The focus of the consortium is actually focussed around catalysis research, however the African partners identified a need for developing their ability to understand and work with crystallographic data.

The workshop began with an introduction to crystallography, illustrating the principles and applications by means of a historical account. The hands-on workshop then began in earnest with a day on solving and refining crystal structures, interspersed with some theory, using the Olex2 software package. Next analysis and graphical representation was addressed, using the CCDC Mercury package. The final day was spent on the CSD system software, querying the database, depositing and validating structures and the application of the Mogul knowledgebase. Around 50 students attended the workshop and were incredibly enthusiastic and engaged – there is no doubt they will all be looking to analyse their own crystallographic data in the future!

Meanwhile, preparations have continued for the First Pan-African Conference on Crystallography to be held in Dschang, Cameroon, from 6-10 October 2016. The starry list of speakers is headed by two Plenary Lecturers: **G. R. Desiraju**, "From molecule to crystal", and **Ron Lifshitz**, "What is a crystal? - New answers to an old question". A keynote lecture will be given by our own **Colin Groom** on "Crystallography data bases". This meeting is sponsored by UNESCO, ICSU, IUCr, ECA, AsCA, CCDC and the Association Francaise de Cristallographie) ... and more than 200 colleagues from more than 30 different African countries are expected to attend. It comes as no surprise that African postgraduate students will struggle to pay for their travel and subsistence expenses. Accordingly, **Claude Lecomte**, the Chair of the IUCr Africa Initiative Commission, has asked for support from further national crystallographic societies. The BCA Council has resolved to contribute 2000 euros in outreach / bursary funding, and we can look forward to reports by the recipients in *Crystallography News* in our conventional style.

Carl Schwalbe

This conference aims at bringing together African crystallographers, mineralogists, solid state and structural scientists to increase the awareness for crystallography and improve the educational opportunities for African researchers and students of all levels.The variety of activities will provide opportunities to engage with (i) the scientific community, from expert crystallographers to young researchers and students of all ages, (ii) government representatives and policy-maker from most African countries.

Scientific program

Chairman: Prof. C. Lecomte, Chair of the IUCr Africa Initiative Commission
claude.lecomte@univ-lorraine.fr

Plenary Lecture: Prof. G. Desiraju, Immediate Past IUCr President India

Microsymposia:

Mineral prospection
Crystal growth
Inorganic materials
Molecular crystals
Crystal engineering
Large facilities
Database
Macromolecular crystallography

Exhibitions booths will be available for companies and individuals

For any question about registration, abstract submission..., please contact Dr Patrice Kenfack at the following address: pancocrys1@gmail.com

Website: http://www.iycr2014.org/capacity-building/icsu2015

PCCr[1] 2016

Dschang 06-11 Oct.

First Pan African Conference on Crystallography

Chairman: Prof. Anaclet Fomethe, Rector of University of Dschang
Co-chairmen: Profs. Ignas Tonle, Jean Ngoune, University of Dschang

ICSU

Natural Sciences Sector

IUCr

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, c.h.schwalbe@hotmail.com . Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

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

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

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

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

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

5-7 September 2016
11th International Conference on Advances in Experimental Mechanics, Exeter.
http://bssm.cmail20.com/t/ViewEmail/r/6E94DAA80A1DFFDB2540EF23F30FEDED/3B177A5D09D7A2F5F6A1C87C670A6B9F

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

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

6-8 September 2016
Advanced data collection for high resolution cryoEM, Diamond.
https://www.biochemistry.org/Events/tabid/379/View/Conference/MeetingNo/td011/MeetingID/2671/Default.aspx

6-8 September 2016
Synchrotron radiation and neutrons in art and archaeology, Chicago, IL, USA.
https://sites.northwestern.edu/sr2a/

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

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

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

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

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

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

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

12-14 September 2016
Physics Meets Biology 2016, Cambridge.
http://pmb2016.iopconfs.org/423120

12-16 September 2016
4th International Soft Matter Conference (ISMC2016), Grenoble, France.
www.ismc2016.org/

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

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

14-16 September 2016
5th Joint Workshop on High Pressure, Planetary and Plasma Physics (HP4), Hamburg, Germany.
https://indico.desy.de/conferenceDisplay.py?confId=14266

19-21 September 2016
RheoSAS2016: In situ rheology for neutron and X-ray scattering techniques, Grenoble, France.
https://indico.ill.fr/indico/event/52/

19-22 September 2016
9th International Workshop on Sample Environment at Scattering Facilities, Gettysburg, PA, USA.
http://seworkshop2016.umd.edu/

19-22 September 2016
E-MRS Fall Meeting, Warsaw, Poland.
http://www.european-mrs.com/meetings/2016-fall

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

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

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

26-30 September 2016
DISCUS Workshop, Erlangen, Germany.
http://www.lks.physik.uni-erlangen.de/DISCUS/index.html

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

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

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

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

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

3-7 October 2016
Modern Trends in Neutron Scattering from Magnetic Systems & Single-crystal Diffraction with Polarised Neutrons, Tutzing, Munich, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/JCNSWorkshops/2016Workshop/_node.html

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

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

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

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

17-19 October 2016
Workshop on SoNDe application in neutron detection, Freising, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/ESS/SondeWorkshop/Scope/_node.html

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

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

28-29 October 2016
Workshop on high-pressure multigrain crystallography, Argonne, IL, USA.
https://sites.google.com/carnegiescience.edu/multigrain2016/home

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

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

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

27 November - 2 December 2016
2016 MRS Fall Meeting, Boston, MA, USA.
http://www.mrs.org/fall2016/

12-16 December 2016
New Trends in Magnetic Structure Determination, Grenoble, France.
https://indico.ill.fr/indico/event/53/

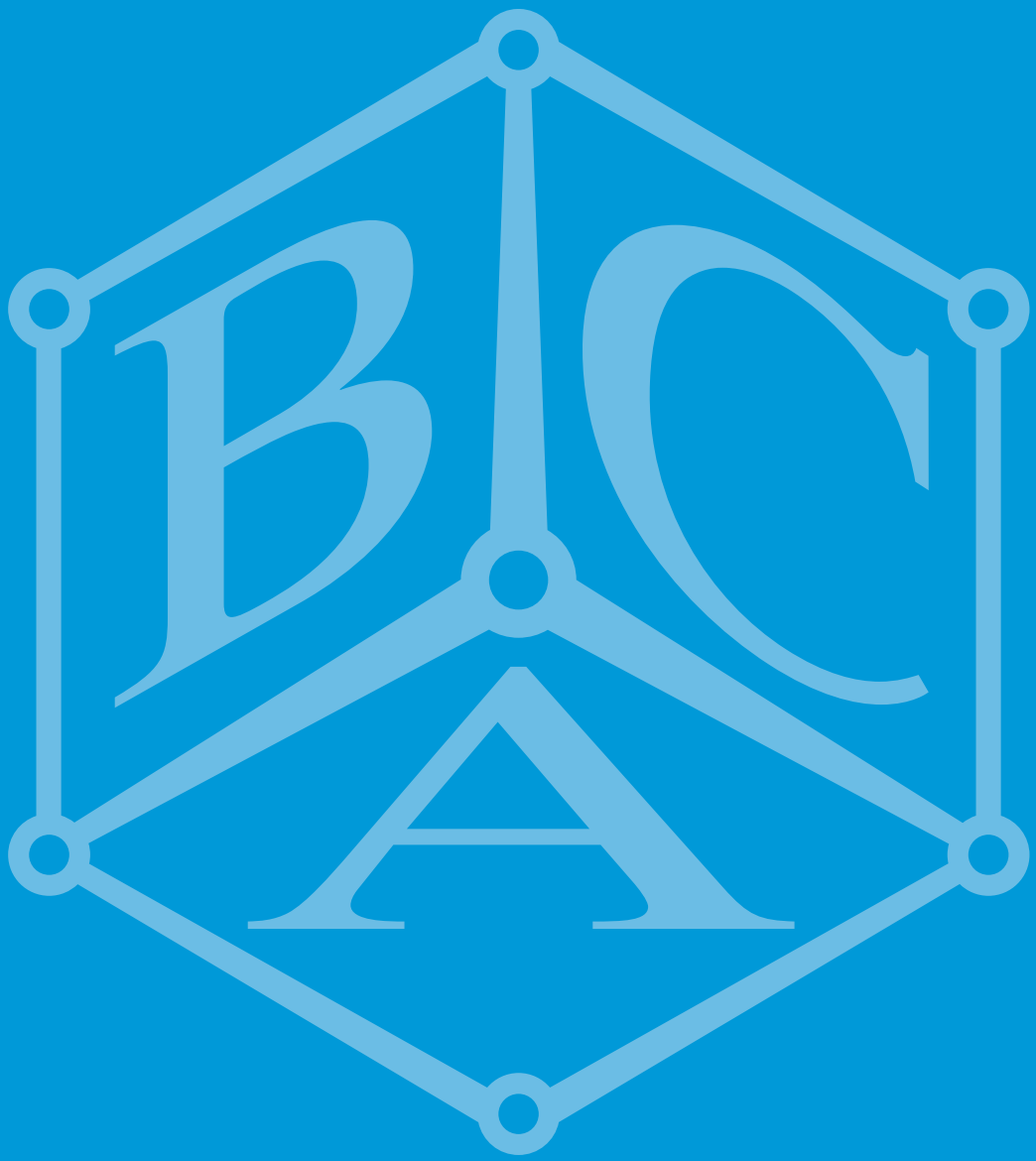
11-15 February 2017
61st Annual Meeting of the Biophysical Society (with new Cryo-EM Subgroup meeting), New Orleans, LA, USA.
https://www.biophysics.org/2017meeting/Home/tabid/6672/Default.aspx

19-22 February 2017
5th Banff Meeting on Structural Dynamics, Banff, Alberta, Canada.
https://banff2017.desy.de/

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

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

17-21 April 2017
MRS Spring Meeting & Exhibit, Phoenix, AZ, USA.
http://www.mrs.org/spring2017/



Arianna Lanza winner of the fourth PANalytical Award

The annual award recognizes innovative X-ray analytical research by young scientists.

THE PANalytical Award 2015 has been won by Ms. Arianna Lanza. She is affiliated to the Department of Chemistry and Biochemistry of the University of Bern (Switzerland) and to the Swiss Light Source, Paul Scherrer Institute in Villigen (Switzerland) and is currently finalizing her PhD. Her article about the dynamic behavior of a flexible and porous metal-organic framework was highly rated by all six members of the selection committee. They were impressed by the convincing and original results, which open the way to even more exciting possibilities in designing metal-organic frameworks. Ms. Lanza's high competence and confidence in X-ray analysis and her scientific leadership were emphasized by the jurors, all leading experts in their fields. The winning article was selected from a record number of more than 90 contributions.

Arianna Lanza and her co-authors **Luzia S. Germann**, **Martin Fisch**, **Nicola Casati** and **Piero Macchi** were delighted by the good news. She will receive the PANalytical Award at this year's Meeting of the European Crystallographic Association (ECM 30) in Basel at the end of August where she will present her work to the professional community.

PANalytical, world's leading supplier of analytical X-ray instrumentation and software, seeks to reward early-career scientists who have demonstrated innovative thought to their research when using an X-ray analytical technique with a €5,000 prize. There are no restrictions on the manufacturer of the laboratory X-ray equipment that was used.

The PANalytical Award 2016 is now open for submissions. Applicants must publish a paper in print during the period 1 January 2015 until 1 December 2016 that demonstrates groundbreaking thinking in a topical field and required the use of a laboratory X-ray diffraction, X-ray fluorescence or X-ray scattering instrument as the primary analytical technique. The prize will be decided by a selection committee that includes established research scientists unaffiliated to PANalytical.

Applying for the award is easy via www.panalytical.com/award, with a closing date of 1 December 2016. Correspondence or questions about the award can be addressed to award@panalytical.com.

Scientists capture neon in an organic environment for the first time

IN a new study, researchers from the Cambridge Crystallographic Data Centre (CCDC) and the U.S. Department of Energy's (DOE's) Argonne National Laboratory have teamed up to capture neon within a porous crystalline framework. Neon is well known for being the most unreactive element and is a key component in semiconductor manufacturing, but neon has never been studied within an organic or metal-organic framework until now. The results, which include the critical studies carried out at the Advanced Photon Source (APS), a DOE Office of Science user facility at Argonne, also point the way towards a more economical and greener industrial process for neon production.

Neon is an element that is well-known to the general public due to its iconic use in neon signs, especially in city centres in the United States from the 1920s to the 1960s. In recent years, the industrial use of neon has become dominated by use in excimer lasers to produce semiconductors. Despite being the fifth most abundant element in the atmosphere, the cost of pure neon gas has risen significantly over the years, increasing the demand for better ways to separate and isolate the gas.

During 2015, CCDC scientists presented a talk at the annual American Crystallographic Association (ACA) meeting on the array of elements that have been studied within an organic or metal-organic environment, challenging the crystallographic community to find the next and possibly last element to be added to the Cambridge Structural Database (CSD). A chance encounter at that meeting with **Andrey Yakovenko**, a beamline scientist at the Advanced Photon Source, resulted in a collaborative project to capture neon – the 95th element to be observed in the CSD.

Neon's low reactivity, along with the weak scattering of X-rays due to its relatively low number of electrons, means that conclusive experimental observation of neon captured within a crystalline framework is very challenging. *In situ* high pressure gas flow experiments performed at X-Ray Science Division beamline 17-BM at the APS using the X-ray powder diffraction technique at low temperatures managed to elucidate the structure of two different metal-organic frameworks with neon gas captured within the materials.

"This is a really exciting moment representing the latest new element to be added to the CSD and quite possibly the last given the experimental and safety challenges associated with the other elements yet to be studied" said **Peter Wood**, Senior Research Scientist at CCDC and lead author on the paper published in Chemical Communications. *"More importantly, the structures reported here show the first observation of a genuine interaction between neon and a transition metal, suggesting the potential for future design of selective neon capture frameworks".*

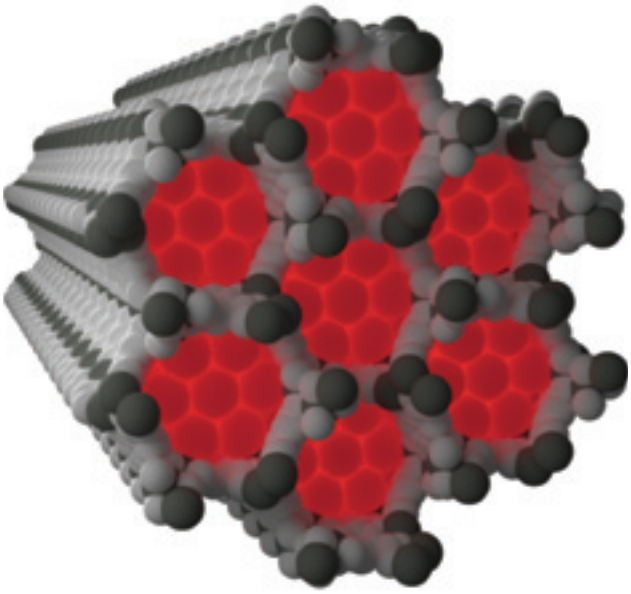
The structure of neon captured within the framework known as NiMOF-74, a porous framework built from nickel metal centres and organic linkers, shows clear nickel to neon interactions forming at low temperatures significantly shorter than would be expected from a typical weak contact.

Andrey Yakovenko said *"These fascinating results show the great capabilities of the scientific program at 17-BM and the Advanced Photon Source. Previously we have been doing experiments at our beamline using other much heavier, and therefore easily detectable, noble gases such as xenon and krypton. However, after meeting co-authors Pete, Colin, Amy and Suzanna at the ACA meeting, we decided to perform these much more complicated experiments using the very light and inert gas – neon. In fact, only by using a combination of in situ X-ray powder diffraction measurements, low temperature and high pressure have we been able to conclusively identify the neon atom positions beyond reasonable doubt".*

Summarising the findings, **Chris Cahill**, Past President of the ACA and Professor of Chemistry, George Washington University said "*This is a really elegant piece of in situ crystallography research and it is particularly pleasing to see the collaboration coming about through discussions at an annual ACA meeting".*

The paper describing this study is published in the journal Chemical Communications, **http://dx.doi.org/10.1039/C6CC04808K**. All of the crystal structures reported in the paper are available from the CCDC website: **http://www.ccdc.cam.ac.uk/structures?doi=10.1039/C6CC04808K**.

This research used resources of the APS, a US DOE Office of Science user facility operated for the US DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02- 06CH11357.



Neon observed experimentally within the pores of NiMOF-74 at 100 K and 100 bar of neon gas pressure.

(Reprinted from https://www.ccdc.cam.ac.uk/News)

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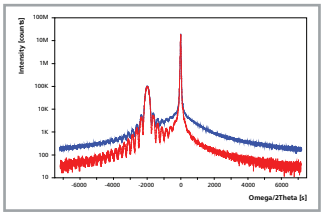

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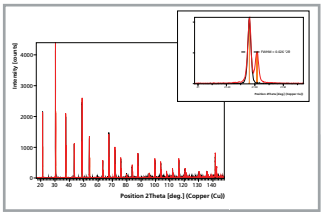

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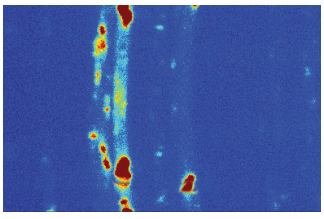

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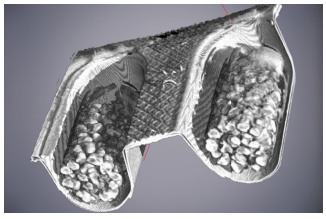

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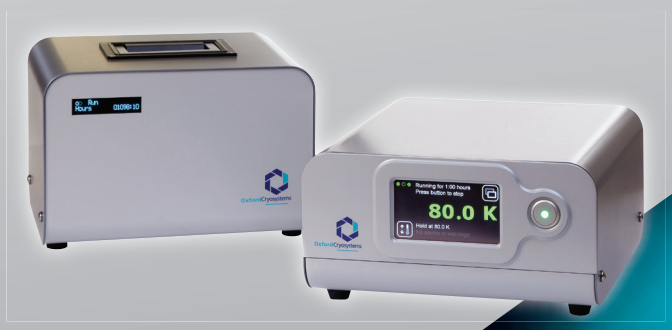

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