Crystallography News

British Crystallographic Association

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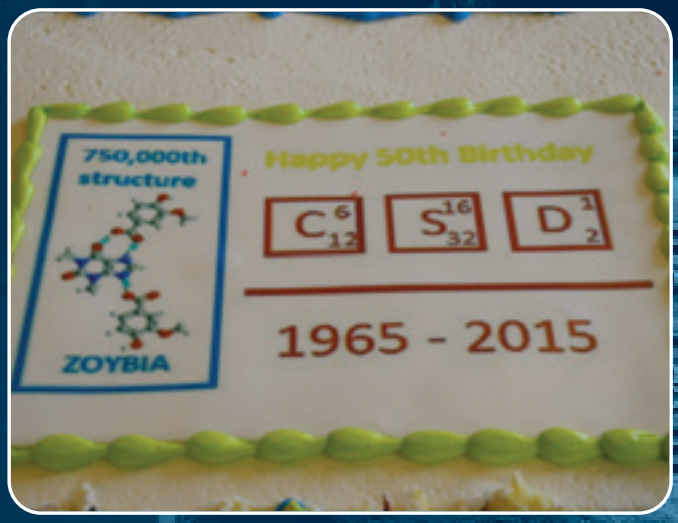

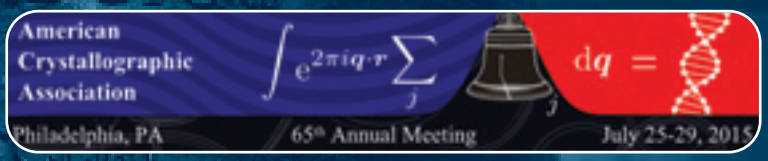

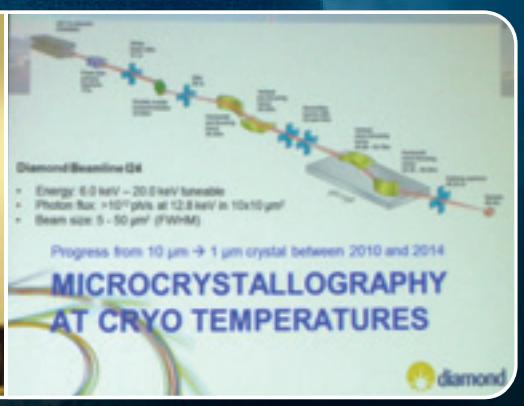

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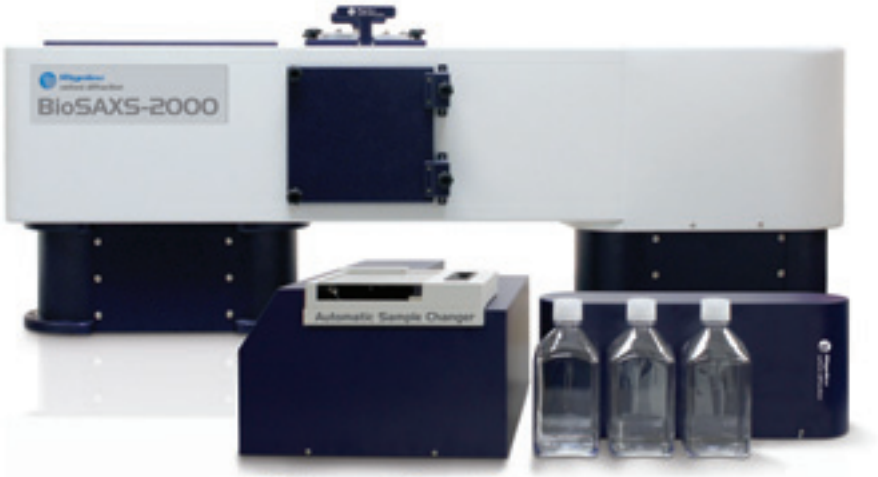
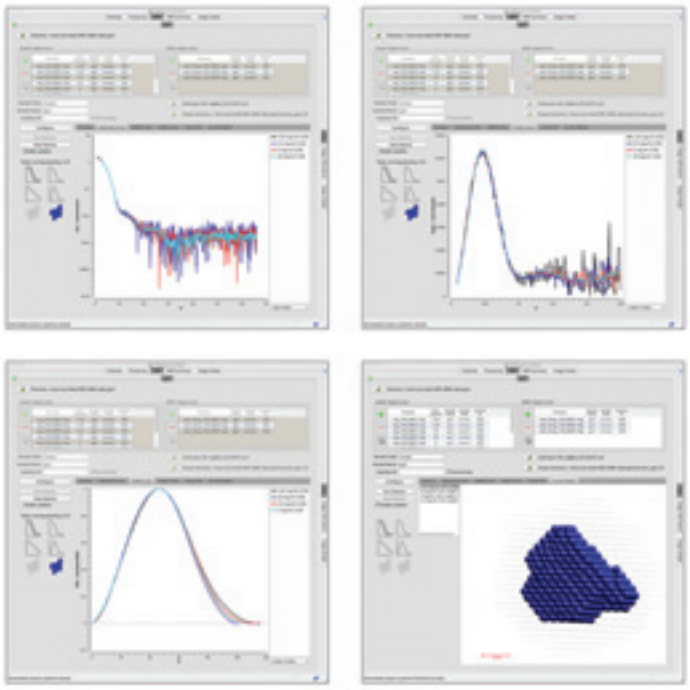


(ASC) Automatic Sample Changer



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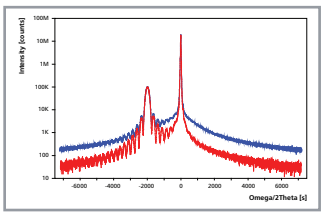
0D



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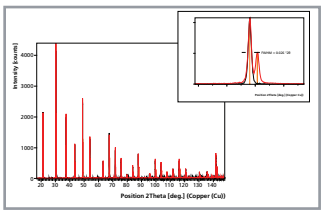

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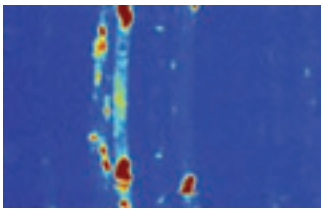
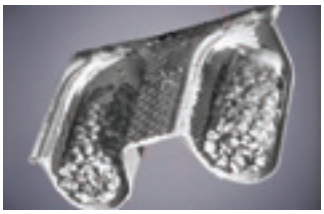


3D



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Contents

This month's cover:

CCDC cake, IUCr Editor's doughnuts, Diamond light by Danny Axford, Liberty Bell photo by J. Fusco for Visit Philadelphia™

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Please ensure that items for inclusion in the December 2015 issue are sent to the Editor to arrive before 25 October 2015.

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These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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From the President

SINCE my last CN column, plans have moved forward regarding the 2016 BCA meeting in Nottingham. The programme committee, chaired by Phil Lightfoot, held their planning meeting on June 24 at the conference venue at the University of Nottingham. This allowed everyone the opportunity to look round the site, which is well suited for the meeting with lecture/meeting rooms, poster and exhibition space all in close proximity in one building. Accommodation, dining area and bar are also close by.

The meeting programme is taking shape, and I'm very pleased that we will have Prof. **Arwen Pearson** (Hamburg Centre for Ultrafast Imaging, University of Hamburg) to give the Lonsdale Lecture and Prof. **Christer Aakeröy** (Kansas State University) to give the BCA Prize Lecture, as well as a strong line-up of plenary lectures and invited lectures already confirmed. The preliminary programme is available via the BCA meeting website and will be updated as the programme develops.

At the beginning of July I had the pleasure to attend the CSD50† symposium, held in very pleasant surroundings at Downing College, Cambridge, over the course of 3 days, to celebrate the 50th anniversary of the establishment of the Cambridge Structural Database (CSD). The symposium brought together many current and former CCDC staff along with colleagues from around the world who have had interactions with the CCDC over its long history. The presentations were an enjoyable mix of talks on the history and development of the CSD and talks related to the diversity of research and education facilitated by the CSD and the associated software developed and supported by the CCDC. It was a pleasure to see **Olga Kennard** and **Jack Dunitz** at the symposium, both of whom I hope will not mind my revealing are now beyond their 90th year. Having established the CSD in 1965 and then the independent Cambridge Crystallographic Data Centre (CCDC) in 1987 and served as its first director until 1997, it was fitting that Olga Kennard gave the opening lecture. Jack Dunitz, who has strong links to the CCDC throughout its existence, and is also a former CCDC governor, contributed insightful comments after many of the lectures from his regular seat near the front of the auditorium. The symposium concluded with a lecture from current CCDC director **Colin Groom**, who looked into his crystal ball and provided a sequence of predictions about the future of crystallography and the CSD with a timeline spanning the next 50 years. Everyone in attendance was invited back for CSD100 in 2065. I'm not overoptimistic of being able to take up the invitation myself, but would be fascinated to know where our field will be 50 years hence. Details of CSD50, including videos of the presentations, can be found on the CCDC website at **http://www.ccdc.cam.ac.uk/CSD50/**.

A few weeks ago I attended an excellent lecture given by **Mike Glazer** (Oxford) entitled "The Legacy of the Braggs: 100 years of Crystallography," which was part of an Institute of Physics lecture series at University of Sheffield, conveniently just a short walk across the road from the Chemistry department for me. Mike also recently stepped in to help the BCA on another project when our help was requested by a BBC documentary producer. The documentary, produced by the BBC Arts division focusing on the work of M. C. Escher, and featuring Roger Penrose, was in need of input to show the links between Escher's periodic drawings and crystallography. I'm sure many of us who teach crystallography make some use of Escher prints to illustrate concepts of periodicity or symmetry and I think there has long been an affinity for the work of Escher among crystallographers. As is often the case with requests like this one, they weren't quite sure what was needed, but needed something quickly as filming was taking place within a couple of weeks. I'm grateful to **Simon Coles** in his capacity as BCA Education & Outreach Officer for leading discussions to put together something that the BBC could use and to Mike for putting together a set of slides and consenting to be filmed. The documentary will be part of the BBC4 series Secret Knowledge (**http://www.bbc.co.uk/programmes/b01rfzgy**) and I am told is likely to be broadcast in August, which is a few weeks after the time of writing this column, but will be before the time that *CN* is published in September. Hopefully if you missed it, those of you in the UK at least may be able to find it on BBC iPlayer. Fingers crossed that Mike's contribution made the final cut. A further BBC article on Escher can be found at **http://www.bbc.co.uk/programmes/articles/1TXskHdW0Hrtng1bYgzRBRf/chaos-is-present-everywhere-the-mysterious-world-of-mc-escher**

I would like to congratulate **John Helliwell**, former BCA Vice-President, on receipt of the **8th Max Perutz Prize**, presented at the ECM meeting in Rovinj, Croatia. John has been honoured for his long, generous and fruitful dedication to developing all aspects of the use of synchrotron radiation for crystallography and for his boosting support to global development of synchrotron and neutron facilities. I would also like to congratulate **Elspeth Garman**, former BCA President, on receipt of the **2015 Mildred Dresselhaus Award** from the Hamburg Centre for Ultrafast Imaging. Elspeth was honoured for her pioneering contributions to structural biology, especially in leading the field of radiation damage during macromolecular X-ray diffraction, and in recognition of her outstanding contributions to mentoring and training of a generation of crystallographers.

I am grateful for the contributions of **Elizabeth Shotton** (Diamond Light Source) as IG representative to BCA Council. Her term of office has just come to an end and we welcome **David Beveridge** (Harman Technology Ltd) as the new IG rep.

The BCA Council will be meeting on September 16 and we would welcome input from the membership on any matters that you think should be discussed. Please contact one of the BCA Officers if you have ideas or suggestions. I'm particularly interested to know what the membership would like to see on the BCA website and in what ways we could make it more visible and more useful to the membership.

I'd like to finish with a mention of 3D printing, which has gradually become much more accessible and affordable, and offers the opportunities to print 3D models of crystal

structures. There are now a number of programs available to convert CIFs to suitable output for 3D printers and, although computer graphics offer tremendous tools for crystal structure visualisation, there is obviously something tangible about having a molecular model that you can rotate in your own hands. Thus, I was delighted when recently my research group gave me a 3D printed model from the crystal structure of $[Mo(C_{12}H_{14})(\eta^5\text{-}C_9H_7)]CF_3SO_3$ in my first publication as a PhD student. The model of the cation is shown here in a view that emphasises the agostic (C–H→M) interaction to the molybdenum centre (*J. Chem. Soc., Chem. Commun.* **1985**, 1411).

I look forward to seeing some of you at upcoming meetings this summer, starting with the ECM in Rovinj, Croatia.

Lee Brammer

† Curiously, if you search for CCDC50 in a well-known search engine you will be directed to information on Coiled-coil domain-containing protein 50.

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From the Editor

AS I write this column, we are well into the summer conference season. I am pleased to include a comprehensive report on the XRF meeting in June that was co-sponsored by our Industrial Group. Then, at the beginning of July, we celebrated the Golden Jubilee of the Cambridge Structural Database. This database, and the Cambridge Crystallographic Data Centre that curates it, embody the willingness to share information that is so prominent in the ethics of the crystallographic community. I am grateful to a number of participants at this meeting for the report that appears in this issue.

Unfortunately I was unable to attend this celebration because a long time ago I had made a non-cancellable booking for Joan and me to fly to Philadelphia on July 1 and stay until the conclusion of the American Crystallographic Association meeting at the end of the month. I report on this meeting later on in this issue. Our long stay gave me, a native of Ohio, the chance to join Joan in visiting a lot of places in the eastern USA where, despite the close proximity, I had never set foot before. It also enabled us to attend the commemoration on July 1-3 of another anniversary, the 152nd of the Battle of Gettysburg and the 150th of the end of the Civil War. Although there were a lot of displays of uniforms and weaponry and illustrations of strategy and tactics, crystals could not be forgotten.

We attended a fascinating presentation about Civil War medicine. When this topic is mentioned, most people think of amputations. Indeed, aided by the use of chloroform and ether as anaesthetics, amputations were very common. We saw a demonstration of a mock amputation using the appropriate instruments. Although surgeons at that time had no idea of germs and the importance of sterility, nevertheless the survival rate was around 70%. Disease was a greater killer than wounds, and here the doctors had some drugs from botanic and mineral sources. Two "wonder drugs" of the period came in crystalline form. Quinine was well-known as an effective remedy for malaria, and much of the fighting took place in malaria-prone areas of the South. Although quinine was ineffective against other infectious agents, it reduced fever and made patients feel better. Quinine in the form of powdered cinchona bark had been used for centuries, but adulteration was easy to disguise, the remedy was unpleasant to take and the concentration of active ingredient could vary. By the 1860s quinine was efficiently extracted from cinchona bark and crystallised as the sulfate to a reliable standard of purity. Made from imported material and packaged by the nascent American pharmaceutical industry, mostly in Philadelphia, it was supplied to Union troops on a regular basis as a precaution. Frequently it was made palatable by dispensing it in bourbon whiskey (an American version of the G&T?). Because of the Union blockade, the Confederates had a shortage of quinine. Blockade runners attempted to smuggle it in, sometimes hiding it in the heads of girls' dolls, and some women attempted to cross the battle lines with it hidden under their hoop skirts. Does any of this sound familiar? Chief among the inorganic drugs was the notorious calomel. We now know that its unit cell contains Cl-Hg-Hg-Cl units with their distinctive metal-metal bond. Although calomel does have some anti-infective activity, its overuse afflicted far too many patients with mercury poisoning.

We can look forward to some very interesting meetings, too. First up are our Group Meetings in the autumn. As usual, our Physical Crystallography Group will hold a meeting at Cosener's House extending over two days, which will be the 19th and 20th October this year. Our Industrial Group will meet at AstraZeneca in Macclesfield on 12 November to discuss the topic "Cracking Challenging Crystals". This year's autumn meeting of the Chemical Crystallography Group will be in Glasgow on Wednesday the 18 November with "Functional Materials" as its theme. The BSG Winter Meeting, "Reactive Macromolecules", will take place on December 16, 2015, in Manchester. For additional details, keep checking the BCA website. Looking further forward to the 4-7 of April next year, the programme for the BCA Spring Meeting in Nottingham is taking shape. The description provided in this issue shows that it will be another exciting event with content that will appeal to every type of crystallographer.

Then, in late August, the European Crystallographic Meeting will take place in Basel. Having been given a trip to Basel as a retirement present which I greatly enjoyed, I count this city as one of my favourite places in the whole wide world. It features beautiful buildings, both old and new, set along a scenic stretch of the Rhine. Adjacent to France and Germany, it offers culture and cuisine of both countries, augmented by a generous dose of Swiss individuality. There is a wealth of museums, starting with the must-see art museum that is considered the most significant in Switzerland. If you wanted to see the collection this year, you would be disappointed. The Main Building is currently closed for renovation, and its main masterpieces have been dispersed. However, it will reopen in April 2016, ready to dazzle us with its gleaming freshness. Given my background in medicinal chemistry, the Pharmacy Museum is another favourite of mine; but there is a museum to suit every taste. One cannot deny that Switzerland is expensive, but Basel does its best to mitigate the expense by providing a free Mobility Ticket transport pass to hotel guests staying there.

Looking ahead 2 years, we can anticipate the next Congress of the International Union of Crystallography, to be held in India in the city of Hyderabad. Pleasantly situated on hilly terrain among numerous lakes, this city offers both tradition and modernity. Hyderabad is called the "City of Pearls" because of its record in trading these precious commodities; but it now is home to important technology industry and has been nicknamed "Genome Valley". Preliminary information is presented in this issue.

I close by referring a request that **Bruce Foxman** made to everyone attending the ACA meeting. Bruce's research deals extensively with twinned products of solid-state reactions. He relies on software to elucidate all possible binary twin laws within maximum index and maximum obliquity for a given material without missing one or proposing a wrong one. A program by Yvon LePage called *OBLIQUE* does the job, but Bruce only has an early version. *OBLIQUE* was presented at IUCr XVIII in Glasgow and published as Le Page (2002) *J. Appl. Cryst.* **35**, 175-181. Frustratingly, the abstract and article contain a link to the program; but this link is no longer valid. Would anyone be able to supply the definitive version to Bruce?

Carl Schwalbe

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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 4-7 April 2016

From the BCA 2016 Programme Committee

WITH the 2nd century of X-ray diffraction now well underway, the BCA 2016 Spring Meeting programme will take stock of the current state-of-the-art and continue to look towards the future. The Programme Committee has been working hard, and we already have the majority of Plenary and several Keynote speakers in place, spanning a diverse range of subject matter across the four subject groups. The 2016 BCA Prize Lecture will be given by Prof Christer Aakeröy and the Lonsdale Lecture by Prof Arwen Pearson.

The meeting will follow a similar session format to last year, with parallel sessions and a range of Workshops, allowing plenty of choice for delegates. Each of the parallel sessions will incorporate a Keynote plus three, rather than two, contributed lectures, in order to allow more opportunities for speakers, in particular younger colleagues. If your talk doesn't fit with the proposed Group Sessions, don't panic! There will be an additional 'Ad hoc' session, with content to be chosen from submitted abstracts.

Lonsdale Lecture (Tuesday pm)

Professor **Arwen Pearson** (Hamburg)
Visualising molecules in motion: crystallography as a tool to probe structure and dynamics

BCA Prize Lecture (Wednesday pm)

Christer Aakeröy (Kansas State University)
From molecular sociology to functional materials

Biological Structures Group (BSG)

The central theme of the 2016 BSG sessions will be **Antimicrobial Resistance (AMR) and Cell Processes**. AMR is an emerging and growing threat to western healthcare providers and the general population. A unique cross council initiative, involving the MRC, BBSRC and EPSRC, has recently been launched to 'jump start' research in this area. The Wellcome Trust also supports research into AMR under the Infectious diseases part of their funding portfolio. Given the importance of this topic we have devised a program that seeks to highlight the role that structural biology can and should be playing in the pursuit of strategies to tackle AMR. This includes understanding the roles that membrane transporters play in giving resistance to current antibiotics and their potential as drug targets themselves. We have also identified a number of recent studies on molecular machines that are also highly relevant to AMR.

Renewed interest and applications of EM, Mass Spectrometry, Small Angle and Wide Angle X-ray scattering to understanding dynamic macromolecular complexes has led to some dramatic advances in our understanding of key cellular processes, such as mitosis and cell division. Another growth area in structural biology is EM tomography, which has the capacity to place atomic structural information into the broader cellular context. To highlight some of these advances we have included a separate session on '**Structural Insights into Cell Processes**' and '**Molecular Machines**' to highlight recent successes from UK based groups.

We hope these topics will highlight some of the world-class structural biology being undertaken in the UK and provide stimulating discussions.

BSG Plenary (Wednesday am)

Prof **Susan Lea** (Oxford)
Chair: ***E J Dodson*** (York)

BSG sessions

Tuesday Session 1. Antimicrobial Resistance.
Chair: ***Ben Luisi*** (Cambridge).

Tuesday Session 2. Developing New Therapeutics.
Chair: ***Colin Kleanthous*** (Oxford).

Wednesday Session 3. (joint with PCG) Future of Structural Science.
Chair: ***Xiadong Zhang*** (Imperial). *Co-chair:* to be confirmed.
Keynote: **Xiaodong Zhang** (Imperial).

Wednesday Session 4. (joint with PCG) Future of Structural Science.
Chair: ***Mike Glazer*** (Oxford).

Thursday. Session 5. Structural insights into Cell Processes.
Chair: ***Richard Bayliss*** (Leicester). *Co-chair:* to be confirmed.
Keynote: **Richard Bayliss** (Leicester).

Thursday Session 6. Molecular Machines.
Chair: ***Susan Lea*** (Oxford)

Chemical Crystallography Group (CCG)

CCG Plenary. Tuesday pm.

Professor **Mike Zaworotko** (Limerick): **Crystal Engineering: Form to Function**
Chair: ***Pete Wood*** (CCDC)

Tuesday Session 1. (joint with IG) From Amorphous to Crystal.
Chairs: ***Katherina Fucke*** (Durham), ***Ghazala Sadiq*** (CCDC/Pfizer)

This session will cover research into the transitions from amorphous, e.g. solution, glass or gas state, into the crystalline state, the connections between the extremes, and the transition states between them. Special interest is taken in the correlation of these topics with the final crystal structures. This session aims at bridging the fields of pharmaceutical solid-state, organic and inorganic chemistry as well as process engineering, the problems that are encountered in these fields and the solutions that crystallographic methods can offer.

Tuesday Session 2. (joint with IG) Interactions and Materials.
Chairs: ***Graham Tizzard*** (Southampton), ***Cheryl Doherty*** (Pfizer)

Keynote: ***Robert Doherty*** (Pfizer)

This session will aim to encompass the flourishing and diverse fields of crystal engineering, the design of structures from first principles by directed assembly, as well as the related areas of polymorphism and co-crystal research. This is a joint session between the CCG and IG that will include a broad range of topics of interest to both these communities.

Wednesday Session 3. NMR Crystallography.
Chair: ***Gareth Lloyd*** (Heriot-Watt), *Co-chair:* ***Paul Hodgkinson*** (Durham)

Keynote: ***Yaroslav Khimyak*** (East Anglia)
Understanding structure of molecular organic solids: combining crystallography with insights from NMR

Nuclear Magnetic Resonance (NMR) Crystallography uses the exquisite sensitivity of NMR frequencies to local environment in order to elucidate crystallographic information. DFT-based methods now allow NMR measurements to be directly correlated with molecular packing, and a range of NMR experiments can be used to probe questions of disorder, dynamics, structure and crystallography.

Wednesday Session 4. Complementary Techniques
Chairs: ***Helena Shepherd*** (Bath/Kent), ***Andrew Stewart*** (Limerick)

Keynote: ***Graeme Day*** (Southampton)

There are many techniques that can give complementary information to traditional crystallographic approaches. This session will explore the use of techniques including computational studies, electron diffraction and microscopy, spectroscopy and scattering to allow a more complete understanding of the molecules and materials we study.

Thursday Session 5. Tips, Tricks and Trials
Chairs: ***Mike Probert*** (Newcastle), ***Iain Oswald*** (Strathclyde)

This session will aim to span the crystallisation journeys of various samples through to the measurement of their diffraction patterns, aiming to explain various Tips Tricks and Trials that the speakers have employed under different circumstances.

Keynote: ***David Allan*** (Diamond)

Thursday Session 6. (Joint with YCG): Would you Publish This?
Chairs: ***Pascal Parois*** (Oxford) and ***Jorge Sotelo*** (Edinburgh)

Keynote: ***Iain Oswald*** (Strathclyde)

Following last year's success, this interactive session of unusual format is aimed for discussing problematic crystal structures that can be hard to interpret and publish. After an opening talk on the challenge of publishing difficult structures, anyone present can briefly describe one or more structural results that raise the session title question for the audience to discuss, with the aim of constructive rather than negative criticism. Problems might include charge imbalance or other chemical issues, poor resolution or data completeness, complicated disorder, highly restrained models, unexplained residual electron density and other artefacts, 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; we will request 1–3 slides for concatenation into a single session presentation. Contributions from Young Crystallographers are particularly encouraged.

Industrial Group (IG)

IG Plenary. Tuesday pm.

Dr Rolf Hilfiker (Solvias AG): *Title* TBA
Chair: TBA

Tuesday Session 1. (joint with CCG) From Amorphous to Crystal.
Chairs: ***Katherina Fucke*** (Durham), ***Ghazala Sadiq*** (CCDC/Pfizer)

Tuesday Session 2. (joint with CCG) Interactions and Materials.
Chairs: ***Graham Tizzard*** (Southampton), ***Cheryl Doherty*** (Pfizer)

Keynote: ***Robert Doherty*** (Pfizer)

Wednesday Session 3. (joint with BACG) Application of Crystallography to Crystal Growth.
Chair: TBA

Keynote: ***Roger Davey*** (Manchester)

continued overleaf.

Physical Crystallography Group (PCG)

The final 'Centenary' of the current cycle is perhaps the birth of powder diffraction. To celebrate this, Prof Bill David will give the PCG Plenary, entitled '120 Years of Powder Diffraction'; for the final 20 years, Bill will presumably take out his (poly)crystal ball and invite us to gaze into the future!

PCG Plenary: Thursday am.
Professor **Bill David** (Oxford and ISIS): *120 Years of Powder Diffraction*
Chair: Matt Tucker

Tuesday Session 1. **Advanced Functional Materials**
Chair: ***Matthias Gutmann*** (ISIS)
Keynote: ***Paolo Radaelli*** (Oxford)

The development of advanced functional materials is critical to underpinning the development of modern technologies. This session covers such materials with current or potential use in cutting-edge applications. This may include magnetic and electronic materials, such as multiferroics, energy related compounds, for use in solar cells or batteries and modern alloys.

Tuesday Session 2. **Modelling Crystals and Crystallographic Data**
Chair: ***Anthony Phillips*** (QMUL)
Keynote: ***Carole Morrison*** (Edinburgh)

Recent developments in data acquisition, computing power, and our understanding of the fundamental forces at play within crystals have transformed the concept of crystallographic refinement. Among the many "unusual" techniques that are becoming increasingly commonplace are, first, refinement of non-standard parameters: mode amplitudes instead of atomic positions, or thermodynamic properties instead of lattice parameters. Second, refinement against non-standard data is also common: more scattering information than just Bragg intensities, or information from complementary experiments such as NMR or EXAFS, can be incorporated into a crystallographic model. Finally, both empirical and *ab initio* modelling are increasingly necessary to make sense of complex crystallographic information. This session will focus on using modelling techniques such as these to predict, interpret, and generally get the most out of crystallographic data.

Wednesday Session 3. **(joint with BSG) Future of Structural Science.**
Chair: ***Xiadong Zhang*** (Imperial). *Co-chair:* to be confirmed.
Keynote: ***Xiaodong Zhang*** (Imperial).

Wednesday Session 4. **(joint with BSG) Future of Structural Science.**
Chair: ***Mike Glazer*** (Oxford)

In the last few years important advances have been made in techniques to investigate the structures of crystals and molecules. In particular the advent of the free electron laser has shown that it is possible to gain structural information on macromolecules without the need to grow large single crystals. Another area of advance is in the field of electron microscopy, where the development of new aberration-free lenses enables individual atoms to be imaged; the use of freezing methods as in CryoEM enable at least protein molecules to be imaged even when not in crystalline form. Alongside the rapid advances in other experimental and computational techniques this raises key questions about the nature of the future of structural science including whether in the future crystals will be needed at all. It is time that crystallographers think about this and consider the impact of these new techniques on their subject.

Thursday Session 5. **Phase Transitions**
Chair: ***Christoph Salzmann*** (UCL)
Keynote: ***John Evans*** (Durham)

Phase transitions are at the very heart of solid-state chemistry, crystal engineering and mineralogy. The aim of this session is to cover as many aspects of this important phenomenon as possible including phase transitions between crystalline as well as amorphous materials. Particular emphasis will be put on the real-time and in-situ detection of phase transitions as well as the description and parameterisation of symmetry changes.

Thursday Session 6. **Local Structure-Property Relationships**
Chair: ***Matt Tucker***

The local structure of materials often plays a critical role in determining their properties yet cannot be perceived easily by conventional crystallographic analysis; this is particularly pertinent in amorphous and nanocrystalline systems which lack the requisite long-range order. This session will focus on materials where such understanding of the local structure is vital, discussing results from techniques sensitive to these length-scales, such as Pair Distribution Function (PDF) data, Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy, diffuse electron scattering and computational modelling. Where possible, it will highlight the complementary nature of these techniques and the way in which they can be combined to address difficult problems.

YCG Satellite meeting:-

Monday pm

Plenary speaker 1: **Professor Sally Price** (UCL)
Plenary speaker 2: **TBA**

Tuesday am

Special Session: **Forgotten Methods in Crystallography**

Three Invited speakers, including: **Mike Glazer** (Oxford), **Paul Raithby** (Bath)

The aim of the Programme Committee is to present the very best in contemporary crystallography, emphasizing the growing significance of the subject to more diverse areas.
Please see the Conference website **http://bca2016.crystallography.org.uk** for up-to-date details. The deadline for Abstract submissions will be 22 January 2016.

The full Programme Committee is:-

Phil Lightfoot (Chair)
Alex Cameron (BSG)
Simon Newstead (BSG)
Mark Roe (BSG)
Pascal Parois (CCG)
Lynne Thomas (CCG)
Qendresa Osmani (IG)
Ghazala Sadiq (IG)
Nicholas Funnell (PCG)
Paul Saines (PCG)
Horst Puschmann (Workshops)
Scott McKellar (YCG)
Natalie Johnson (YCG)
Lee Brammer (BCA President)
Richard Cooper (BCA Vice President)
Claire Wilson (BCA Secretary)
Pamela Williams (BCA Treasurer)

Phil Lightfoot & **Richard Cooper**
Chair of BCA 2016 & BCA Vice President
pl@st-and.ac.uk richard.cooper@chem.ox.ac.uk


Business School: the venue for sessions


Business School: the venue for sessions


Exchange building


Exchange foyer

BCA 2016
Nottingham

Puzzle Corner

OUR Industrial, Chemical and Biological groups will hold their Autumn Meetings in Macclesfield, Glasgow and Manchester. **In Victorian times, what was the product for which each of these places was best known? What is its main constituent, and what is the space group of this constituent?**

Answer to June Puzzle Corner

Here are the letters to fill the grid.

1 A	2 T	O
G	4 E	3 M
5 A	X	I
A	T	6 S
7 R	8 A	T
E	10 T	9 S
11 M	A	S
A	O	12 S
13 P	14 I	C
I	16 M	15 O
17 T	18 E	R
XXXX	XXXX	A

Boxes 2, 4, 8, 10, 14, 16, 18 tell you to go ahead and have a cuppa!

XRF Meeting Report 17 June 2015

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

Delegates at the XRF meeting.

Overview of Event

THIS year's XRF meeting was held at the University of Leicester in collaboration with the Royal Society of Chemistry and gathered together 57 delegates along with 12 vendor stands presenting their products.

Summary of the Morning Session:

In the beautiful surroundings of Victoria Park backing onto De Montfort Hall it is pleasant for the XRF user to arrive at this one day event which gathers together the XRF community from academics to industry users and of course instrument and sample preparation vendors.

As an industrial XRF user I relish the chance to escape the lab, albeit for one day, to discuss my current XRF issues with likeminded individuals and hear of their experiences and challenges that are so similar yet from a completely different world. The outside and a telephone free environment to do this is such a rarity.

The day did not disappoint in this respect. From the moment I arrived and signed in, the usual faces greeted me and the 'challenging' conversations ensued. Along with meeting new XRF users and interested parties it really is a good mix for thought provoking ideas.

The formal talks began as follows with a good mix of breaks to continue these thoughts and ideas.

Morning Session

Morning Speakers: left to right

***Dave Taylor** (Chair), **Heather Harrison**, **Peter Webb**, **Neil Eatherington**, **David Beveridge**, **Ros Schwarz** (Chair) and **David Maclachlan**.*

Neil Eatherington, PANalytical Ltd, Environmental Science Centre, *(formerly British Geological Survey whom PANalytical have recently acquired after closing their Cambridge demo labs in the UK)* gave a talk on combining EDXRF and WDXRF to optimise the analysis of a range of elements in soils and sediments.

This was a very relevant talk to all XRF users at choosing your instruments to their strengths and made me think more about the use of the instruments at my disposal.

Specifically, Neil centred on As and Sn mapping in SW England utilising the Zetium (WDXRF) and ProTrace package from PANalytical to deliver 41 trace elements in one application and a measurement time of ~50 minutes.

ED(P)XRF (polarised ED) was then presented using the Epsilon 5 to deliver low level analysis on elements that proved problematic for the Rh tube of the WDXRF. The choice of tube target combined with the fact that the high energy K-lines can now be selected on the Epsilon 5 delivered better LLD's for these elements using a 2 target, 17 minute analysis. Interestingly the new PANalytical WDXRF (Zetium which replaces the Axios) can be configured with an EDXRF channelset.

Peter Webb, Open University, delivered a thought-provoking talk on reporting XRF results at concentrations approaching the detection limit. This talk was dedicated to **John S Watson** who was a familiar face within the XRF community and recently passed away.

Running the GeoPT scheme which has so far delivered 37 rounds of proficiency testing on more than 40 samples delivers some very useful data to interrogate.

Elements showing poor fit to the consensus (As, Sb, W, Cd, Mo) were looked into further and a breakdown by instrument technique was presented. ICP-MS was used alongside EDXRF and WDXRF along with other techniques and the data

Exhibitors at the XRF meeting.

was of interest to all. Further discussions later in the day and between delegates brought up the idea that manufacturer presented detection limits could be considered by some as lower reporting limits and further education of XRF users could be beneficial to calculate lower limits of quantification and the associated uncertainty of measurement close to the detection limit.

Exhibition Session

From sample preparation to fusion and pellet production to analysis with handheld (including a LIBS handheld from Oxford Instruments) across to benchtop ED and full WDXRF were all on show. A first look at all the exhibitors as well as the vital discussions between delegates were then followed by a further two talks.

David Maclachlan, Johnson Matthey, presented a summary of JM divisions and then an interesting insight into the world of catalyst analysis. For the researcher who has limited sample but wants to know everything about the sample, XRF provides an essential part in this. The challenges that also arise from analysis taking place across multiple techniques and sites proved that the environment plays a large part in analytical accuracy and the associated measurement uncertainty.

The results from DOT-2 – David Beveridge presented the results from DOT-2, the sample that delegates were provided with last year. This meeting is a good arena for trialling samples of types that delegates are not used to, but this sample was so unfamiliar that only 3 sets of results were presented. **Heather Harrison** from British Gypsum provided this year's sample, DOT-3, which should prove more popular. I have challenged my XRF trainee to provide her best analytical results by thinking through all aspects of material identification and analysis and hopefully all the well-spent training will make me a very proud mentor.

In between talks the time is spent digesting the information in a work/hassle free environment and the nature of the day makes the bouncing of these ideas across many different minds a very useful event indeed.

Judith Bain
Alfred H Knight International Ltd

Afternoon Session

Afternoon Speakers: left to right

Frederic Davidts, Nick Marsh** (local organiser), **Ade Band, Raphael Yerly, David Beveridge** and **Heather Harrison** (Chairs) and **Rainer Schramm.

After lunch, **Raphael Yerly** from Thermo Scientific gave a talk on **a new application of WD-XRF**, analysing small samples, or small areas of larger inhomogeneous samples, using an internal mask to restrict the take-off beam. He first showed that it is possible to get good quantitative results from 0.5 mm diameter fused beads made with as little as 0.05g of sample. Raphael then discussed the analysis of inhomogeneous samples, moved on a slider across the internal mask to pick out different regions, exemplified by point analysis on a defect in stainless steel. He illustrated the mapping capability with examples from a weld between two different steels and a limestone with a dolomite vein, adding the usual caveat that mapping takes a long time, and that a line scan can give much of the same information. He finished by showing us some more examples of the versatility of the technique.

Next, **Rainer Schramm** from FLUXANA introduced his company's new electrical fusion system and gave us some examples of its use. He showed us very good results from oxidic materials and then discussed more difficult materials such as ferroalloys. Ferroalloys, which must be oxidised before fusion, can either be placed with the vanadium pentoxide oxidant on top of the flux in one step, or oxidised first and then the flux added in a two step procedure. Adding

tungstic oxide as an internal standard for silicon in ferrosilicon gave impressive precision. Lids on the crucibles retain splashed material and a quartz window is available so that the melting can be observed without contamination of the furnace, particularly during method development. Lastly, Rainer talked about the analysis of continuous casting powders that can contain up to 20% carbon which must be burnt off and which require fluorine analysis. Because the furnace is small and closed, loss of fluorine (and other volatiles such as chlorine and sulphur) is controlled and good results can be obtained.

After a break for a welcome cup of tea, **Frederic Davidts** from SOCACHIM gave a comprehensive discussion of the care of platinumware. He pointed out the advantages of using platinum including its high melting point, high strength and resistance to corrosion at fusion temperatures, and its good formability; and he outlined the different alloys. He suggested some basic precautions such as using platinum-tipped tongs, clean refractories and oxidising furnace conditions, showing some dramatic pictures of what happens when things go wrong. Elements including Sb, As, P, Se and Te (and their compounds) poison platinum and must be avoided; the more common troublemakers, including sulphides, metal powders, ferroalloys and silicon carbide must be fully oxidised or they will not dissolve properly in flux and will damage the platinum. Frederic showed some data to illustrate the importance of a flat casting dish (mould) and discussed the best technique for polishing. He outlined the acids used for cleaning platinumware, such as boiling dilute HCl or 20% w/v citric acid in an ultrasonic bath. Finally, he pointed out that if you have to spend a long time on cleaning and polishing or you suspect that problems with the flatness of your beads is beginning to affect your results, then that is the time to trade in for new labware. And, of course, it is fully recyclable!

For the last talk of the day, we had a reminder of the uses of our technique. **Adrian Band** from the University of Leicester described his PhD research on tracing the history in deep time back to the Early Palaeozoic of the re-arrangements of the ocean basins, using the different chemical domains of the depleted mantle that erupts to give mid-ocean ridge basalts (MORB). However, it is very important that these ancient rocks are unmodified by subsequent geological events such as subduction, obduction or weathering. After setting the scene by showing what these rocks, known as ophiolites, look like and where they are found, he described screening his MORB material, looking at the behaviour of the ratios of elements determined by XRF and of each element to the rock to loss on ignition of the material. Detailed ICP-MS work at levels below the range of XRF and finally isotope analysis gave data that Adrian used as new evidence for widespread and early Indian-type MORB with a possible shallow origin. The meeting finished with a question and answer session which included a discussion of the results that Peter Webb presented earlier in the day and answered several questions from the audience.

Ros Schwarz

The Academic Family Tree

MIKE Glazer introduces us to the website http://academictree.org/crystallography , which aims to explore the influence of mentorship on trainee research programs (and possibly vice versa!). The beta site now provides a simple overlay of research similarity on the tree display. Mike suggests to BCA members to enter their details so that mentor-trainee interactions in crystallography can be characterised.

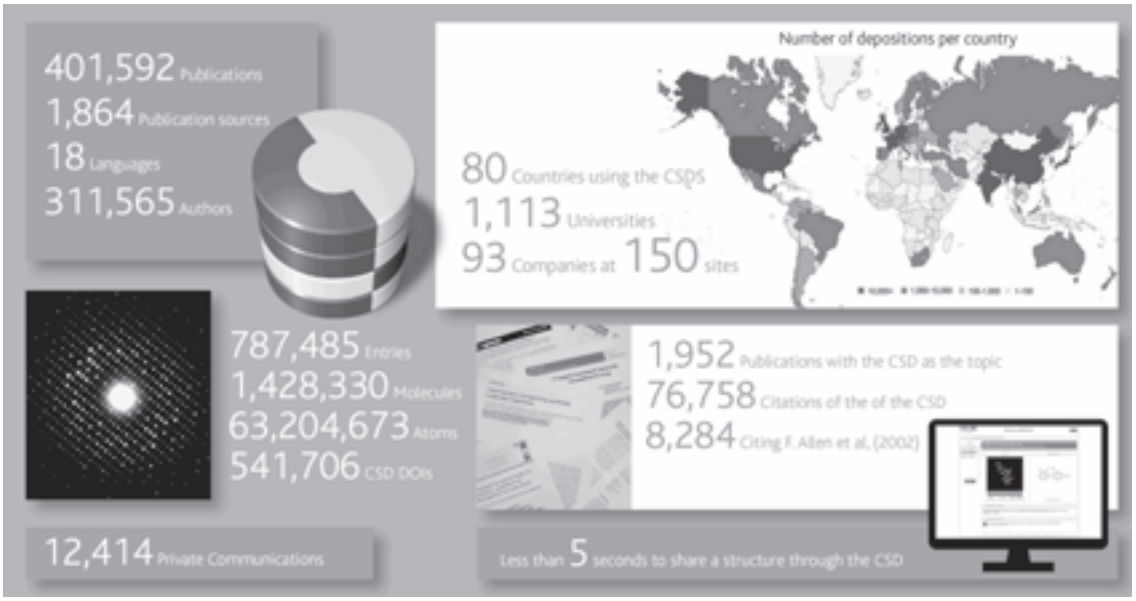
Celebrating 50 years of the Cambridge Structural Database

THE beginning of July in Cambridge saw crystallographers from around the world gathering to celebrate the first fifty years of the Cambridge Structural Database. From the opening lecture by Olga Kennard, the Founder and first Director of the Cambridge Crystallographic Data Centre to the closing session when the current Executive Director, Colin Groom turned his crystal ball to the next fifty years, attendees were taken on the journey from Olga's vision for one of the first scientific databases to the creation of a vast curated resource of immense value to scientific research. With over ¾ million curated crystal structures, the CSD is now used by researchers and educators worldwide to answer questions in structural chemistry, drug discovery, materials science, formulations, and much more.

The symposium program celebrated the community achievement that is the CSD with presentations from CCDC staff past and present, and our colleagues in industry and academia. Sessions explored current applications in molecular recognition and design, solid form informatics and structural chemistry. You can access the program and the CSD50 newsletter at http://www.ccdc.cam.ac.uk/csd50/

▲ *CSD50 Symposium attendees gather in the garden of Downing College Cambridge.*

▼ *50 years of the CSD in a snapshot.*



50 Years of Sharing Structures

Opening lecture by **Olga Kennard**, Founder of the CCDC

Ian Bruno (CCDC) – *"Sharing research data and knowledge – a fifty year perspective"*

Helen Berman (PDB) – *"The evolution of the Protein Data Bank"*

Suzanna Ward (CCDC) – "A journey through the Cambridge Structural Database

Report by **Hannah Bruce Macdonald**, University of Oxford

Olga Kennard describing the founding of the CSD.
Picture courtesy of Caroline Hancox, Department of Chemistry, University of Cambridge.

Every seat was filled for the opening talk of the 50th anniversary of the Cambridge Structural Database (CSD): **Olga Kennard**, the first Director and one of the founders of the CCDC in 1965. She began by talking of JD Bernal and his belief that huge scientific gain could be made by bringing together the results of many individual experiments, and how this idea lay at the foundation of the CSD. Looking back at how one post-doc would process 100 structures onto punch cards using knitting needles gave context as to how far the information had come. The Royal Society saw the early work and Olga was invited to present their work in Washington, which led to the funding that allowed for one postdoc and the beginning of the CSD. She attributed the success to the talented and energetic group who started the daunting task of work with the database, to whom users of the CSD owe so much. Olga talked of being offered an existing database, which hadn't been checked but this was turned down, as she wanted to build a reliable database, which people could use with confidence. She closed by telling the room how 'the basic ideas still hold good' and how much of the dream had been realised. Her talk of the history of the Cambridge Crystallographic Data Centre (CCDC) illustrated the highlights of the 50 years she has seen of the company, setting the scene for the talks of the scientific successes and working to come, which have all been made possible by the database.

Ian Bruno, a senior manager at the CCDC followed, giving a 50-year perspective of the CCDC. He talked of the flood of information the CSD faced, and the methods used to handle it. He discussed the data formats used to help that – the introduction of the CIF files, and the positives and the negatives of human-readable file formats. The Public Library of Science now expects all data to be submitted with a journal submission, and Ian described how this is already compatible with the CSD system. He debated the addition of raw data to the database, and how this could be beneficial with improvements to analysis techniques allowing information to be revisited, but came at a storage cost. He closed, talking of the licences available for the database, and how no institution would be denied access to the service based on funding.

Helen Berman, former Director of the Protein Data Bank talked about the PDB and how the CSD was instrumental to its development. She attended the 1971 Cold Spring Harbor Symposium where the PDB was born through a petition. When Walter (Hamilton) established the archive, the first step he took was to fly to England and discuss the CSD with Olga. The PDB was made possible by recognising the importance of the CSD in its field. The PDB now receives 210 new entries a week, from a broad community. She echoed Ian's discussion of raw data, stating how despite the benefits the funding and resources are limited. The parallels between the two databases are now reflected nicely as they now both have offices in the same building in New Jersey.

Suzanna Ward, Cambridge Structural Database Manager at the CCDC, closed the first session of the Symposium, discussing the numbers of the CCDC (784,428 was the current number of structures in the database) and how the R-factor had decreased over time, and looked at how publications were now split between many more journals. There are now many more authors per crystal structure, and the average cell volume has now doubled in size. The increase in size and complexity in the structures reflects the improvements in techniques, and there are very few elements left, that are not present in a CSD structure. She discussed the alphabetical bias by the users of the database, with a 7% increase in looking at early alphabetical structures. She finished by discussing some of her favourite structure refcodes, including CARPET, BIKINI and BADBOY.

Suzanna Ward closing the first session of the Symposium.
Picture courtesy of Caroline Hancox, Department of Chemistry, University of Cambridge.

50 Years of Science & Software

Robin Taylor (CCDC) – *"CSD research at the CCDC: a voyage through the years"*

Angelo Gavezzotti (University of Milan) – *"Twenty-five years of Cambridge Structural Database mining: Chemical bonds and chemical bonding"*

Jason Cole (CCDC) – *"The development of the CSD System: The challenges faced and the milestones achieved"*

Report by **Andy Maloney**, University of Edinburgh & the CCDC

Having woken up at the crack of dawn to endure the hustle and bustle of an early morning flight to get from Edinburgh back to my CCDC base of operations (and being only slightly delayed), I was extremely glad to arrive at the tranquillity and grandeur of Downing College. A truly fantastic setting for what promised to be a truly excellent conference.

After a nice spot of lunch in the sun spent catching up with some old friends and some fascinating talks discussing the journey of the CSD so far, of particular note the opening lecture from Olga Kennard, it was time to settle down to the late afternoon session – "50 Years of Science and Software". Our session chair, Ian Bruno, took to the stage to introduce the first speaker, the CCDC's own **Robin Taylor**, and his talk "CSD research at the CCDC: A voyage through the Years". During his introduction, Ian was quick to point out the caveat in Robin's abstract: "Only a fool would attempt to summarise these fifty years of CCDC research in just thirty minutes." How would our speaker fare, having made such a rod for his own back?

Robin began by reminding us why research is done at the CCDC – to develop our software and understand our users, to maintain our contacts and our own high profile and, of course, because we are scientists and simply enjoy doing it. He noted that the research at the CCDC is becoming more and more diverse with each passing year before taking us on a timeline of a set of papers that illustrated this point magnificently, and highlighted how important the CSD and the research the CCDC provides are to the scientific community. All the famous papers from through the years were there, from the evidence of C-H···O hydrogen bonds to the tables of derived bond lengths (cited over 12,000 times!) and the introduction of the Crystallographic Information File, and many more besides. More recently, last year's paper "Knowledge-based approaches to co-crystal design" showed how far the CSD and the CCDC have come in terms of harnessing the huge amounts of data at our disposal to tackle complex problems, highlighting the importance of several high-profile collaborations along the way. Clocking in at just under half an hour, Robin had summed it all up perfectly, foolishly proving himself wrong in the process.

Our next speaker was **Angelo Gavezzotti** of the University of Milan, with his talk titled "Twenty-five years of Cambridge Structural Database mining: Chemical bonds and chemical bonding". After a historical preamble, he challenged the audience with two questions. The first of these was to ask if we know what a chemical bond is. Fortunately, courtesy of the CSD, we do (to some extent anyway). The second question was a bit trickier. "What is not a chemical bond?" Angelo went on to stress that, while the distribution of intramolecular bond lengths across the CSD is quite narrow, intermolecular bond lengths for hydrogen bonds and "the sons of a lesser god" (other short contacts, to you and me) have considerably wider distributions. A stark warning, perhaps, that it is very important to investigate energies as well as geometries before making any assertions about bonding.

This session was rounded off by **Jason Cole**, a member of the CCDC's staff ever since completing his PhD, with his talk, "The development of the CSD System: The challenges faced and the milestones achieved." It must be said, Jason was ideally suited to give such a presentation, having contributed to the majority of the software involved. I have to admit, although I've used the CSD system almost every day for the last five years, I hadn't ever really thought about the journey it had taken. From the hefty tomes of the early days which had to be pored through manually, to the sleek searches that can be performed in the blink of an eye today, the CSD System has come a long way. Jason spoke with great insight into how the changing scientific world has led to numerous data explosions over the years that the CSD has had to cope with.

And cope it has. The CSD, through some pieces of remarkably clever software, has always managed to stay ahead of the curve. Perfectly summed up by Professor Gavezzotti, "the CSD is to the structural chemist what lavender is to the bumblebee."

Molecular Recognition

Martin Stahl (Roche) – *"Mining the treasure trove: Interaction and conformation searching in structural databases"*

Chris Hunter (University of Cambridge) – *"Quantification of non-covalent interactions"*

Gerhard Klebe (University of Marburg) – *"From structure correlation in the CSD to the prediction of molecular recognition in protein-ligand complexes"*

Report by **Christin Schärfer,** CCDC

The first speaker of this session was **Martin Stahl** who just recently joined the board of the CCDC's trustees. He started his talk "Mining the treasure trove: Interaction and conformation searching in structural databases" by explaining how he became interested in chemical structures. As a child he collected stamps, some of them with pictures of molecules. He really enjoyed it but later realised that it is much more fun to look at structures than at stamps and he started wondering what people know about conformations and how we can share knowledge. Martin suggested that in order to expand our knowledge about conformations we should use analogies between structural motifs and we should think in series of structures rather than individual cases. In an application example he explained how they successfully used this methodology at Roche to look at conformations of Suvorexant to find out what the overall shape looks like. CCDC tools like ConQuest were really helpful during this process. In the second half of his talk Martin described and showed applications of a new pharmacophore query tool that has been developed in collaboration with the CCDC. Results are provided almost in an instant by the new tool, allowing iterative searches and making them highly interactive. Martin finished his talk by showing more examples that illustrate how crystal structure data can be used to gather knowledge that helps analysing structures.

The next talk "Quantification of non-covalent interactions" was given by **Chris Hunter**. He introduced himself by saying that although he shares a birthday with the CSD he is more a solution guy. To start his talk Chris showed a slide with his first

contribution to the CSD which is probably also the last molecule he ever made with his own hands. Chris's group perform quantitative measurements of the thermodynamic properties of aromatic stacking, hydrogen bonding and halogen bonding interactions in the liquid phase. They use IsoStar and quantum chemical calculations in the gas phase to corroborate their findings. Chris established a system to use interaction potentials for functional groups derived from the liquid phase experiment to screen for compounds that form co-crystals with a particular drug molecule. This co-crystal prediction project is done in collaboration with Neil Feeder at the CCDC. This approach simplifies complex systems by approximating the overall energy of association as a sum of individual interaction energies, which are rigorously benchmarked against experimental data. Klaus Müller asked whether the model can explicitly model the cooperative effects of weak interactions. Chris answered that it cannot, but that it is rather accurate nonetheless.

The session was finished by **Gerhard Klebe** and his talk "From structure correlation in the CSD to the prediction of molecular recognition in protein-ligand complexes". Gerhard is a former CCDC trustee and started his talk by telling us that his first encounter with the CSD was during his PhD in 1979 and a book written by Jack Dunitz. He then talked about his time at BASF where he got acquainted with computational methods for generating conformations. Looking at these conformations they realised that the conformations often didn't correspond with crystal structures and so they came up with the idea to solve this problem by using torsion angle distributions from the CSD. In his next slides Gerhard showed how they predicted interaction sites in protein pockets by mapping crystal field environments in the CSD which later resulted in the development of IsoStar. Next he talked about a problem that occurred while looking at preferred atom-atom distances in protein ligand complexes for scoring functions. At that time, there were not enough entries in the PDB and the resolution of the entries was not very good. To make the best possible use of all the information present, Gerhard and members of his group including Manfred Hendlich developed Relibase and Relibase+ in collaboration with the CCDC and others. One of Relibase's very well received features is the ability to store positions of conserved water molecules. Gerhard showed an impressive example of how the quality of the water network in a binding site affects the potency of a drug. He finished his talk by saying that the CSD is a great tool which everyone in Marburg is very thankful for and that their research really depends on the CSD.

Molecular Design

Klaus Müller (Roche) – *"The CSD and Roche's early entry into structure-based drug discovery"*

Terry Stouch (Science for Solutions) – *"The CSD: A fundamental resource for molecular modeling"*

Alberto Gobbi (Genentech) – *"We need Champagne, other drinks are not enough!"*

Report by **Florian Roessler**, University of Cambridge

The session was opened by the chair, Beth Thomas, who introduced **Klaus Müller** (Roche) as the first speaker of the session. In his talk Dr. Müller told the compelling story of how structure-based drug design at Roche was influenced from the beginning by very fruitful collaborations with the CCDC and the PDB. This is exemplified by the shared 50th birthday of the CSD and Roche's small-molecule X-Ray structure analysis efforts. He continued describing his early career at Roche, where he made access to structural databases a condition of his involvement. While in the early years Roche was using its own relational database version of the CSD (ROCSD), they abandoned this project in the 1990s in favour of the powerful CSD software suite. The early years in the area were made challenging by the lack of sufficient crystal structures and it took a significant amount of time and effort to develop the necessary molecular models needed in their ongoing projects. He illustrated this by drawing the listeners' attention to their efforts in producing sufficiently hinged small-molecule structures in order to target the E. coli DHFR-MTX complex. Their model existed as early as 1982 but it took until 1986 until the first compound (CSD REFCODE: DUZHEL) was produced and showed sub nano-molar activity. Previously found compounds had shown no activity at all. He continued by stating that underrepresentation of conformational polymorphs due to crystal packing effects still exists despite today's large number of structures in the CSD. He summarised his talk by saying that because of the growth of the data in the CSD and the software that is built around it, previous challenging questions can nowadays be answered more easily and elegantly than before.

The second speaker of the session was **Terry Stouch** who works as a consultant with Science for Solutions. Dr. Stouch shared his great insight into the early days of force-field development and his involvement therein. He described the early advances in the field and the close interactions with researchers working on the CSD. As his talk continued he highlighted milestones like the acquisition of energy parameters from crystal data in 1979 and the work by Donald E. Williams on deriving non-bonded potential parameters from crystals. The lack of crystal data representing substantial volumes of chemical space along with the rise in availability of computational resources then led to the emergence of force-fields that were parameterised using quantum-mechanical approaches. While over the past decade these types of force-fields have shaped development in the area he stressed that it has come to a point where crystal data has again become more relevant. He attributed this to the significant improvement in availability and quality of crystal data. As an example he discussed the dihedral angle of ligands in a structure-based drug optimisation context. In this example, the difference in steepness of the energy profile between CSD and QM dihedrals nowadays can provide valuable information and influence the outcome significantly. The talk was concluded by his emphasis on the significance of the CSD as an educational tool and the need to promote interaction between Modellers and Crystallographers as exemplified in a successful RCSB workshop in 2009 at Rutgers University.

Alberto Gobbi was introduced as the last speaker of the session. Along with the previous speakers, Dr. Gobbi presented a convincing story of the importance of the use of crystal data in a drug development context both in the past and for the future. His talk focused around the importance of the correct assessment of strain energy between bound and unbound ligands and its relevance in determining the strength of ligand binding. He provided insights into cases where the calculation of strain energy using modern force-fields still performs below expectations. In particular considering the time and resources that are involved in providing accurate dihedral parameters, classical force-field approaches are seen as a bottleneck in this aspect of Structure-Based development. He presented examples of the trade-offs that current approaches encompass. While quantum-mechanical approaches at high

level of theory provide good insights into the accurate potential energy surface of ligands, the time involved in running these calculations (from 30 min up to 12 hours per dihedral) render them unusable in a high throughput context. On the other hand, force-field approaches while providing a much quicker result, still struggle with a lack of accuracy due to the generality of their parameters. Besides this, Dr. Gobbi also highlighted how force-field based approaches can massively reduce the time spent on drug optimisation problems. In addition to this he stated that only by comparing the relevant calculations to data from small molecules of the PDB (bound) and CSD (unbound) can we ensure that our models provide the best results possible. All this contributes to better tools that with their interactive capabilities significantly improve the understanding of the role of strain energy in protein ligand binding. He concluded his talk and the session by emphasising that champagne and much praise reflect only part of the appropriate way to celebrate the 50 year anniversary of the CSD and its contribution to the scientific community.

Solid Form Informatics

Susan Reutzel-Edens (Eli Lilly and Company) – *"Lessons learned in structure-based solid form design"*

Joel Bernstein (Ben-Gurion University of the Negev & NYU Abu Dhabi) – *"The CCDC and me"*

Aurora Cruz-Cabeza (Roche) – *"From desmotropy to conformational polymorphs*"

Report by **Luca Iuzzolino**, University College London

This session of talks during the '50 years of the Cambridge Structural Database' event was focused on the role the CSD solid form informatics tools have had in aiding scientific research and the understanding of organic-solid state behaviour both in industry and academia. This series of talks was characterised by a combination of personal experiences, anecdotes and scientific information that made it extremely interesting for the audience.

Susan Reutzel-Edens who works as a Senior Research Advisor for the pharmaceutical company Eli Lilly and Company, gave the first talk. It was focused on how the CSD helped to solve some important drug-development problems during her career at Eli Lilly. A very interesting example she gave regarded the synthesis of pruvanserin, a drug used to treat insomnia: during the development it was realised that its crystals lost weight with increasing temperature, which suggested the presence of water within the crystal structure. Although this intuition was backed by NMR studies, she struggled to make her management believe this theory since there was no way to see the presence of water in the crystal structure. But the CSD informatics tools solved the problem by allowing a change in perspective that made it possible to see the presence of water in the voids between molecules, which would have not been possible without that presence. She also reminded the audience of how the Blind Tests of organic crystal structure prediction organised by the CCDC have increased the credibility of computational methods in industry leading to her collaboration with Sally Price's group at UCL.

The second talk was given by **Joel Bernstein**, currently serving as a Professor at New York University in Abu Dhabi and at the Ben-Gurion University of the Negev. After an interesting anecdotal introduction about how a piece of homework in his youth made him understand the importance of finding the right information when needed, he went on to talk about some major developments in our scientific understanding of solid state organic chemistry that would not have been possible without the presence of the CSD. In particular the fundamental role of the CSD in making the scientific community accept the physical existence of the weak C-H···O bond despite the famous Jerry Donohue's "it isn't" was outlined. Professor Bernstein also expressed his gratitude to the CCDC for having made the hydrogen bonding graph sets become lingua franca of chemistry through their implementation into the CSD informatics tools. This was very important to him: the idea of graph-sets had been developed by his colleague Margaret C. Etter before her death in 1992, and he was grateful to the CCDC for having allowed her intuition to be spread out in the scientific community.

The final talk of the session was given by **Aurora Cruz-Cabeza**, who is currently working at Roche in Basel. It was focused on how the CSD has helped her throughout her career as a researcher to investigate some solid-state phenomena. In particular she gave a very interesting exposition of how the use of the CSD allowed her study of how to control tautomerism via supramolecular selectivity. The main section of the talk was focused on her recent study conducted together with Joel Bernstein on polymorphism. In particular mining the CSD with the aid of its informatics tools has allowed them to collect a large enough set of data to be able to demonstrate how certain common beliefs about polymorphism do not have any statistical base: the occurrence of polymorphism appears to be totally independent of molecular flexibility, molecular size and hydrogen bonding. The final part of the talk was focused on how the CSD was vital in categorising and studying conformational polymorphism, which occurs when a molecule crystallises in two different conformers separated by an energy barrier. Data-mining with CSD informatics tools has also made it possible to produce some simple cut-offs to recognise conformational polymorphs.

Overall it was a very interesting session, which gave every person in the audience a very good idea of the importance of the informatics tools developed by the CSD in scientific and industrial research.

Structural Chemistry

Paul Raithby (University of Bath) – *"The use of the CSD in understanding and designing solid-state organometallic reactions"*

Greg Ferrence (Illinois State University) – *"Permeating the Cambridge Structural Database into chemical education"*

Nick Funnell (University of Oxford) – *"Disorder and dimensionality"*

Zéphirin Yav (University of Kinshasa) – *"CSD use at the University of Kinshasa in D. R. Congo"*

Report by **Rachael Skyner**, University of St Andrews

The structural chemistry session, chaired by the CCDC's own Pete Wood, was kicked off by **Paul Raithby**, Professor of Inorganic Chemistry at the University of Bath. Paul was introduced by Pete as a 'Giant of British Crystallography", and his talk certainly emulated this introduction. Paul's discussion had a focus familiar with the rest of the conference; where have we come in the last 50 years – specifically in structural

chemistry? Quoting the experienced words of Jack Dunitz, Paul reminded us all that "Crystals do not contain an array of rigid molecules"; and it is the movement of molecules in crystals that Paul believes to be a future focus of structural chemistry. The movement of molecules in the solid state is key to Paul's research, which focuses on reactions in the solid state.

Paul discussed his lab's tried and tested method of using Christmas tree lights (!) to induce photochemical reactions. This sort of reaction has been known since the late 19th century, with the first example in the solid state being Cohen and Schmidt's light-induced 2 + 2 cycloaddition reactions (1964). Paul has used the topochemical postulate that the reaction process follows the minimum energy pathway, meaning the least atomic movement is the most favourable pathway for preservation of the crystal in a solid-state reaction, to investigate further. Assuming the structure of the product is related to the orientation of the reactant monomer, Paul searched the CSD, finding 67938 hits corresponding to parameters for 2 + 2 cycloaddition, with around 2600 of these containing the necessary parallel double bond. Of these structures, 4 structures were found which hadn't previously been investigated for the photochemical 2 + 2 cycloaddition reaction, which Paul's group went on to investigate. This sort of example reminds us all of just how far and wide the use of the CSD stretches, and of how the potential applications of the vast amounts of data we have at our fingertips are far beyond what many of us would dream of!

The second talk of the session was given by **Greg Ferrence**, Professor of Chemistry at Illinois State University, who has been collaborating with CCDC since 2006, focusing on how to use the CSD in education. In 2004, Greg noticed that the CSD was absent from teaching the principles of chemistry at the undergraduate level, which he thought was particularly absurd. In 2006 Greg surveyed the literature for examples of the use of the CSD in chemistry education, and found 15 mentions of the CSD, of which only 3 were related to the use of it. Greg set to work in collaboration with the CCDC to select a subset of structures representative of the topics covered in undergraduate chemistry. This set is now openly and freely accessible via the CCDC.

Greg also showed us some examples of the specific modules designed by himself and the CCDC to aid teaching. One particular example that sticks in my mind is using the CSD to search for the existence of the bromonium ion, in order to help students understand the mechanism of Br_2 addition to alkenes. If I had been taught about this mechanism with the aid of the CSD for visualisation, maybe I would have really understood it, instead of sitting at the back of the lecture theatre giggling at "backside attack" - but maybe that's more a reflection of my attitude than my lecturer's teaching style!

The penultimate speaker of the session of the session was **Nick Funnell**, who works as a Post Doctoral Research Associate in Prof. Andrew Goodwin's group at Oxford, and the winner of this year's CCDC Chemical Crystallography Prize for Young Scientists. Nick discussed some of his fantastic work focusing on disorder and dimensionality in three separate systems – an organic hydrate, a framework material and an inorganic nanosheet – all very different materials, yet all very interesting. Nick promised us that he really does use the CSD a lot, even though his presentation focused on the nitty gritty details of how he went about solving the disorder in the materials he discussed. Disorder is something that most crystallographers have to deal with at some point, and the methods that Nick discussed certainly had our minds working overtime on how we could improve our own structure solutions!

The final speaker of the session was **Zéphirin Yav** from the University of Kinshasa, Democratic Republic of Congo. The University of Kinshasa first started its relationship with the CCDC in 2007, when the CCDC granted a CSD license to the Sciences Faculty as part of a collaboration whereby over a 24 month period, academic staff and students were introduced to and trained to use the CSD for both training and learning. In 2013, a research collaboration between CCDC and Kinshasa was established, allowing the sponsorship of a number of students in the area of structural chemistry. The CSD plays an important role in supporting the QM calculations conducted by researchers in Kinshasa.

Yav discussed some of the difficulties encountered by his university, and exemplified the responsibility of researchers from top-class institutions to aid the development of research programmes in the rest of the world. When asked "What can we do to help?" Yav simply responded, "Collaborate with us and help us where you can". Certainly food for thought, and a perfect close to the session. We started the session thinking about where we have come, and ended the session wondering where we would go in the future.

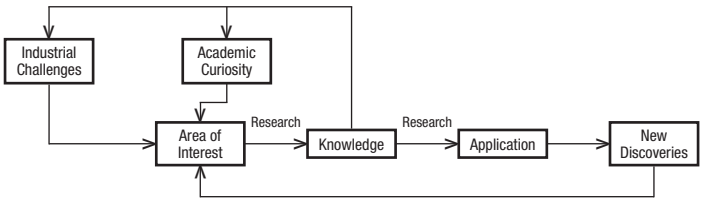
Structural knowledge in a changing world

Chick Wilson (University of Bath) – *"From structure to crystallisation and manufacturing: a journey from fundamentals to flow"*

Bob Docherty (Pfizer) – *"Towards computational product and process design"*

Report by **Elena Kabova**, University of Reading

It is often stated that academia and industry are very different – and indeed they are. Academia is (historically) largely curiosity driven, whereas industry is driven by economic imperatives. However, there are clear underlying similarities, as demonstrated by the talks of Prof. **Chick Wilson** and Prof. **Bob Docherty**, which focussed on the area of solid-state science in (mainly) the area of pharmaceuticals. Both speakers described their personal journey (very X Factor!), their key drivers and the underlying principles of their work, and these were remarkably similar throughout. My interpretation of these various elements is outlined below:



In Chick's case, the cycle began with sheer curiosity: to discover the fundamentals of the hydrogen bond from a structural viewpoint. This knowledge is then applied to design and create new materials with improved properties. By way of example, his group discovered (with a little bit of serendipity) a crystallisation route for paracetamol form II (Thomas et al., 2011), a form that had previously proved quite elusive. One of his main focus areas is now the continuous flow manufacturing of crystalline forms, which is of course of considerable industrial interest; efficiency, sustainability, reduced production times,

decreased costs and quality control. With low-solubility pharmaceuticals increasingly being formulated as co-crystals, salts and solvates, the aspect of applying continuous flow crystallisation to multi-component systems is also under investigation.

Bob then proceeded to show how industry successfully exploits the accumulated knowledge and proactively utilises it in current developments. The importance of the aforementioned hydrogen bond and the CSD, together with its tools, was demonstrated by his referencing of a number of articles – he must have highlighted around 20 papers in his talk. In an early paper of Margaret Etter for example (Etter, 1990), the predictability of hydrogen bonds is discussed, and empirical hydrogen bonding rules are established based on the CSD derived information about intermolecular contacts. This structural knowledge was shown to play an integral role in all stages of the "molecule to crystal to particle to drug" journey, and helps tackle specific problems, an example of which is polymorph stability (Feeder et al., 2015).

Unsurprisingly, both speakers strongly linked their journeys to developments in the CSD, which in just 50 years has advanced from a few hundred simple crystal structures (from which information was extracted manually) to a remarkable 750,000+ crystal structures that can (in many cases) be interrogated automatically. Perhaps most importantly, many tools for extracting and evaluating this 'library' of information have been developed by the CCDC, allowing non-expert users to benefit from this invaluable source of experimental information. Interestingly, the CSD was described as the 'fire' which catalysed discussions and ideas over the last 50 years. This resonated strongly with me as, without the CSD, my own particular research area (leveraging prior structural information to improve the performance of crystal structure determination from powder diffraction data) would be even more challenging, denied of a source of valuable experimentally-derived structures that function as an ensemble.

The overall emphasis was that, as new challenges arise, better collaborations between the industrial and academic communities will be needed to overcome them. And with academic funding increasingly placing emphasis on the 'impact' that will result from the funding, it is hard to argue against this.

Etter MC (1990) Encoding and decoding hydrogen-bond patterns of organic compounds. Accounts of Chemical Research **23**:120-126.

Feeder N, Pidcock E, Reilly AM, Sadiq G, Doherty CL, Back KR, Meenan P and Docherty R (2015) The integration of solid-form informatics into solid-form selection. J. Pharm. Pharmacol. **67**:857-868.

Thomas LH, Wales C, Zhao L and Wilson CC (2011) Paracetamol Form II: An Elusive Polymorph through Facile Multicomponent Crystallization Routes. Crystal Growth & Design **11**:1450-1452.

The Next 50 Years

Christer Aakeröy (Kansas State University) – *"What are we going to do with all this information?"*

Colin Groom (CCDC) – *"The CSD at 50: How will structural science look in another 50 years?"*

Report by **James McKenzie**, University of Cambridge

Following an excellent display of how the CSD has been utilised past and present, the closing session of the CSD50 looked towards the future. **Christer Aakeröy** opened the session with his talk titled "What are we going to do with all this information?". The talk addressed some of the key issues that may arise in the future of an ever expanding CSD. The interesting question of "how much data is enough?" was raised. Does the CSD already hold enough data to answer all of our questions? Christer argued that we are still extremely far away from this point as there are still many classes of molecule or functional groups for which there is little data available. A comment from the audience furthered this point, adding that the content of the database is not uniformly distributed throughout the chemical space and we need crystallographers to fill in the missing gaps. The growth of the CSD will therefore remain vital for the continued elucidation of behavioural patterns which help guide industry and academia to making correct decisions.

"You can't just put data out there" – Olga Kennard

With the growth of the CSD comes a larger need for data curation. Christer acknowledged the fantastic work the CCDC do in scrutinising published structures to ensure their quality. This can only be achieved by a team of dedicated experts who are in constant contact with authors. Encouragingly, complementary technologies to crystallography may arise in the future, such as crystal structure prediction and microscopy. Christer argued that in order to consolidate all this information it will become even more important for the CCDC to curate, organise and distribute these data to the public.

The second and final talk was by **Colin Groom** who gave his predicted forecast of the changes that are likely to occur in the CSD, and how the CCDC will adapt accordingly. Colin predicted that the way in which that database is accessed will become easier, a point which was emphasised throughout the conference by numerous people viewing structures on their mobile phones and tablet devices. The types of structures that are deposited are likely to change with an increasing number of MOFs and nanoparticles being crystallised. Due to the increased size and complexity of these structures new graphics will be required to visualise them and new programs will be needed to analyse them. Additionally the number of deposits of host guest systems will increase due to the growing use of Fujita's crystal sponge method.

Colin explained how alternative funding models are being explored to ensure that the CSD is as far reaching and accessible as possible. The importance of overseas use of the database was highlighted by Colin's prediction that in the near future the largest contributors to the CSD are likely to be researchers in China and India. An earlier talk by Professor **Zéphirin Yav** from the University of Kinshasa (D. R. Congo) explained how through collaboration with the CCDC they were able to access the CSD for not only teaching purposes but also to perform innovative scientific research. Future collaborations like this will be required to give access to the CSD and train people who would be otherwise unable to use it.

Left to right: David Wilson, Olga Kennard and Colin Groom.
Picture courtesy of Caroline Hancox, Department of Chemistry, University of Cambridge.

Collaboration between the CCDC and the IUCr Streamlines Crystallographic Data Deposition into the Cambridge Structural Database

04 August 2015, Cambridge, UK and Piscataway, NJ, USA

THE Cambridge Crystallographic Data Centre (CCDC) announces a new collaboration with the International Union of Crystallography (IUCr) that has integrated checkCIF data validation into the Cambridge Structural Database (CSD) deposition process. The Crystallographic Information Framework (CIF), maintained by the IUCr, is the standard format used worldwide for representing crystallographic information. Combining checkCIF with deposition into the CSD has huge benefits for the scientific community, by further streamlining the workflows for crystallographers, authors, referees and publishers.

Crystallographic data deposition is now even faster and easier as CIF syntax, cell and geometry details, space group symmetry, anisotropic displacement parameters and structure factors can be checked automatically during the CSD deposition process rather than in two separate steps. Depositors can be confident in the integrity of their data with immediate access to both the edited CIF file and the embedded validation report, and reviewers and publishers can read the checkCIF report alongside the deposited data to aid peer review of submitted papers.

Journals that publish small-molecule crystal structures require authors to submit their crystallographic data files to the IUCr's checkCIF system for validation, followed by deposition of the data with the CCDC prior to publication. Over 60,000 crystal structures are deposited annually into the CSD and collaborations with all of the key publishers ensure that structures are available for community access as soon as they are published. CheckCIF is used to make around 1.2 million data integrity checks per year and the resulting report is a mandatory requirement for publication in a number of journals.

Contact:

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PANalytical Award

MR. Matteo Bianchini, affiliated to three French research institutions, was elected as the winner of the 2014 PANalytical Award, which recognizes innovative X-ray analytical research by young scientists. His article about a potential new Li-ion system was listed by all 5 jury members as their number one. The jury was impressed by the comprehensive investigation which was carried out with a masterful understanding of crystallography. Mr. Bianchini is currently finalizing his PhD at the University of Amiens (France) and will use the prize money to support him while looking for new scientific challenges abroad.

The PANalytical Award is presented at the European Crystallographic Meeting (ECM), this year in Rovinj, Croatia on 26 August, and provides the opportunity to present the research to the professional community at this meeting. More details about the award-winning article and its author can be found on www.panalytical.com/award .

PANalytical, 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 2015 is now open for submissions. Applicants must publish a paper in print during the period 1 January 2014 until 1 December 2015 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 2015. Correspondence or questions about the award can be addressed to award@panalytical.com .

Matteo Bianchini, winner of the third PANalytical Award.

American Crystallographic Association Annual Meeting

Your editor up close and personal with the Liberty Bell.

AS usual, this year's meeting of the ACA offered a wealth of stimulating science. I can only give a précis of some talks that I attended and found particularly interesting. The topic chosen for this year's Transactions Symposium was a matter of importance beyond the confines of crystallography: "Crystallography and Sustainability". It included a major contribution by our own John Helliwell. A set of papers based on this Symposium should eventually appear at www.amercrystalassn.org .

A notable feature was the respect given to X-ray powder diffraction (XRPD), starting with a session on the first day. **Andrew Brunskill** described uses of XRPD in pharmaceutical development. Information from XRPD as simple as the unit cell volume helps with the design of solvates and cocrystals. The molecular volume of the active pharmaceutical ingredient (API) can be estimated by the Kempster-Lipson or the Hofmann method and referred to the unit cell contents. Excess cell volume is then attributable to solvent and/or coformer. Comparison of predicted and observed volumes for 100 crystalline anhydrates showed RMS error of 12 $Å^3$ per molecule. Once suitable analytical peaks for anhydrate and hydrate have been identified, XRPD is a useful analytical method in dynamic moisture sorption studies. For instance, a sample can be cycled between 60% relative humidity and desiccation conditions and its state can be monitored. **Simon Bates** took us through the development of a "gold standard" GMP (good manufacturing practice) analytical method based on XRPD. Ideally, the variance of the analytical signal should be due only to phase quantity. A plot of calibrated response *versus* quantity should have slope 1 and intercept 0. As a real-world example where other factors must be considered, mixtures of fructose and calcium carbonate were subjected to rational analysis step by step. Corrections took into account instrumental background, raw response normalised for sample mass, absorption via a miscible matrix model, diffuse background due to defects, thermal motion and Compton scattering. Pure fructose has severe preferred orientation; variance analysis separates components due to $CaCO_3$ and several orientations of fructose. Addressing one of the most challenging areas of data collection, **Julie Quinn** showed us that a synchrotron is not absolutely essential for pair distribution function (PDF) analysis. Useful for materials with limited structural coherence, total scattering is the sum of Bragg peaks and the diffuse scattering which is measurable at high 2θ. The procedure involves 4 steps: collecting data up to a high magnitude of the scattering factor $Q = 4\pi\sin\theta/\lambda$, data correction and normalisation making use of measurements on an empty capillary that are repeated with sample inside, Fourier transformation to a PDF, modelling the PDF. The X-rays must have high energy (typically Mo or Ag radiation) along with high intensity. This combination is achievable with a laboratory source equipped with a focusing mirror. Although the Q range is smaller for a laboratory source than a synchrotron, it is adequate for a variety of disordered crystalline materials such as silicon carbide, TiO_2 nanoparticles, C_{60} fullerenes at low temperature to stop random spinning, quartz at room temperature and high temperature. **Raj Suryanarayanan** returned our attention to pharmaceutical materials. Pharmaceutical properties are affected, often profoundly, by phase transformations such as amorphisation/crystallisation, solvation/desolvation and change between a salt and a cocrystal of acid and base. A requirement arises for analysis of intact dosage forms (usually tablets). An example is the analysis of tablets made by compressing amorphous indomethacin, which may crystallise leading to impaired bioavailability. By X-ray diffraction, tablets were mapped from edge to core to edge and top to core to bottom. After storage at 35°C for 24 hours crystalline indomethacin was detected near the edges, extending closer to the core if the tablets were made under higher pressure. Magnesium stearate, a common lubricant, can be added to the formulation or coated on the die wall. The latter technique reduced crystallisation. Finally in this session, **Jim Britten** demonstrated that single-crystal equipment can be made to provide useful analytical information about polycrystalline powders, solids and films. Phases of corundum and fibre texture of bone were revealed by 2-D XRD. Going to 3-D powder diffraction gives concentric shells which may reveal additional information about texture. Residual stress makes 2θ values change slightly with orientation. An area detector needs to have careful position calibration. The choice of wavelength is important: the bone sample initially acted as a beam stop until more penetrating radiation was used!

The next day, July 27, there ensued a session about publication – a topic of interest to every crystallographer. Under the title "Publication of 1000 Structures a Day"

Suzanna Ward gave a presentation that was both light-hearted and thought-provoking. Her most recent check revealed 787,912 structures in the Cambridge Structural Database (CSD), and the millionth structure is expected in late 2017. This rate of expansion is impressive, and yet there seem to be a lot of missing structures! Estimates based on annual use of CheckCIF and on the number and capability of diffractometers in the world suggest that there should be between 418,000 and 480,000 structures determined every year. If only these structures were all deposited, we would have a better basis for synthon design and crystal structure prediction. Recently the CCDC has done two important things to facilitate deposition of structures by private communication: each structure is given a DOI, which ensures that the author gets due credit; and the Community Deposit website facilitates the process. The ideal would be to incorporate deposition into laboratory workflow. Possible difficulties arising from a surge in depositions would be to increase the load on CCDC informatics (but plenty of capacity is available), to give (perhaps excessively) prolific hits from searches, and to sharpen data quality issues. **Ton Spek** carried on with "Proper Reporting and Archiving of Crystal Structure Data". His one-sentence summary was that all structures should be published with experimental data. He extended this statement by recommending deposition of unmerged reflection data. He warned that "unusual structural features" are likely to be "wrong structural features", and the whole edifice of atom types and coordinates is just the authors' interpretation. He illustrated these points with a recent structure published in a prestigious journal purporting to be a bicarbonate salt with a C-O bond distance of 1.563(6) Å and no hydrogen bond acceptor for the OH group. Reinterpreting this anion as acetate with CH_3 instead of OH brought it into line with expectations. An organometallic structure thought to contain Mn atoms with unusual tetrahedral coordination had residual density at the metal sites. Changing the metal to Zn (probably picked up from the reaction vessel) matched the observed density and the expected coordination. He concluded by stating emphatically that CheckCIF is intended to be helpful, not annoying. **Phillip Fanwick** looked at crystal structure determination from 3 sides: (1) chemists doing their own compounds, (2) service crystallographers and (3) reviewers. The chemists know their compounds better than anyone else, but there is a danger that they may have such strong preconceived ideas about the structure that they may twist the facts. The service crystallographers have an independent perspective, but they do not wish to upset the chemists. Phillip gave us a memorable quote from **John Huffman**, "Consider everything on the submission form as fiction". It is not cheating to use other methods, such as mass spectroscopy or NMR, to guide the crystallography. Finally, the referees have to identify incorrect structures while avoiding the temptation to correct them, making them "their" structures. Reinforcing Ton Spek's point, Phillip pointed out that Fourier transformation of the intensity data yields the electron density. Atoms are merely our interpretation. The use of atoms by SHELX is intuitively appealing and works well most of the time; but where there is diffuse density, one has to make do with partial atoms. Finally, **Sandy Blake** introduced the significant new developments in the IUCr journals. There are new covers, article designs and web pages. *IUCr Journal* has been successfully launched as the new flagship journal covering all aspects of crystallography and sciences that employ crystallography. Download statistics are available, a GUI leads to supporting information and there is a smooth 3D viewer. By adding crystal engineering and materials to structural science, *Acta Cryst. B* does what it did before, but hopefully better. New authors are being pulled in by special issues and the opportunity to write lead, feature and perspective articles. Moves to exploit graphical abstracts and use colour have been made to maximise impact, visibility and attractiveness. *Acta Cryst. C* is at the centre of chemical space. It publishes not only structures that are well done, but also poor structures that have sufficiently interesting consequences. The idea that there is a cut-off on R factor, above which structures will be refused, is completely mythical. *Acta Cryst. E* was re-launched in spring 2014 and will be re-evaluated for an impact factor this year. Articles can report a single structure or can encompass more than one structure and make side-by-side comparisons if appropriate. From 2016 Data Reports will be replaced by IUCr Data.

An important theme in these presentations was the validation of small molecule structures. Two contributions to the General Interest sessions dealt with validation of macromolecular structures. **Heping Zheng** introduced the CheckMyMetal server. The 98,333 structures in the PDB contain a variety of blobs, which could be water, a metal ion or other things. Generally, water or ammonia can be identified by examining the hydrogen bonding environment. Metal ions, however, can be alkali, alkaline earth or transition. The orientation of ligands, normally tetrahedral or octahedral, helps to narrow down the possibilities but is not conclusive. Furthermore, clusters can occur, as in proteins binding Fe-S. Bond distances further help with identification of the metal and, in suitable cases, the spin state: Fe(II)-N is about 2.2 Å if the iron is high spin, 2.0 Å if low spin. Even so, an anomalous signal is needed to identify a metal unambiguously. Unfortunately the quality of metal ion locations is not improving; the number of transition metal sites with problems has actually been increasing over time. CheckMyMetal evaluates a variety of factors starting with composition and valence and takes hints from the binding environment. **Bradley Hintze** told us about the latest enhancements to MolProbity, dealing in particular with the orientation of side chains in proteins. Conformations of side chains are described by a succession of torsion angles χ starting at the N atom. A quality filtered empirical distribution is derived from structures in the Protein Data Bank which satisfy the filters: resolution $\leq$ 2.0 Å, structure factors available, $\leq$ 5% of geometry outliers, along with additional filters for individual residues: no clashes, B-factors $\leq$ 40, atomic coordinates that match peaks in a $2F_o$-DF_c map. One still has no right to ask whether a particular observed conformation is definitely correct or incorrect, but one can ask if it matches the empirical distribution and seek an explanation if it does not.

As a small-molecule crystallographer I was interested in the session on "Important Science from Small Molecular Structures". **Brian Dolinar** presented a series of bimetallic

Poster session making waves, along with the carpet.

Modern architecture in historic Philadelphia.

paddlewheel compounds. Along with a description of the structures, Brian showed us that appropriate ligands could be designed by invoking the concept of hard and soft acids. **Carolyn Brock** reported her latest findings about crystal structures with high Z'. She searched the CSD for all structures with Z' > 4, excluding those with faults revealed by PLATON. She found that, although high Z' structures are very diverse, there are just a few relatively simple organising principles: (1) hydrogen bonding, (2) translational modulations (not necessarily along exes with small indices), (3) formation of layered structures, (4) layers often having higher symmetry than the overall structure, the stacking of layers breaking symmetry, (5) ordered faults and (6) self-inclusion compounds. The frequency of occurrence of space group $P2_1/c$, which is about 35% for the totality of structures, drops to about 10% for structures with Z' > 4. **Colin Groom** began with a statement by Rutherford quoted in a biography by Birks: "All science is either physics or stamp collecting." Colin effectively dispelled any prejudice that analysis of the CSD amounted to stamp collecting. He cited the simplistic view of solubility of drugs: the more lipophilic the molecule, the less its aqueous solubility. Quinoline structures in the CSD vividly disproved this idea. Comparison of the molecules with refcode RUDZAT and RUDYUM shows that the latter is more lipophilic and also more water-soluble. RUDZAT stacks well, while RUDYUM has a methyl group perturbing the stacks, creating voids and lowering the melting point. The less stable crystals have higher solubility. Plainly, comparison of crystal structures provides essential insight into the physics of solubility. **Amy Sarjeant** began by debunking two myths: over time R factors for crystal structures have been getting better and better, and the more prestigious the journal, the worse the average R factor. Her analysis of the CSD showed that, presumably due to improvements in both instrumentation and instruction, average R factors decreased to around 5% by 1997; but they have remained around this value ever since. There used to be a positive correlation between impact factor and R factor, but any correlation has become insignificant in the last decade. Amy went on to investigate the "fried calamari effect." This was the subject of a famous study of recipes and restaurant reviews in the *New York Times*. A graph plotting the number of appearances annually of this delicacy following its first mention showed a steady increase to peak popularity, followed by a decline. Amy carried out CSD searches for boranes, metallocenes, porphyrins, fullerenes and MOFs appearing annually. Expressed as numbers of structures, no drop-off was observed in any of the categories. Re-expressed as percentages of the database, the statistics do show a peak followed by a decline for several of the categories, although MOFs have not yet reached a peak after 15 years (almost 1 Standard Calamari Unit) and fullerenes are also still increasing. Incidentally, the Fried Calamari Index is described at **http://www.nytimes.com/2014/08/12/upshot/special-sauce-for-measuring-food-trends-the-fried-calamari-index.html?_r=0&abt=0002&abg=1** .

In the final General Interest session **Timothy Ramadhar** kept a sizeable audience in their chairs by describing improvements and giving us practical guidelines on the Crystalline Sponge Method, which caused great excitement when published in *Nature* in 2013 by Fujita's research group in Tokyo. As described in an article in *Chemistry World* recently, **http://www.rsc.org/chemistryworld/2015/05/crystal-free-x-ray-crystallography-axial-planar-chirality** , some small molecules that resist all attempts at crystallisation can be taken up as ordered guests in a special MOF and subjected to X-ray diffraction. Fujita and coworkers had characterised chiral molecules by this technique. However, widespread application by other researchers has been hindered by the difficulty of synthesis and the poor quality of data obtained (both resolution and R factor). Timothy and colleagues in the Clardy research group at Harvard have devised an easier synthesis using chloroform as solvent and taking only a few days without heat. A complex is made by soaking in neat guest. With the use of synchrotron radiation reasonable R factors are obtained. Varying the terminal ligand in the zinc-based MOF from the iodide used previously to bromide or chloride has produced more tractable crystals with menthyl acetate as guest. Results have recently been reported in *Chemical Communications* 2015, **51**, 11252-11255. The ensuing discussion elicited answers that 6 or 7 guests have been studied, their maximum allowable size corresponds to a molar mass of about 500, but shape matters, too.

Carl Schwalbe

XXIV Congress and General Assembly of the International Union of Crystallography

Dear colleague,

I would like to inform all crystallographers in the UK that the XXIV Congress and General Assembly of the International Union of Crystallography will be held in Hyderabad, India between 21 and 28 August, 2017. I would like to invite you to attend and participate in this meeting. I would also like to obtain your suggestions as to how to secure the maximum participation of UK crystallographers and structural scientists in the congress.

The program will be fixed next March and will cover all areas of crystallography.

We are making every effort to have a nice conference package for students and scientists which will include registration (including lunch) and accommodation in 3- and 4-star hotels on sharing basis or individual occupancy. This would come at a rate that is definitely affordable by students and faculty. Details will be known next year. It is also certain that the exhibition area, the poster area and the lunch area will be in the same large hall in the convention centre. It is also quite possible that we will introduce electronic posters in this IUCr congress.

Please be aware that there is a non-stop air connection between London Heathrow and Hyderabad (9.5 hours).

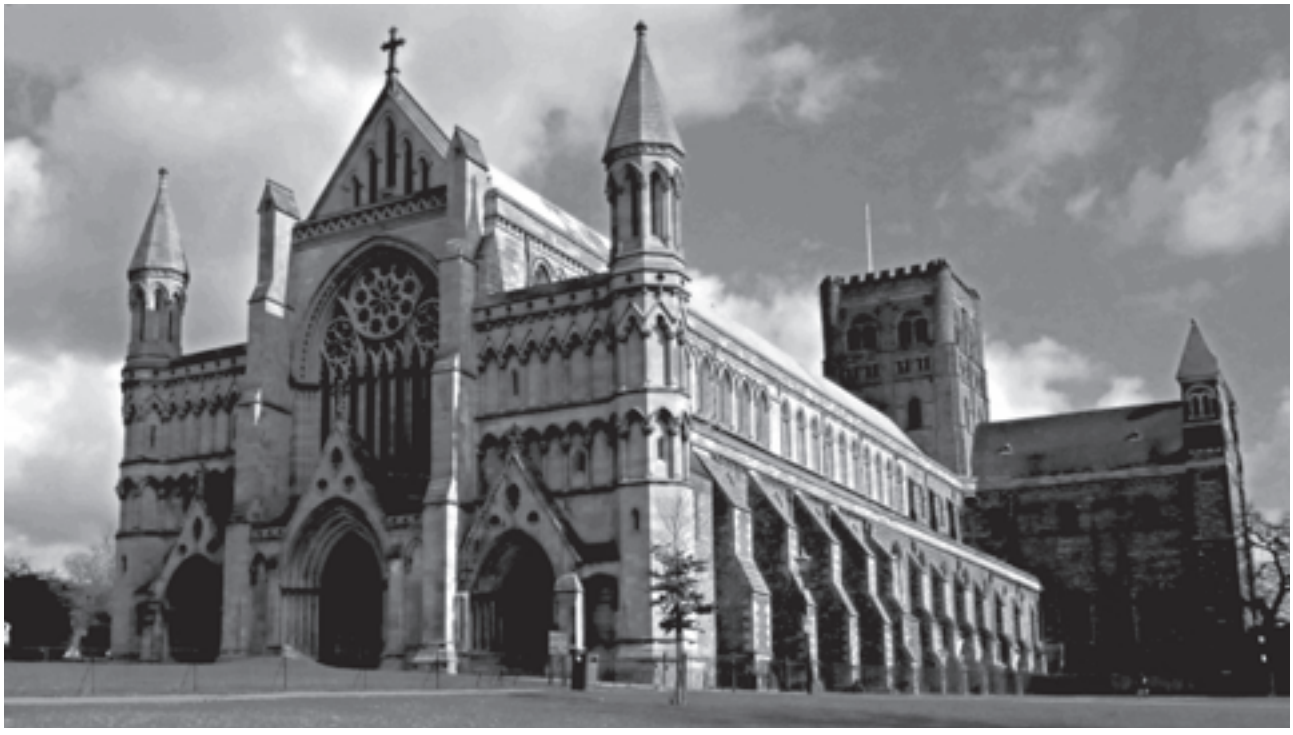
Preliminary information is given in our web page at www.iucr2017.org

You may find this picture to be of interest. This is a site that is around 30 miles from the congress centre in a small place called Medak.

http://tourmet.com/wp-content/uploads/2014/03/medak-church.png

I hope to see you in Hyderabad in 2017!

With best wishes,
G. R. Desiraju



http://ecm30.ecanews.org

ECM-30 will be a four-day vibrant and intensive scientific meeting held between **August 28 and September 1, 2016 in Basel**, **Switzerland** and will provide many learning opportunities in every current aspect of crystallography.

In addition, there will be a Young Crystallographers meeting, workshops and user meetings, lunch meetings, and a social program, which will allow scientists from all over Europe and the world to meet, connect and exchange. Besides the satellite meetings, a visit to the free electron laser SwissFEL is planned.

Basel is a welcoming, active and enterprising city of open minded citizens who excel in business as well as in the arts. The famous Basel mathematicians Bernoulli and Euler are of course known to many of you. In addition to the architecturally interesting campuses of some leading pharmaceutical and chemical enterprises, world-renowned museums, like the Beyeler, the Vitra Design or the Tinguely museum with its modern architecture, are ready to welcome you.

The conference is located close to the Basel exhibition area, in the triangle between Switzerland, France and Germany. Within a 30 minute ride on public transportation, more than 1000 hotel rooms are available in Basel, St. Louis (France) or Weil am Rhein (Germany). It is well connected to Europe by car, by plane (Basel-Mulhouse-Freiburg Euroairport hosts many low cost carriers) and has frequent train connections to Germany, France, Italy and Austria.

We look forward to welcoming you to Basel in 2016!

Katharina M. Fromm
University of Fribourg

Jürg Schefer
Paul Scherrer Institute

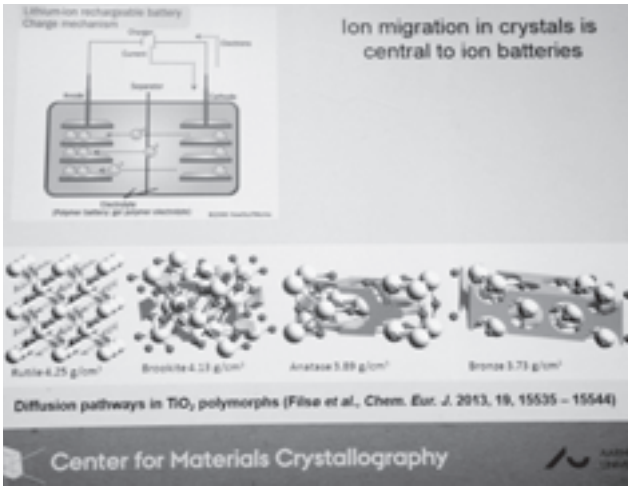
German Crystallographic Society Annual Meeting

THE Deutsche Gesellschaft für Kristallographie held its annual meeting in Göttingen from 16-19 March. Since I had been a postdoctoral fellow there 40-some years ago, I was eager to go back. My first surprise was to find that my old institute, the Max Planck Institute for Experimental Medicine, which had dominated the landscape in relatively lonely splendour, was now almost completely surrounded by student residences. My second surprise came when I scrutinised the programme book, compared it with the BCA's counterpart and found big differences. Four entire microsymposia were devoted to the crystallography of materials, showing the high standing this topic has in Germany. On the other hand, there was no session covering crystal engineering or Cambridge Structural Database analysis. Two microsymposia were entitled "Inorganic Structural Chemistry", but there was no corresponding session on "Organic Structural Chemistry". I must hasten to add that organic structural chemistry *was* given sophisticated treatment in some charge density studies and some structure determinations at high pressure and/or high temperature. The official language of the meeting was English, which helps to explain why speakers from Germany give such lucid talks in English at international meetings.

The venue was the Geoscience Centre of the University of Göttingen. The commercial exhibition was held in a large central area, where crystallographic conference posters were also on display next to large slabs of rock and posters about prehistoric life. A "rock garden" outside featured more slabs of rock with some faces polished to show crystals that sparkled in the warm sunshine that we were enjoying.

Bo Iversen from Aarhus University in Denmark gave the first plenary lecture, simply entitled "Materials Crystallography". Its technological relevance showed why the organisers placed this lecture first and recruited an eminent scientist from outside Germany to give it. Ion migration in crystals is of central importance to ion batteries. Since smaller crystals imply a shorter diffusion path, the obvious extension is to nanocrystals. Nanocrystals of a metal salt can be made in supercritical water, which acts as a nonpolar solvent! A micro fuel cell with a nanocrystalline catalyst on a carbon support can power a hearing aid almost indefinitely. As a material for anodes, $Li_4Ti_5O_{12}$ has many desirable properties, but it is prone to defects. Synthesis by use of the solid-state reaction between TiO_2 in the anatase form and Li_2CO_3 is liable to create impurities by forming Li_2TiO_3 and changing anatase to rutile. Analysis of the product by X-ray powder diffraction showed that too low a temperature (400-650°C) facilitates formation of Li_2TiO_3, while too high a temperature (above 800°C) favours rutile. The second part of the lecture covered charge density studies and probed accuracy as well as presenting results. Comparing thermal parameters for a structure determined with neutrons and X-rays is instructive because wrong U values affect the description of core as well as valence electrons. The suitability factor is related to the ratio of valence to core electrons. Thus a high atomic number implies an unsuitable atom.

The annual meeting commences with a message of welcome



Slide from the talk by Bo Ivarsen presenting crystallographic information relevant to the operation of batteries

The first microsymposium (General Interest) began with a talk by **Claudia Wandke** on invariom based point charges. Invariums featured prominently in this meeting, which is no surprise since much of the formalism has been developed by **Birger Dittrich** and colleagues in Göttingen. Invariums are aspherical atomic scattering factors, available in a database, that enable refinement of more accurate and precise geometries than are obtainable with conventional atomic scattering factors. Readers who wish to learn more about invariums can download the open-access lead article in *Acta Crystallographica*, Section B, at http://journals.iucr.org/b/issues/2013/02/00/issconts.html . Claudia showed that invariums also provide a quick way to calculate molecular electrostatic potential (ESP), given a set of atomic coordinates. She compared these ESP values with ESP's from DFT calculations for 18 angiogenesis inhibitors and also with the results of a charge density refinement on the protein kinase inhibitor sunitinib malate, finding a satisfactory match.

From a point of view based on theory and on data mining **Detlef Hofmann** considered the extension of empirical force fields to extreme conditions. Using (stepwise) linearised

effective potentials he ranked structures from the Cambridge Structural Database by free energy, thereby providing an order of stability for polymorphs. Another method involved the derivation of parameters, particularly for H and D atoms, by recursive fitting. The effective potential of D…N interaction was found to be lowered and shifted to shorter distances, compared to H…D .

Continuing the theme of deuteration, **Anna Kupka** presented cases where deuterium disturbs the molecular arrangement in the solid state. Compared with H_2O, D_2O has a melting point that is 3.82 K higher and a boiling point 1.44 K higher. The maximum density of D_2O occurs no less than 7.14 K higher, with the consequence that D_2O ice sinks! D_2O has stronger self-association, leading to solvation dynamics 25% slower. The zero point energy of D_2O is lower, with a concomitant effect on hydrogen bond distances (the Ubbelohde effect). In some cases deuteration has drastic effects on crystal structure. $CF_3COOH•4H_2O$ is ionic with H but molecular with D. Pyridine forms crystals in space group $Pna2_1$ and Z' = 4, but with d_5-pyridine the space group changes to $P2_12_12_1$ with Z' = 1, a phenomenon known as isotopic polymorphism.

Ultrafast pump-probe studies of a photo-induced electron transfer process were presented by **Sreevida Veedu**. *N,N*-dimethyl-4-pyren-1-ylaniline provides a simple model photosystem which can be pumped with an optical laser and probed with polychromatic synchrotron radiation by the Laue technique. A 62° twist was found between pyrene and aniline rings in the ground state, but this increased to 72° in the excited state.

To any user of crystallographic software, the name Göttingen carries an association with the SHELX suite of programs. **George Sheldrick** gave the first presentation in the microsymposium on "Computational & Theoretical Crystallography". He described how, in SHELXD, the real space part of the dual phase cycle imposes a strong atomicity constraint on phases, which are then optimised in reciprocal space. With typical modesty he concluded that, by chance, this method is good at locating heavy atoms in macromolecules. He pointed out that at low resolution the better phase estimates from MAD rather than SAD can make a decisive difference. SHELXD is highly parallel and scales up well: it is 29 times faster on a 32-CPU machine compared to a single CPU.

Another distinguished non-German speaker presented the next plenary lecture. After setting out the equations for SIR/MIR and SAD/MAD **Wayne Hendrickson** displayed graphs showing trends in the use of methods for macromolecular structure determination over time. As techniques have advanced in recent years, the application of anomalous dispersion has increased while isomorphous replacement has declined. As expected, the increasing number of known structures has facilitated an increase in the use of molecular replacement. Wayne's talk was illustrated with many beautiful structures, including some determined from X-ray free-electron laser (XFEL) data. He stated that if 100 µm single crystals are available, better results are still obtainable on a synchrotron.

The first microsymposium on "Inorganic Structural Chemistry" included some conceptually interesting results and some software that may be generally useful. **Alexander Pöthig** illustrated the idea of hemilability with some results on Ir(I) complexes with *N,N'*-bispyridyl-imidazolylidene (NCN) exhibiting both monodentate and bidentate coordination modes. Hemilabile coordination of attached donor ligands should be a helpful feature in the design of molecular catalysts. **Daniela Schmidmair** presented a new ambient pressure polymorph of $K_2Ca_3Si_3O_{10}$, which appears to be the first example of a structure containing both isolated SiO_4 tetrahedra and Si_4O_{12} rings. The tetrahedra have almost uniform Si-O distances, while the rings are made from four tetrahedra with two longer and two shorter Si-O bonds. **Daniel Kratzert** began by telling us what we already knew: SHELXL is remarkably effective at treating almost every possible kind of disorder, but setting up the appropriate sequences of commands can require a lot of effort. Since around 23% of the entries in the Cambridge Structural Database have disorder, their refinement represents a serious amount of work. Daniel presented a new program called DSR, which transfers a molecular fragment from a database of such fragments to the desired position in the unit cell and generates the appropriate restraints. It can be downloaded from **https://www.xs3.uni-freiburg.de/research/dsr** . Also presenting advances in software, **Holger Ott** described the new APEX3 system. Stages in the structure determination process are dealt with by using plugins. For instance, the Scale plugin comes with GUI support for TWINABS.

The plenary lecture by **Alessia Bacchia**, entitled "Trapping liquid drugs into crystals", addressed the objective of embedding liquid or volatile materials into crystals so as to increase their stability, improve delivery and/or establish new intellectual property. As examples she selected four liquids: the anaesthetic propofol, m.p. 18°C, nicotine, m.p. -79°C, and two compounds added to food at low concentration, eucalyptol, m.p. 1.5°C, and carvacrol, m.p. 1°C. These liquids were taken up in MOFs or incorporated into cocrystals. MOF cavities can be tuned to match the size of the drug. The MOF is formed with solvent in its cavities. While the solvent can be driven off by heating to ≈100°C, this degrades crystallinity. A better method is to remove the solvent with an excess of a more weakly held solvent which can subsequently be displaced by the guest. A MOF containing Cu can reduce the concentration of a standard nicotine solution by two orders of magnitude, the nicotine coordinating Cu. Cocrystals held together by halogen bonds and by hydrogen bonds were described. Examples included propofol with pyridine derivatives, eucalyptol with orcinol and propofol with 4,4'-bipyridine.

An interesting microsymposium had the title "Computational and theoretical crystallography: diffraction versus wave function". **Regine Herbst-Irmer**, a renowned expert on twin refinement, talked about charge density studies, specifically improvements in data processing and refinement. Data quality must be as high as possible. It benefits from high multiplicity of measured data but suffers if weak data are included. Small-molecule crystallographers can benefit from insights obtained by the macromolecular community about when to cut. The 'paired refinement method' aids the decision about rejecting outliers. Refinement of resolution-dependent scale factors improved the residual density. **Birger Dittrich** intrigued us with the title "EXAFS in 3 dimensions". Diffraction data collected at the SLS synchrotron near the Kα absorption edge on single crystals of a zirconium complex showed electron-density rearrangements concomitant with ionisation of Zr. In addition, for refinement of certain complexes of Ni, Cu and Zn with ligands having opposite σ and π donor/acceptor properties, the independent-atom model gave the best R factor with scattering factors from the adjacent atom in the Periodic Table, while aspherical scattering factors gave the lowest R factor with the correct

Poster session enlivened by the rock slabs and drawings of underwater scenes in the Geoscience Centre

choice of element. **Simon Grabowsky** reminded us that the independent-atom model with spherical scattering factors cannot account for bonding density. The use of multipoles, as in the Hanson-Coppens formalism, remedies this defect. An alternative way to achieve the same end is with X-ray wavefunction refinement (XWR). This method has two steps: (1) Hirshfeld atom refinement, and (2) constrained wavefunction fitting. The resulting X-H bond lengths and displacement parameters agree well with neutron data. **Jens Luebben** pointed out that although the Hirshfeld rigid-bond test is important for structure validation, it can give false positives and false negatives. False negatives occur mainly with terminal atoms in linear bonding environments, or rings in planar bonding environments. The RIGU restraint in SHELXL enforces that relative motion of two bonded atoms is perpendicular to the bond vector. Testing how well it is obeyed works as an enhanced Hirshfeld test. **Swastik Mondal** presented an electron density study of boron carbide at 100K. This chemically inert, high-melting and very hard material with a formula of $B_{12+x}C_{3-x}$ fulfills demanding applications such as bulletproof vests. Synchrotron data and a multipole model have yielded details of electron density. **Christian Hübschle** discussed anharmonic thermal motion in glutathione using the Maximum Entropy Method. Refinement against accurate data measured at 100K revealed electron density not described by the model. Extending the model with anharmonic ADPs for carbonyl oxygen atoms gave a better fit but led to a probability density function with unphysical negative regions. A more successful alternative used the dynamic electron density of the Invariom model with harmonic ADPs as prior density for Maximum-Entropy-Method (MEM) calculations with the program BayMEM

The Conference Dinner was held in the agreeable surroundings of the "Bullerjahn" restaurant in the basement of the city hall. Such a Ratskeller would typically serve excellent food and drink to city councillors, university professors and other high-status individuals. We enjoyed a buffet dinner which enabled us to sample a variety of German dishes. It was announced that with 427 participants the meeting was a great success; and we were invited to attend the next meeting, which will take place in Stuttgart from 14-17 March 2016.

Carl Schwalbe

Next ACA Meeting

HOWDY, pardner, the American Crystallographic Association will be returning to the Wild West next year. So giddy up to Denver, Colorado, between July 22 and July 26. This is made easier by the existence of flights from the UK to Denver International Airport. Please note that the start and end of the meeting have advanced by one day, compared to those in recent years. The Program Chairs are Amy Sarjeant from the CCDC in America and Eddie Snell from the Hauptman Woodward Medical Research Institute. I'm certain that these two will put together a highly interesting set of lectures. Keep checking www.amercrystalassn.org for details as they emerge.

Denver is nicknamed the Mile High City because the elevation at its reference point is exactly 5280 feet above sea level. That elevation means that, although summer days can be hot, the nights get pleasantly cool: in July the average high and low are 31.1°C and 13.3°C. Don't forget the suncream if you mean to enjoy your lunch *al fresco!* Denver is located right where the Front Range of the Rocky Mountains rises abruptly from the Great Plains. Spectacular sights are located within an easy excursion from Denver. Rocky Mountain National Park is 69 miles northwest of Denver. On the way is the hiker- and cyclist-friendly city of Boulder, home of the University of Colorado and the National Center for Atmospheric Research. A similar distance to the south is Colorado Springs, where the breath-taking rock spires rising out of parkland in the Garden of the Gods inspire some breath-taking rock climbing; there also are enjoyable hikes and interesting nature trails for the more earth-bound among us.

Book Review

More and Different: Notes from a Thoughtful Curmudgeon

by Philip W Anderson

Singapore, World Scientific Publishing, 2011, ix + 412 pp, ISBN 978-981-4350-13-6.

Scope: large collection of book reviews and articles with some biographies. Level: most for general reader but parts need physics background.

AS his Preface concedes, Anderson knows that publishers don't expect review collections to sell. Reviews may be too dated for useful recommendation or criticism of a new book (biographies here of Crick, Feynman and Gell-Mann are from the 1990s, and 1980 for Landau) but, as Anderson rightly claims, his reviews usually contain some original thoughts. This assembly of over 60 essays is divided into ten groups, which range from Personal and Historical, via Science Politics (mainly Star Wars), to Futurology ('a mug's game') and Complexity Physics; each is usually preceded by a page of introduction. The title arises from Anderson's slogan *More is Different* in a 1972 *Science* article; this opposed the deterministic Laplace approach with a view that simple laws and mechanisms yield new consequences when applied to large assemblages. Broken symmetry, the concept that simplicity of laws is not manifest in their consequences, is a continuing philosophical theme, with a tribute to Nambu Sensei. The final section, headed Popularization Attempts, including Pauling's Resonating Valence Bond Theory and the scope of theoretical condensed matter physics, supports Anderson's admission, despite his wide scientific interests, about limited ability for explanations to a lay public. He writes that, although he had envisaged devoting more time to writing in later years, physics proved too strong.

Philip Anderson (born 1923) was brought up in an academic family in Urbana before taking a wartime degree aged 19 at Harvard. His time in the US Navy as a Chief Specialist (X) at the Office of Naval Research ended after World War II and was followed by a PhD with Van Vleck in the early NMR days. Having married in 1948, he nearly took an academic post in Washington State, but, with no offers from GE or Brookhaven, was glad to join Bell Technical Laboratories (BTL) in 1949 on ferroelectricity under Shockley ('brilliant but arrogant and overconfident'); he stayed for 35 years. The Nobel prize for physics, on the quantum theory of condensed matter, came in 1977. There was a valuable spell 1953-4 with Ryogo Kubo in Tokyo and a visiting chair until 1975 followed 1961-2 at the Cavendish; in formal retirement, research continued at Princeton.

Early historical sections of the book include lengthy articles based on chapters of an unfinished 1960s history of superconductivity but also embrace 20th century physics. Naturally, the people and culture of BTL figure prominently. Anderson uses initials without immediate explanation; I don't think BCS is anywhere explained as the 1957 *Phys Rev* paper of the quietly brilliant Bardeen, the inspired dilettante Cooper and the affluent self-critical Schrieffer (who later suffered a tragic decline). Despite the justified reputation for Nobel prizes (electron diffraction, Johnson noise, etc) from speculative research, Anderson contends that pre-war Bell required the research of such first-rate scientists as Townes and Shockley to be associated with company activities, ie communication systems. During the war, Jim Fisk's group under Shockley developed the British invention of the magnetron microwave generator and Si crystal detector underlying the Allies' superiority in radar. Only in the 1950s did BTL management style relax to become less hierarchical and paternalistic. Physical electronics broadened to include ferroelectricity, while a theorists' subdepartment was set up in 1955. Over the next 30 years came the transistor, maser, laser, LED, fibre optics, MRI, the Josephson effect, etc, although the company rarely exploited them.

After the wartime triumph of physics, Anderson regrets that Big Science was dominant in the proliferation of national laboratories until the end of the Cold War and the decline of the Strategic Defense Initiative (SDI). His case against SDI is that a defensive system costs 10 times as much as an offensive one. As BTL declined and Small Science vastly expanded in the 1980s, he bemoans the decline in quality, excessive specialization, and emphasis on grants and papers from the 1990s. A1985 lecture argued that condensed matter physics was transforming the technology of everyday life while in another article reproduced from 2000 he notes that the theorist must be creative and exercise taste and judgement. For the 21st century, an essay predicts a shift from the reductionist study of detail to the emerging field (1995) of understanding of complexity, the overall title of the penultimate batch of papers. Also envisaged are the merging of physics, technology and biology/medicine and the wider employment of physics-trained people as in econophysics. A 1995 review is included of *Frontiers of Complexity* (Ballantine, 1995) by Peter Coveney and Roger Highfield. There are several references to the Santa Fe Institute founded in the 1980s by some extremely eminent scientists to respond to the observation that most scientific revolutions are outside or between established disciplines.

More and Different has no illustrations but art work by the author's daughter Susan Anderson introduces each chapter. A good contents list, albeit with some enigmatic titles, is no excuse for the lack of an index; more contemporary comment and greater clarity of contribution dates would have been welcome. For the physicist interested in recent scientific history, almost every article has some appeal, whether portraits of Nobel prizewinners by one who knew them or Anderson's reflections (written in the 1970s) on different species of futurologists. More typically, a reader may be interested in one or two of the sections, such as the people involved in the generation of superconductivity theories (Frohlich's contribution to the earlier theory is acknowledged), views on the philosophy of science (labeled Tactics and Strategy), reductionism and complexity, or even the Star Wars debates. Curmudgeon or not, Anderson's Notes are well worth reading, but not at one sitting.

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Obituaries

Passing of Norman A Curry (1929-2015) and Dr Dennis S Beard (1922-2015)

TWO physicists who have made different but notable contributions to British crystallography have died recently: NA Curry (NAC), one of the neutron diffraction (ND) pioneers, and DS Beard (DSB), for his Weissenberg instrument and production of apparatus for schools' electron-physics experiments.

NAC was born in Rotherham in 1929 but soon moved to Stocksbridge, near Sheffield, and went to Penistone Grammar School. After graduating in physics from Balliol in 1950, he became first a National Service assistant at the new and secret AERE, sited on the old Harwell RAF airfield (from which gliders were towed on D-day). Initially in Metallurgy, NAC transferred to Solid State Physics. As mentioned in the notes on GE Bacon, father of neutron diffraction (ND) in Europe (*Crystallography News*, 118, p27, Sept 2011), Curry and Bacon were first to use ND to study hydrogen-bonding in organic molecules (alpha-resorcinol and benzene). [NAC and I attended Bacon's 80th birthday gathering at Abingdon.] Very large crystals were needed for data collection with the manual diffractometers at the heavy-water-moderated DIDO and earlier reactors. Curry regretted that, although there were Bacon and Pease papers, there was not one by the trio Bacon, Curry and Pease!

In 1956, NAC married physicist Margaret Curry, working on fast reactors at AERE. I invited NAC to talk at Bradford (then Institute of Technology) in 1961. Through Bacon (before he left for Sheffield University) I followed JB Speakman as vacation consultant and from the 1960s spent many attachments, each of a week or two, at AERE, with NAC, slowly collecting neutron data; the process was so slow that 3-week family summer attachments were appropriate. After a gap of several months, NAC and I could immediately go into a quiet scientific discussion as though the next day. Our last paper was in *Zeitschrift für Kristallographie* 181, 205-214, 1987 on extinction corrections from reactors of increasing flux: BEPO, PLUTO and DIDO with the Badger-Dyer and Hilger-Ferranti diffractometers. In 1966, NAC left AERE to become a programmer at EEC, Leicester, before moving to the School of Computing Science at Leicester Polytechnic, later De Montfort University.

The Currys were staunch (though different) Methodists (NAC was a Local Preacher while at AERE) and NAC was longtime main organist at the Christchurch, Leicester, until 2010. Encouragement of the musical and conscientious pastoral traditions has found a ready response in successive family generations, through daughter Frances and son Andrew. Norman died in a Methodist Care Home on 26 Feb 2015, aged just 86, within three weeks of the death there of his wife, Margaret Curry.

DSB was born on 6 August, 1922, at Clapham, London. Following wartime graduation in Physics, 1940-42, from ICL, he was sent first to Hard Metal Tools at Coventry, developing spectrographic analysis of tungsten carbide for armour-piercing tank shells. X-radiography of warship hulls for the Naval Constructors' Department at Bath was next in a series of diverse skilled occupations which seemed to direct him towards his later enthusiasm for devising portable apparatus for demonstrating X-ray diffraction and other electron-physics effects in schools and colleges. From spectrographic analysis of precious metals at Sheffield Smelting Co and more ship X-radiography for the Admiralty at Bath, DSB was awarded an ICI fellowship in Cox's Chemistry Department at Leeds, 1947-1951. Here, he worked on several devices (including the cold room) for crystal structure analysis and the development of the Leeds Weissenberg goniometer (including an integration device), used into the 1970s, described in *Crystallography News* 123, p20-21, Dec 2012 and 124, 13, Mar 2013. His 1955 PhD was actually in Chemistry. After spells at NRDC (precursor of British Technology Group), 1951-1954, farming, and teaching at Norwich Tech, DSB joined Griffin and George (under Nobel prizewinner AJP Martin as Director), becoming Technical Director in1961, devising schools' apparatus, then became Technical Director of Teltron, 1964-74, developing tubes for electron diffraction and atomic physics for schools, culminating in the Tel-X-ometer. Thereafter, under Ideas for Education (initially in collaboration with Eagle Scientific[Nottingham]), DSB ran a small independent outfit in Northern Ireland, manufacturing mobile apparatus for schools to demonstrate X-ray diffraction, electron physics, cloud chambers, etc, until shortly before his death, aged 92.

Dennis Beard had been a hefty and talented Rugby Union enthusiast, having played for Headingley, Sheffield and Bath. His activities were restricted in recent years, made more companionable with his late wife Mary, and greatly helped by their daughter Anne Marie; he died in Kesh, Northern Ireland, on 10 Jan 2015, aged 92.

Derry W. Jones

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.

5-8 September 2015
ESCG. European School on Crystal Growth, Bologna, Italy.
http://escg2015.eccg5.eu/

6-10 September 2015
European Conference on Molecular Magnetism (ECMM2015), Zaragoza, Spain.
http://ecmm2015.unizar.es/

6-18 September 2015
14th Oxford School on Neutron Scattering, Oxford.
www.oxfordneutronschool.org/

7-9 September 2015
Design and Engineering of Neutron Instruments, Budapest, Hungary.
www.bnc.hu/denim2015/

7-10 September 2015
VI International Conference of Synchrotron Radiation in Polymer Science, Madrid, Spain.
http://srps6.com/

8-10 September 2015
Physical Aspects of Polymer Science, Manchester.
http://paps15.iopconfs.org

8-11 September 2015
3rd International GISAS Conference, Nice, France.
http://gisas2015.univ-lemans.fr/fr/index.html

9-11 September 2015
8th European Conference on Mineralogy and Spectroscopy, Rome, Italy.
http://www.ecms2015.eu/

9-11 September 2015
Fifth European Conference on Crystal Growth, Bologna, Italy.
http://www.eccg5.eu/

12-16 September 2016
4th International Soft Matter Conference.
http://www.eccg5.eu/

13-17 September 2015
35th Symposium on Dynamical Properties of Solids, Munich, Germany.
https://webapps.frm2.tum.de/indico/conferenceDisplay.py?confId=18

13-18 September 2015
SAS2015. 16th International conference on Small-Angle Scattering, Berlin, Germany.
www.helmholtz-berlin.de/events/sas/

14-16 September 2015
FMC2015. Frontiers in Medicinal Chemistry 2015, Antwerp, Belgium.
www.ldorganisation.com/v2/produits.php?langue=english&cle_menus=1238915914&cle_data=1360153416

14-16 September 2015
Materials Science and Engineering. 4th International Conference and Exhibition, Orlando, FL, USA.
http://materialsscience.conferenceseries.com/

14-18 September 2015
23rd International Congress on X-ray Optics and Microanalysis (ICXOM23), BNL, Upton, NY, USA.
www.bnl.gov/icxom23/

14-18 September 2015
Neutrons and Synchrotron Radiation for Magnetism. Hercules Specialized Course HSC18, Grenoble, France.
http://www.esrf.fr/events/conferences/HSC/HSC18

14-18 September 2015
PULSE summer school, Porquerolles, France.
http://pulse-school.sciencesconf.org

14-18 September 2015
XLIV Congress of the Italian Crystallographic Association, Università del Piemonte Orientale, Vercelli, Italy.
http://www.cristallografia.org/congresso2015

14-25 September 2015
13th School on Synchrotron Radiation, Grado,Italy.
www.synchrotron-radiation.it

15-18 September 2015
2015 E-MRS Fall Conference & Exhibit, Warsaw, Poland.
www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=13&Itemid=1651

16-19 September 2015
XIIIth International Symposium on Biomineralization, Granada, Spain.
http://granada-en.congresoseci.com/biominXIII

16-23 September 2015
5th International Conference Nanomaterials: Applications & Properties, Lviv, Ukraine.
http://nap.sumdu.edu.ua

20-24 September 2015
XXIII Conference on Applied Crystallography, Krynica Górska, Poland.
www.cac.us.edu.pl/

21-24 September 2015
Size-Strain VII. Diffraction Analysis of the Microstructure of Materials, Oxford.
http://www.size-strain2015.org/

21-25 September 2015
Application of Neutrons and Synchrotron Radiation in Engineering Materials Science, Hamburg, Germany.
http://www.hzg.de/matrac

24-25 September 2015
PDBe Workshop for Programmers, Hinxton near Cambridge.

28-30 September 2015
Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.
www.icdd.com/education/rietveld-workshop.htm

28-30 September 2015
4th International Workshop on Neutron Delivery Systems, ILL, Grenoble, France.
www.ill.eu/nds2015

28 September – 2 October 2015
ICESS-15. International Conference on Electron Spectroscopy and Structure, Stony Brook, NY, USA.
www.stonybrook.edu/commcms/icess/index.html

28 September – 3 October 2015
International Rietveld School, Sofia, Bulgaria.
www.bgcryst.com/RS2015/

1-2 October 2015
Basic & Advanced Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.
www.icdd.com/education/rietveld-workshop.htm

5-6 October 2015
Neutron Imaging and Tomography: New Applications and Developments, Evian les Bains, France.
www.sfn.asso.fr/jdn/site-jdn-23/

6-8 October 2015
Powder Diffraction of Organic Compounds, Frankfurt/Main, Germany.
http://web.uni-frankfurt.de/fb14/Anorg_Chem/AK_Schmidt/chemkrist2015/ws_ck/ChemKrist2015_Flyer_English.pdf

12-16 October 2015
Structural Bioinformatics. An EMBL-EBI Course. Hinxton near Cambridge.
http://www.ebi.ac.uk/training/course/structural-bioinformatics

12-16 October 2015
8th International Conference on Electromagnetic Processing of Materials, Cannes, France.
http://epm2015.sciencesconf.org/

19-20 October 2015
BCA Physical Crystallography Group Autumn Meeting, Cosener's House, Abingdon.

19-23 October 2015
Maud School on Combined Analysis, Trento, Italy.
http://maud.radiographema.com/

21 October 2015
International Workshop on Liquid-Liquid Interfaces, Grenoble, France.
www.ill.eu/liq2015

26-28 October 2015
International Conference on Protein Engineering, Chicago, IL, USA.
http://protein-engineering.conferenceseries.com/

2-6 November 2015
3rd Euro-Mediterranean Conference on Materials and Renewable Energy, Marrakech, Morocco.
http://www3.emcmre.com/

9-13 November 2015
Fifth Annual Niels Bohr International Academy Workshop on ESS Science: Condensed Matter Theory and Advanced Software, Copenhagen, Denmark.
https://indico.nbi.ku.dk/conferenceDisplay.py?ovw=True&confId=815

12 November 2015
BCA Industrial Group Autumn Meeting, AstraZeneca, Macclesfield.

17-19 November 2015
In Situ Serial Crystallography Workshop, Villigen, Switzerland.
http://indico.psi.ch/conferenceDisplay.py?ovw=True&confId=3677

18 November 2015
BCA Chemical Crystallography Group Autumn Meeting, Glasgow.

29 November – 4 December 2015
Materials Research Society 2015 Fall Meeting, Boston, MA, USA.
www.mrs.org/fall2015/

5-8 December 2015
AsCA2015. The 13th Conference of the Asian Crystallographic Association, Science City, Kolkata, India.
http://www.asca2015.org/

6-10 December 2015
4th Nano Today Conference (Nano Today 2015), Dubai, United Arab Emirates.
www.nanotoday-conference.com/

14 December 2015
NMR Crystallography, Institute of Physics, London.
www.iop.org/activity/groups/subject/brsg

16 December 2015
BCA Biological Structures Group Winter Meeting, Manchester.

13-15 January 2016
Bio-XFEL STC 3rd Annual International Conference, San Juan, Puerto Rico.
https://www.bioxfel.org/events/details/64

9-11 March 2016
9th International Workshop on X-ray Radiation Damage to Biological Crystalline Samples, Lund, Sweden.
http://indico.maxlab.lu.se/event/67/

4-7 April 2016
BCA Spring Meeting, Nottingham.
http://www.crystallography.org.uk/bca-spring-meeting-2016/

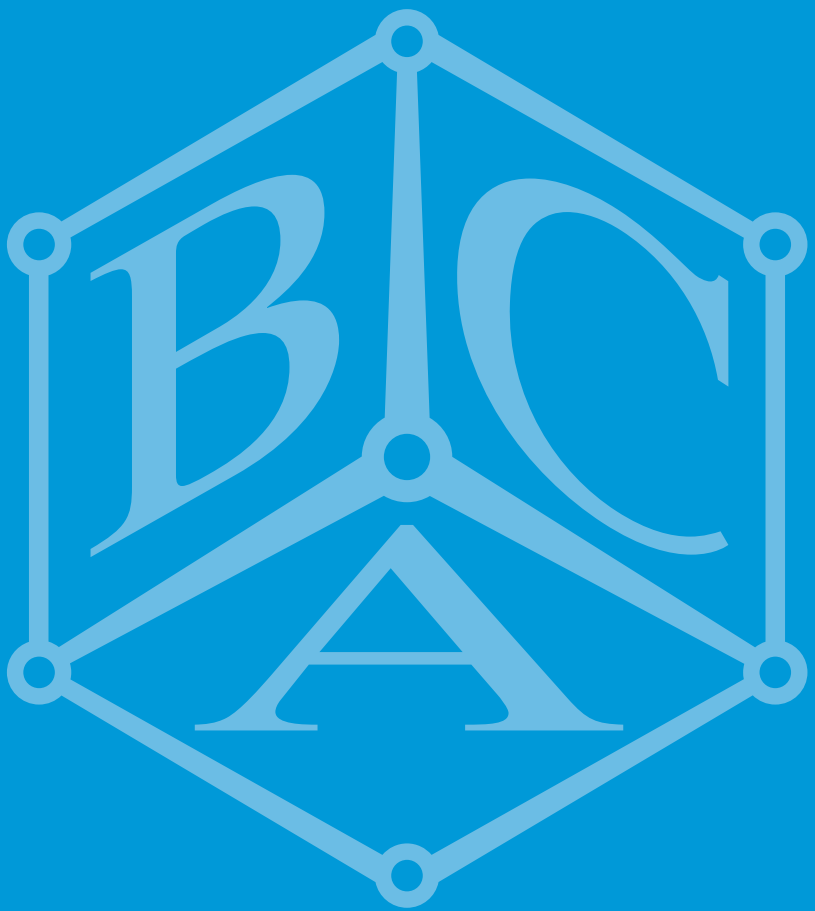
27 May - 5 June 2016
High-Pressure Crystallography: Status Artis and Emerging Opportunities. 49th Erice Course, Erice, Sicily, Italy.
http://www.crystalerice.org/2016/

3-8 July 2016
ICCBM-16. 16th International Conference on the Crystallization of Biological Macromolecules, Prague, Czech Republic.
http://www.iccbm16.org/

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

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

2 October 2016
MEDSI2016. Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation, Barcelona, Spain.
https://indico.cells.es/indico/event/42/



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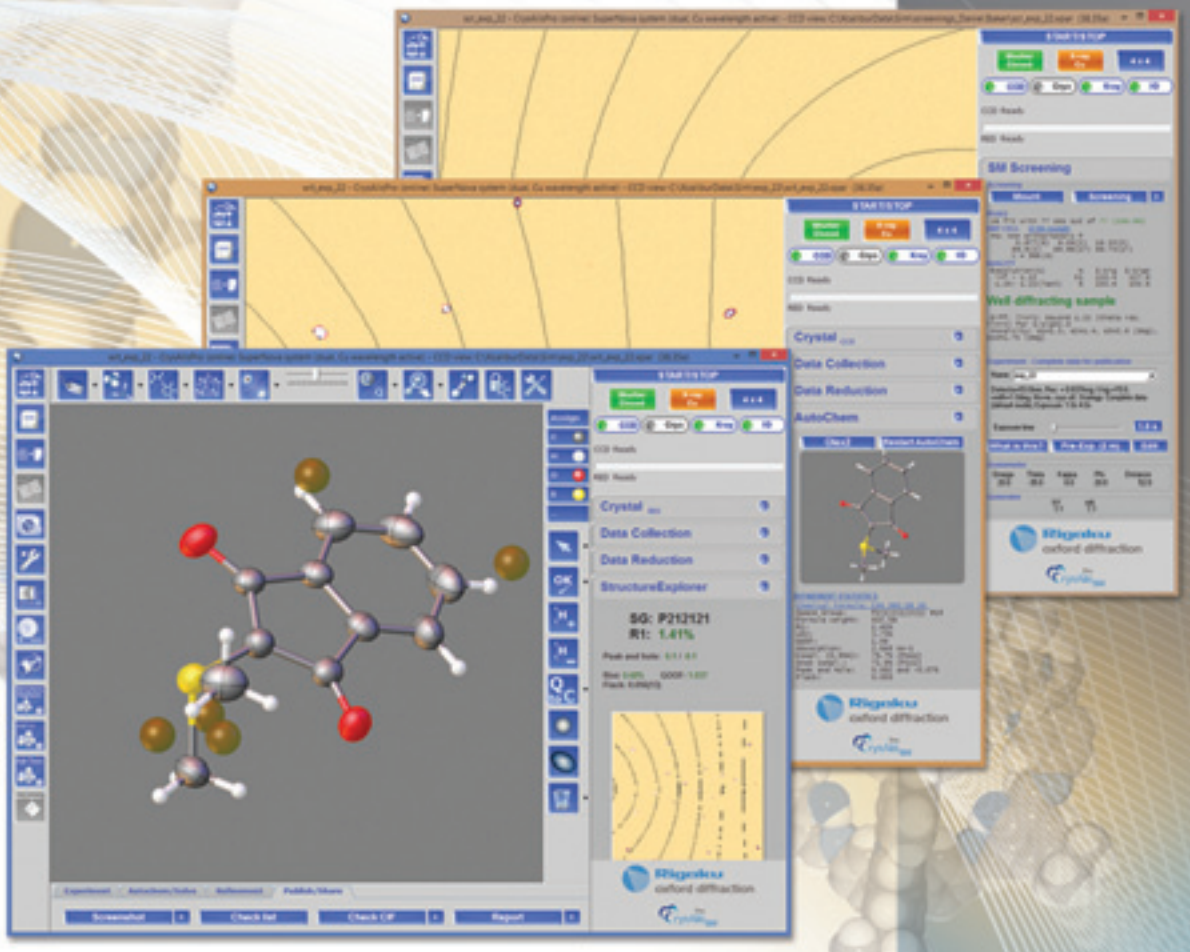

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