# Crystallography News

## British Crystallographic Association

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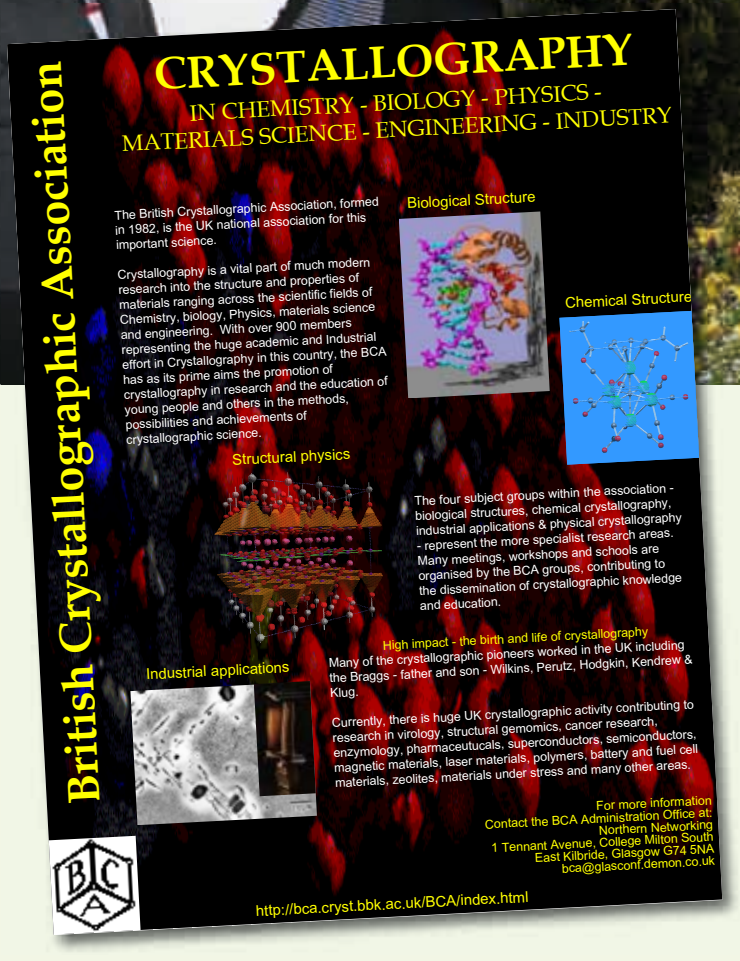


# BCA SPRING MEETING 2010 p6

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**Crystallography News** June 2010

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***This month's cover:***

*Kudos to Bill Clegg and Dave Taylor, seeing Stephen Moggach in stereo, classic poster*

# From the Editor

**I am writing this column just after another very successful and stimulating BCA Spring Meeting. Our expectation that the "Data Matters" theme would provide a unifying thread was amply fulfilled. From informative coverage of data collection to a final very lively session on publication followed by a Cambridge Structural Database user forum, the progress of structure determination was well documented. As we arrived, shy spring sunshine was illuminating the flower beds and blossoming trees on the beautiful Warwick University campus. As we left (or should that be attempted to leave?), a plume of volcanic ash and glass passing overhead enforced the cancellation of all flights. It seems ironic that we had assembled a group of the scientists most able to study the structure of this material, yet some of us fell victim to its effects.**

I had been resigned to the idea that the interval between the close of the meeting and the copy deadline would be too brief for any well-considered accounts of the sessions to appear in this issue, and I would have to fill it with waffle. How wrong I was! I am very grateful to so many contributors, especially bursary recipients, for the timely submission of their reports. I hope you will enjoy reading them while memories of the meeting are still fresh.

The conclusion of the BCA meeting was followed on the same evening by the first TV debate among the prime ministerial candidates. Perhaps I missed one due to post-conference fatigue, but I did not register a single sentence about science. There was plenty about budget-cutting, though. Sadly, often the first activities to be cut are those, like science, which require patience and mainly pay off in the long term. Therefore we owe it to science to explain the benefits of our work when we have the opportunity. However, **Elspeth Garman** told a cautionary tale in her very stimulating lecture to the Young Crystallographers. An announcement of space-based research to grow crystals under conditions of microgravity of an enzyme from HIV targeted for drug discovery led to an accurate article in a broadsheet newspaper. The next day a tabloid reported that mad scientists had put AIDS in space, where there was a danger that it would collide with an out-of-control Russian nuclear-powered satellite and start a nuclear-fuelled AIDS epidemic!

One important event at the BCA Spring Meeting was the changeover of Vice Presidents. **Sandy Blake** reached the end of his term of office. We have appreciated Sandy's wit, his unquenchable enthusiasm for crystallography, and his willingness and ability to examine the By-Laws minutely and spot errors and archaisms. This is a rare combination of qualities, and we hope that Sandy will continue to participate as a "private citizen." We are delighted to welcome **Dave Allan** as the newly elected Vice President. We admire Dave for his contribution to the outstanding success of the Diamond synchrotron. As a Principal Beamline Scientist (i.e. technical wizard), he could have been part of an aloof priesthood, deriding the mucky crystals that we brought to his beautiful machine. Instead, he has always been friendly to users and approachable, sharing our delight with the results we obtained from synchrotron data. A possible problem for the unwary is the spelling of Dave's surname. Over the years we have felt immense gratitude to **Frank Allen** for his leadership of the Cambridge Crystallographic Data Centre. Now we have to distinguish AllAn from AllEn. If anyone can do this, it is people who can distinguish Pmmn from Pnnm!

I was particularly impressed with the Commercial Exhibition at this year's Spring Meeting. Twenty exhibitors filled all of the available space. Their displays showed an impressive amount of innovation in both hardware and software. At a time when the recession has made so many companies over-cautious, we can be very grateful for the community of suppliers that we have. Plainly they are motivated by a zest for crystallographic technology, not just money making or capital conservation. Their payments for exhibition space made it possible to avoid any cost increase for conference delegates.

The location of this exhibit was ideal for all but one person. It was on a bridge providing access to the various lecture rooms. Good coffee, tea and lunches were also served there. The only person who suffered was your poor Editor/photographer. The exhibits backed onto a wall of windows, so that our "angels" and their displays appeared in deep shadow surrounded by a bright halo. Fortunately a spell of anticyclonic gloom during an otherwise sunny week made it possible to improve the signal-to-noise ratio. I encourage you to look for the smiling exhibitors on the centrefold pages.

Featured on our cover is the BCA poster, a design classic created around the turn of the millennium. In the place occupied by our usual Puzzle Corner are details of the opportunity for readers to design an eye-catching new poster that does justice to the advances in crystallography since then.

**Carl Schwalbe**

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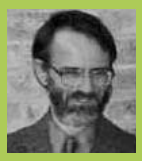

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Full committee details on the BCA website **www.crystallography.org.uk**

Spring Meeting Registration and Subscriptions:
**www.crystallography-meetings.org.uk**

# From the President

**DEAR MEMBER**,

**BY the time you read this, some of you will either be in the thick of exam marking or finished all teaching responsibilities for this academic year. You may be breathing a sigh of relief that you can now get going with your research again and can enjoy the summer weather. Certainly the recent bright sunshine has been welcome after our long and (even in Oxford) snowy winter.**

The recent Spring meeting on 'Data Matters' in Warwick attracted over 270 delegates, and at least 70 of them were `Young Crystallographers', who held their day-long symposium before the main meeting commenced and then gave a very welcome youthful feel to the atmosphere once diluted by the older crystallographers. I really enjoyed the YC talks on a diverse range of crystallographically related topics. There is no doubt that whatever else one thinks about the effect of Microsoft Office on our lives, the standard of presentations has definitely improved over the last 10 years, since we switched from overhead and slide projectors to computer based talks and all the contributing speakers at the YC sessions were extremely adept at this form of presentation. The Inaugural Parkin lecture was given by Professor **Simon Parsons** on 'Phase Transformations in Simple Molecular Solids': very appropriate for the occasion since Simon was **Andy Parkin's** PhD supervisor. The only regret for me was that there was only one Macromolecular Crystallography (MX) talk (given, incidentally, by my own research student) out of 14, not because of any oversight by the organisers in the selection but because there were no other volunteers. The YC forum is a wonderful place to gain valuable experience in communicating to a 'mixed' crystallographic audience, and I would encourage more MX students to step up to the plate next year in Keele. Many thanks go to **Graham Findlay** and **Helena Shepherd** for organising the YC part of the proceedings, and also to the EPSRC for helping to finance the event.

The masterminding and coordination of the main meeting was led by **Simon Coles**, the Chair of the Programme Committee to whom we owe much gratitude, as well as to the the Session Chairs from the Groups: **Vilmos Fülöp** and **Neil Isaacs** (BSG), **Ross Harrington** and **Hazel Sparkes** (CCG), **Martin Gill** and **Matthew Johnson** (IG), **Sarah Lister**, **Matt Tucker** and **Andrew Willis** (PCG) and the last but not least member of the Organising Committee, our Vice-President, **Sandy Blake**.

Northern Networking provided their usual efficient level of organisation for the meeting, including expediting the silencing of some particularly noisy drinks machines in the Exhibitors space. They were supported ably (and it seemed to me smoothly, but perhaps I was being shielded from any complications!) by the local Warwick staff. We are particularly grateful to our 20 exhibitors (see list and photos later in this issue) for their support of the Meeting despite the current chilly financial climate. Without them we could quite simply not be able to run the Meeting in its present form. We were also glad to be sponsored for various aspects of the Meeting by Bruker-AXS, the ICDD, PANalytical, Rigaku, Incoatec and Oxford Diffraction.

The main meeting started inspirationally with the Dorothy Hodgkin Prize lecture given by Professor Dame **Louise Johnson** FRS who gave a wonderful overview of 'Forty Years of Structural Biology: where have we come from and where might we be going?', ending with a brief mention of some exciting unpublished results hot from the LCLS in Stanford. Our Bragg Prize lecturer, Professor Sir **John Meurig Thomas** FRS, also did us proud with his energetic and informative lecture on 'The promise and essence of 4 D microscopy'. I much enjoyed the glimpse he provided into the world of catalysis design and complementary imaging techniques, as well as his vision of future possibilities in relation to the latter. Sir John, who is also an elected Member of Gorsedd of Bards of the Royal National Eisteddford of Wales, treated us at the Meeting dinner by starting the meal with a Welsh grace.

Three crystallographers were made Honorary Members of the BCA at the Meeting: **Bill Clegg** and **Dave Taylor** to acknowledge their significant contributions to the fields of chemical crystallography (BC) and XRD as well as XRF (DT) over many years, and also their great service to the BCA as Council Member and Treasurer respectively. Our third Honorand is **Venki Ramakrishnan**, winner of the Nobel Prize in Chemistry in 2009 for his work in solving the structure of the ribosome. He delivered a riveting plenary lecture on his research at the BCA Spring Meeting last year in Loughborough.

At the BCA AGM our redoubtable Vice President, **Sandy Blake**, retired after his three year term. I would like to repeat the thanks of the BCA which were expressed both at the AGM and the Meeting dinner to Sandy for his wisdom and foresight, and to add my personal thanks to him for the quiet and much appreciated support he has given me, particularly in the last 6 months. Our new Vice President is **Dave Allan** from Diamond, who is the Principal Beamline Scientist on the small-molecule single-crystal diffraction beamline, I19, and the BCA are fortunate to have him as an Officer. At Warwick two of our Co-opted Council members, **Paul Raithby** and **Bill Clegg**, attended their last Council meeting. We are really grateful to them both for their long standing and very positive service to the BCA. According to a scheme

agreed last year by Council, we are staggering the election of new ordinary members of Council at one a year, instead of electing a completely new triplet every three years. To achieve this, one Ordinary Council Member kindly stepped down (**Andres Goeta**) and was then co-opted back onto Council, and **Arwen Pearson**, a macromolecular crystallographer working at Leeds University and our next Spring Meeting Programme Chair, was elected onto Council.

The Icelandic volcano stranded several of our speakers in the UK and gave them difficult journeys home. We hope this has not put them off travelling too much!

On the wider front, this summer ECM26 is being held in Darmstadt, Germany from 29th August - September 2nd. The programme looks varied and should have something of interest for all crystallographers. At this meeting, the BCA will have a booth manned by Northern Networking and any Council members who happen to attend to advertise the 2013 ECM in Warwick.

Lastly, for those of you who were at the BCA conference dinner, you might have noticed that another conference (the Joint Spring Meeting of the British Society for Cell Biology and the British Society for Developmental Biology) who were holding their conference dinner in a neighbouring banqueting room, had a lively ceilidh after their dinner was over. Would there be any takers (apart from me!) for such activity after the Spring Meeting dinner at Keele next year?

# TIME FOR A CHANGE...


**Can you do any better than this?**
Approximately fifteen years ago, Chick Wilson designed a fabulous poster (see the front cover for the full colour version) to attract new delegates to the BCA. Both crystallography and graphics programs have developed considerably since then so maybe it's time for a new marketing campaign!

Are you a budding graphic designer, or have you just got a bit of free time while waiting for your crystals to grow? There is a competition to design a new poster which would be used in full or in part to advertise the BCA.

*Information:*
The poster will be printed in sizes up to A0 so graphics must be of appropriate quality. Please send your entries to **alex.griffin@oxford-diffraction.com**

## BCA Corporate Membership

**The BCA values its close ties with commercial companies -involved with crystallography. To enhance these contacts, the BCA offers Corporate Membership. Corporate Membership is available on an annual basis running from 1 January to 31 March and includes the following benefits:**

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# BCA Spring Meeting 2010

## Participants' impressions

**"HOW much can I assume you know about Crystallography?"... a question apparently asked of Sir Lawrence Bragg by a young researcher and recounted by Sir John Meurig Thomas in his Bragg lecture. As this is my first spring meeting it is difficult to know what to assume and how to judge what's new and important. I thought therefore that it might be of interest to give my perspective as a naive and impressionable young researcher attending my first BCA meeting.**

The first was thing that really struck me was the degree of innovation going on in crystallography. 3D glasses were obviously the most important development at this year's conference, although a number of people did comment that it was easier to see the structures if you closed one eye. As a small molecules crystallographer I am always amazed by what can be achieved with protein crystallography. I attended a session on high throughput and membrane proteins and, besides being bombarded with acronyms I didn't understand, came away inspired by projects with a clear purpose and the resources and experience to make progress. Whilst the oversized sample changing robots at Diamond at first appeared excessive, they reflect an era where mounting the crystal has become the limiting factor for productivity, a far cry from single point detectors where it took a week to collect data. I was fascinated to hear about the efforts of **Simon Coles** and the eCrystals project at Southampton in collating crystallographic and chemical information and making it widely accessible through the internet, something crystallography is already leading the way on with the CSD. However, it was the point at which I heard Dame **Louise Johnson** talk about the development of X-ray free electron lasers which are $10^{10}$ x brighter than current synchrotron sources and capable of imaging nano-sized objects where I really got a taste of the next generation of crystallography.

The second theme that struck me was the increasing importance of complementary techniques alongside traditional crystallographic data as we investigate ever more complex structures. This was illustrated most clearly by Dr **Lynne McCusker** with her 'Witch's brew' of XRPD, charge flipping and electron microscopy. The use of electron microscopy in crystallography seemed particularly prominent with an entire session devoted to electron diffraction as well as Professor Sir **John Meurig Thomas**'s eminent talk on four-dimensional electron microscopy. At the Young Crystallographers (YC) meeting, **Mark Eddleston**'s excellent talk describing his work imaging beam-sensitive pharmaceutical crystals won him the IG YC prize for best talk. Computational techniques appeared throughout the conference with talks on structure prediction, the use of charge flipping to solve powder structures and incorporating information from the CSD into models and in validating structures.

A thank-you to Sandy Blake

The final area I would like to highlight is the emphasis the BCA obviously put on training younger researchers. There were a number of talks which sought to pass on practical expertise and best practice on everything from collecting data through to validating structures and writing up papers. The Young Crystallographers meeting provided an excellent chance to present research and meet other crystallographers. I found that the Industrial stands and conference dinner provided a great opportunity to network and learn more about opportunities in industry. Last, but not least, I'd like to thank the BCA for their generous initiative in getting young researchers to write up the conference proceedings.

**Jonathan Foster**
**Durham University**

On Wednesday night everyone got dressed up, to varying extents, for the BCA conference dinner. There was a great buzz in the room as everyone filtered in, claimed a seat using jackets of other people and then went to the bar. It was my first conference dinner and I didn't know what to expect, but it didn't disappoint me at all. The food was of a really high standard, even for those with dietary requirements. The wine disappeared far too quickly but luckily the food appeared just as quickly to fill the void. The prize giving was a nice break in the middle of proceedings and I was lucky enough to win a prize for my poster, which I think may have given the night a bit more of a rose tinted feel. The friendly atmosphere continued well into the following morning, for some later than others (a certain spray bottle comes to mind), and I saw a few blood-shot eyes for the session on the Thursday morning. The whole night and really the week for me were a big success. As a young crystallographer it was a great experience to witness what is going on in the rest of Britain and around part of Europe, as well as having the opportunity to show off what we are doing in our group. I know it's wrong to say it, but I am looking forward to next year.

**Alexander Graham**
**University of Edinburgh**

## PLENARY LECTURES

### Hodgkin Lecture

Prof. Dame **Louise Johnson** FRS painted a vivid picture of the "Forty Years of Structural Biology: Where Have We Come From and Where Might We Be Going?". Starting with an introduction to **Dorothy Hodgkin** and the research she carried out to further the field of macromolecular crystallography, Dame Louise showed some fascinating pictures from the "early days" when the first crystallographically solved structure of an enzyme (Lysozyme) was presented at the Royal Institution at a scale of 2 cm to the Å. What followed was a walk-through of the next 40 years, often from a very personal perspective documenting the advancements not only in the crystallographic techniques but also the DNA cloning and protein purification, which make the process of structure determination possible. There was a fascinating insight into the future of the subject also, allowing crystallographers to explore larger proteins and smaller crystals with the use of third generation synchrotron sources and the development of free electron lasers. The talk finished with a letter written from Dorothy Hodgkin to a research colleague who was applying for a position at The University of Oxford in which she showed her pragmatic and encouraging nature in the furthering of the careers of others.

Hodgkin Lecture

**Alexander Graham**
**University of Edinburgh**

### Alun Bowen Lecture

This year's lecturer was a very popular member of the BCA, **Dave Taylor**, whose long and loyal service is appreciated by many. To enable this lecture to provide an introduction to the ICDD Workshop, it was moved to an earlier time. Some members of the audience were hastily swallowing the last of their lunch, but this did not spoil their enjoyment. Dave's lecture, "Phase Identification Data – How it's Changed Over the Years", along with his presentation at the Exhibitors' Forum, provided a link from the past to the future of phase identification. Dave paid tribute to Alun Bowen, who as chair of the Industrial Group stimulated his own involvement. He described the progress made since the early days of the Powder Diffraction File, when only peak matching could be carried out on the relatively small number of tabulated phases. Thanks to collaboration with CCDC, ICSD, NIST and the Pauling File as well as progress in powder diffraction, the number of available phases will exceed 700,000 from September. The round-robin exercises organised by Dave have driven up the quality of data. With storage of entire patterns now becoming a reality, the prospects for phase identification are indeed bright.

**Carl Schwalbe**

## PCG Plenary Lecture

The PCG Plenary lecture was given by **Lynne MuCusker** (ETH Zurich) and chaired by **David Keen**. Lynne stated the problem facing powder diffraction: a powder crystallite has a volume ca. 1 $\mu m^3$ instead of $10^6$ $\mu m^3$ for a single crystal. She outlined a 'witch's brew' of techniques available for structure solution from powder diffraction data in her talk entitled "Polycrystalline Materials, Powder Diffraction, Electron Microscopy and Charge Flipping – A Remarkable Brew. " Lynne demonstrated the benefits and drawbacks of electron diffraction compared to X-ray diffraction with reference to complex zeolitic structures. When X-ray reflections overlap, the total intensity has to be partitioned, and initially there usually is no sensible alternative to arbitrary equipartitioning. Lynne also highlighted the advantages of repartitioning data midway through a charge flipping refinement where no symmetry is assumed.

**Samantha Callear (ISIS) and Carl Schwalbe**

## Bragg Lecture

Presentation of the Bragg Lecturer's trophy

In a year when the Bragg lecture is given, it automatically becomes one of the highlights of the meeting. This year's lecture, given by Prof. Sir **John Meurig Thomas** FRS, fully lived up to its star billing. Talking about "The Confluence of Microscopy, Unconventional Crystallography and Electron Energy-Loss Spectroscopy", he began by showing that unconventional crystallography actually predates conventional crystallography. Sir **William Bragg**'s notebook, compiled while a professor at Leeds and held in the University of Leeds library, records observations of diffuse scattering several pages before what we know as Bragg scattering. Building on structural and spectroscopic information, Sir John showed how it is possible to design materials with open structures. Applications include environmentally benign catalysts. One of his triumphs was a porous material with acidic and oxidation sites that forms caprolactam, a building block for nylon-6, from cyclohexanone, ammonia and air without the need for strong acids or high temperatures. The author of many books, he has just collaborated on another one, A. H. Zewail & J. M. Thomas, "4D Electron Microscopy: Imaging in Space and Time", published this year by Imperial College Press.

**Carl Schwalbe**

## IG Teaching Lecture

The teaching plenary lecture has always been an excellent environment within which to learn about new techniques and this year was no exception. **Simon Billinge** lectured on "Structure at the Nanoscale: Atomic Pair Distribution Function Analysis of Nanostructured Materials". He introduced his thoughts and approach by weaving background technical information together with case studies from both the organic and inorganic disciplines. The technique has been applied to crystalline samples, but it also promises to be an invaluable tool for characterising the structures of so called "X-ray amorphous" materials (nanomaterials), which previously may have been ignored or left poorly understood. Short range structural information can be extracted by using the pair distribution function (PDF), providing enough information to fingerprint and in some cases determine the local molecular structure. Simon described a number of case studies to highlight the key advantages of this technique from the structure solution from purely PDF data of C60 (buckyball), to the determination of layer thickness of atomic sheets within Xerogels, to characterising stacking faults and stress within the nanostructure of CdSe quantum dots and finally to identifying the melt quenched amorphous form of carbamazepine as containing the ß form with a domain size of 4.5nm. This is a technique that has a strong scientific base that is currently spreading wider than its initial development field and is crossing both the laboratory and the synchrotron scales.

**Matthew Johnson**
**GSK**

# Group Sessions

## PHYSICAL CRYSTALLOGRAPHY

### Resonant X-ray Diffraction

The first PCG session of the 2010 BCA Spring Meeting, entitled "Resonant X-ray Diffraction" was chaired by **Peter Hatton** (Durham University) and gave a fascinating demonstration of the kind of complex systems that can be investigated using resonant diffraction and other complementary techniques. **Manuel Angst** (Forschungszentrum Jülich) began the session with an interesting talk on the "Interplay of electronic and structural degrees of freedom in lutetium ferrite" which focused on the magnetoelectric multiferroic $LuFe_2O_4$. Manuel explained how resonant X-ray diffraction at the Fe K edge had been used to confirm charge ordering of $Fe^{2+}$ and $Fe^{3+}$ cations and explain its antiferroelectric structure, whilst polarised neutron diffraction had been used to investigate orbital ordering in the material. **Paulo Radaelli** (Oxford University) followed with a fascinating talk entitled "X-ray and neutron studies of multiferroics and frustrated magnets" which showed how subtle structural effects can be elucidated using resonant scattering. Paulo began by looking at the delafossite $AgNiO_2$ and demonstrated how resonant scattering at the Ni K edge had revealed charge disproportionation of nickel to $Ni^{2+}$ and $Ni^{4+}$ which had helped to explain the magnetic structure of the material. He then went on to discuss some $RMn_2O_5$ multiferroic materials and how their domain structures had been investigated using neutron spherical polarimetry and resonant scattering. The final talk of the session was given by **Sean Langridge** (ISIS) under the title "Observing interfacial magnetism in nanoscale films". Sean spoke about some FeRh multilayered systems with a magnetostructural phase transition which was investigated using neutron and resonant X-ray scattering and magnetic dichroism techniques. These nanomagnetic systems are of considerable technological importance and can help in the understanding of magnetic behaviour in other systems of reduced dimensionality.

**Emma McCabe**
**University of Durham**

### New Approaches to Structure Solution

The New Approaches to Structure Solution session, chaired by **David Keen**, was started by **Sarah Lister** (University of Durham) whose talk entitled 'The Use of Complementary Techniques in Structure Solution from Powders' introduced the benefits of using NMR to probe the local structure. Discussing the $(Mo^{VI}O_2)_2P_2O_7$ system which forms superstructures, the information gained from NMR studies was used to aid structure solution. Following this, **Maryjane Tremayne** (University of Birmingham) discussed the use of a new direct space global optimisation technique for structure solution known as differential evolution in her talk 'Structure Solution of Multicomponent Systems from Powder Diffraction Data.' Using co-crystals as examples, Maryjane demonstrated how the differential evolution technique offers a fast and robust method for convergence of powder X-ray diffraction refinements (from laboratory data) by 'exterminating' three-quarters of the solution minima population. The session was finished with a talk by **Paul Midgley** entitled 'Towards Routine Structure Solution using Precession Electron Diffraction.' Paul discussed the use of precession in electron diffraction experiments and noted that although the obtained intensities are not strictly kinematical, they can be used for structure solution. The effectiveness of this technique was shown to be improved when employed in combination with a new charge flipping algorithm that includes the crystal symmetry.

**Samantha Callear**
**ISIS**

### Electron Diffraction

Chair **Kirsten Christensen**

**Ute Kolb**'s presentation entitled 'Enhanced Electron Diffraction Data for "Ab Initio" Structure Solution Using Automated Diffraction Tomography (ADT)' illustrated how ADT can be successfully used to solve structures on a nanoscale. In these cases single crystal and powder X-ray diffraction techniques can fail but ADT solely and in combination with other complementary methods, has proven to work for materials with small particles and domains, and some beam sensitivity. Structures solved by this technique were compared to solutions found by traditional methods; examples included $BaSO_4$, $Zn_{1-\sigma}Sb$, the zeolite structure ZSM-5. Combination with PED (precession diffraction) improves the data, and direct methods can be used. The more beam sensitive organic-inorganic hybrids (for example Basolite) have been solved with a combination HRXRD and ADT. Importantly the rapidity of the calculations was highlighted with some structures only taking a few days to solve.

The advantages and disadvantages of employing Electron Diffraction as a technique to solve structures on a nano-scale were discussed by **Sven Hovmöller** in his talk 'Single Crystal Diffraction from Powders Using Electrons.' The most striking feature of this technique is the ability to investigate powdered samples in a single crystal manner removing common problems such as peak overlapping. The disadvantages associated with discerning between relative intensities and multiple scattering effects generally caused by sample thickness were also discussed.

**Wuzong Zhou** presented experimental techniques to aid in the collection of data from beam sensitive materials in his talk 'Electron Diffraction of Some Beam Sensitive Materials.' Initially common problems associated with beam sensitive samples were highlighted: knock-on damage, ionisation damage and heating damage. Since low temperature sample holders offer an effective yet expensive solution, several alternative sample treatments were presented: keep the sample dry; remove adsorbed contaminants by annealing in an electron beam; determine maximum irradiation dose; determine a desirable experimental

arrangement by initially setting a low magnification and irradiation dose. These factors were proven invaluable in the study of C60/trimethylbenzene nanowires, zeolites and metal organic frameworks all of which would normally decompose under electron beam irradiation.

**Lisa Simmons**
**Salford University**

### PCG Prize Lecture

Chair **David Keen**

The PCG Prize was awarded to **Christoph Salzmann** (Durham University) who gave a talk discussing his work mapping the phase diagram of ice: 'Ice XV and Other Forms of Solid Water.' Christoph discussed the structural complexity of the solid forms of ice and how its hydrogen ordering phenomena leads to either ferroelectric or antiferroelectric ice structures. Focussing on the medium pressure ranges of the ice phase diagram Christoph discussed the methods used to determine the structure of ice XV and compared the results to other ordered ice structures and discussed the disagreement of the structure with that predicted by DFT calculations.

**Samantha Callear**
**ISIS**

### Pair Distribution Function: Local Structure

Chair **Matt Tucker**

**Andrew Goodwin** gave the first talk of the Pair Distribution Function (PDF): Local Structure session, entitled 'From shells to solar panels – 'solving' the structures of amorphous materials using PDF'. He presented a range of materials and showed that by modelling the PDF for each of these, information on local structure could be obtained. In one example, a zeolitic imidazolate framework material (ZIF), underwent a thermally-induced transition to an amorphous phase and then surprisingly re-ordered at higher temperatures to give a new denser crystalline phase. PDF analysis showed that the sample actually retained the same local environment although the long range order differed between the crystalline polymorphs. Andrew also demonstrated the possibility of structure 'solution' using amorphous $CaCO_3 \cdot H_2O$ as an example. Starting with an ordered atomic configuration and introducing disorder produced the same PDF that was obtained when starting from a random configuration of atoms and introducing order instead. The resultant atomistic model could be regarded as a 'solution' of the amorphous structure. **Daniel Shoemaker**'s talk 'Locating atoms in disordered crystals' highlighted exactly why 'interesting things happen when crystals are disordered'. The complex $Bi_2Ti_2O_7$ possesses a cation 'off-centring problem' where bismuth and oxygen atoms are displaced from their ideal positions. This disruption on long range ordering meant accurate information on the structure could not be obtained from Rietveld analysis alone. Reverse Monte-Carlo (RMC) modelling of the PDF produced a 'snapshot' of the local structure showing the instantaneous deviations in bismuth and oxygen positions. Daniel highlighted another advantage to the PDF method – in the complex $CuMn_2O_4$, disordered copper and manganese atoms adopt both octahedral and tetrahedral geometries. Rietveld refinement would constrain the coordination geometries of manganese and copper to be the same but this is not the case when using the PDF approach. In fact it predicted the existence of $Cu^{3+}$, which occurs via charge disproportionation in order to avoid Jahn-Teller distortions. **Samantha Chong** gave the final presentation of the session 'Investigating disorder in a pure Bi A site perovskite using total scattering and RMC modelling'. Samantha presented a perovskite structure that featured a mixture of titanium, iron and magnesium occupying the 'B' site. However, similarly to the problem described by Daniel, Rietveld refinement constrained all B site atoms to be the same, which led to incorrect bonding coordination according to bond valence sums analysis. Using the RMC method but utilising bond valence sums as constraints on the atomic configuration, the disorder in the system could be more accurately modelled. The results showed there was no significant long or short range ordering for the B-site atoms and that the B-site itself had little structural consequence on the Bi-O bonds.

**Nicholas Funnell**
**University of Edinburgh**

## INDUSTRIAL CRYSTALLOGRAPHY

### Data: What Goes In

Chair **Matthew Johnson**

The first speaker was **Ross Harrington** of Newcastle University, whose talk was titled "Getting the Best Possible Data from Your Crystals". The talk provided a guide to what to look for from crystals before, during and after data collection. Basic subjects such as how crystals or a diffraction pattern should look were covered, through to topics such as what radiation to use and how to deal with twinned data sets and other commonly encountered problems. The talk gave many useful tips from an experienced crystallographer's perspective on matters from the crystal growth stage through to structure determination. Example tips delivered by Ross, which are intuitive but often neglected, included keeping single crystals in the crystallisation growth medium to maintain the crystal in its current solid state form prior to mounting, to have confidence in the X-ray data not in the diagram submitted by the chemists, and to maintain your diffractometer and use your knowledge of chemistry when refining.

The second speaker was **Sarah Barnett** from the Diamond Light Source. Her talk explained the advantages of using the I19 beamline for small molecule single crystal diffraction. The synchrotron offers various advantages over lab sources due to the higher flux and tuneable energies of such x-ray sources. This allows for relatively high speed data collection even from small or poor quality crystals. It also offers a vast improvement in data resolution over lab sources making it

ideal for disorder or charge density studies. As a beamline scientist who is well aware of the potential pitfalls that can befall the unwary user, Sarah then went on to give advice to future users of I19 on what preparations should be made beforehand and how to identify problems early on in the data collection process. The guidance went from a description of the storage ring status and the need to monitor this throughout your experiment, simply because without the white beam there are no X-rays; to a detailed description of the I19 beamline, its beam size when focused (128 x 190μm), the ability to change wavelength depending on the experimental goals (0.5-2.5Å) and the automated robots for mounting and alignment of t he crystals. Sarah wanted the audience to consider carefully the experimental proposal and the planning of the beamtime so that a successful experiment is completed in the limited time available and not wasted. If in doubt when planning an experiment, contact the beamline staff.

The final speaker was **Alastair Florence** from the University of Strathclyde who spoke about "XRPD Data in Physical Form Identification and Structure Determination". Alastair began by discussing the role of physical forms in the pharmaceutical industry and how powder x-ray diffraction is routinely used for physical form identification. He set out his thoughts for maximising the chance of success when applying XRPD data to fingerprinting, phase identification and structure determination from powder diffraction data, through optimisation of the instrument, sample and the data collection. Collecting the best data, he suggested, should involve a calibrated instrument which has a well prepared and aligned sample to minimise errors such as inaccurate $2\theta$ peak positions and sample errors (such as peak broadening, difficult peak shapes and preferred orientation); such errors can lead to poor pattern matching and failed indexing attempts. He then went on to say that although single crystal diffraction is the method of choice for structure determination, structure determination from XRPD is becoming more common. He explained the XRPD data collection process for structure determination, which normally involved variable count times with longer steps at high angle to improve the quality of the data to allow for Rietveld refinement. He presented examples of solving structures using the DASH software, explaining the simulated annealing process of adjusting all degrees of freedom within the structure, such as molecular positions and torsion angles, to find the global minimum. His results showed that although the crystal structure obtained was close to the actual structure, it was not always as accurate as we would like. He then demonstrated with his example how software tools such as Mogul can overcome this problem by using CSD data to generate probability distributions for bond angles, lengths and torsion angles and applying constraints based on this data.

**Craig Wales**
**University of Glasgow**

**Matthew Johnson**
**GSK**

## Data: What Comes Out

Chairs **Brett Cooper and Cheryl Doherty**

**Trevor Rayment** from Diamond gave the first talk of the session: Food, Formulation, Foams and Fabrication – Modern Applications of Synchrotron Radiation for Industry. Trevor introduced synchrotron facilities as an essential tool for the modern economy. He went on to discuss the challenges in providing a resource which attracts such a wide variety of interested parties: academics, industry and facility staff. He further described recent developments such as the pseudo real time analysis of samples using the Pilatus detector and also the introduction of remote control operation at Diamond.

The second talk of the session was presented by **Robert Hammond** from the School of Process, Environmental and Materials Engineering at the University of Leeds. His talk was entitled: A Molecular-Scale Perspective: New Insights into the Assembly of Crystalline Particles. Robert started by discussing the drive to understand the properties of materials, and that it is possible to apply molecular modelling techniques with inputs from crystallography to achieve this. He introduced the use of a molecular mechanics approach to model the critical clusters of the growth phase in nucleation. He then showed that it is possible to use these techniques to further explore the intermolecular interactions of pre-nucleation clusters with a variety of different solvents.

The third and fourth talks of the session were the winner and the runner up of the Industrial Group Prize awarded to the best Industrial Relevant Presentations from the Young Crystallographers Meeting held on Monday and Tuesday.

The winner of the prize was **Mark Eddlestone** from the University of Cambridge. His talk was entitled: Analysing Pharmaceutical Materials by Transmission Electron Microscopy (TEM). Mark introduced the technique of TEM and highlighted some of the issues including the difficulties involved in sample preparation and stability in the electron beam. He went on to describe how the technique could be applied to the analysis of pharmaceuticals including obtaining information on morphology, phase ID as well as crystal structure and defects. He described how individual crystals could be examined and phase determined with a possible application to patent infringement cases.

The runner-up for the Industrial Group prize was **Jonathan Foster** with his talk: Supramolecular Gels; a New Medium for Crystal Growth. Jonathan described a new range of bis urea gel forming agents that could be used as media in which to grow crystals. He described the advantages to growing crystals in the gels which slow down the crystal growth; this can lead to preferentially forming a more thermodynamically stable form where normally a kinetically favoured form may predominate. The gel structures can easily be broken up by the addition of a gel disrupting agent such as a simple anion. Once the gel had been disrupted, the crystals could then easily be recovered by filtration and could be used for single crystal studies. By varying the type of gel formers and the solvents it may be possible to grow a variety of crystalline phases.

Industrial Prize Lecturers plus chairpersons
**Cheryl Doherty and Brett Cooper**

### Complementary and non-Ambient Techniques
Chair **David Beveridge**

**Tim Hyde** from Johnson Matthey opened with the first talk of the session: Catalysis Studies using Complementary Techniques at Johnson Matthey. Tim highlighted the fact that catalysts often do not operate at room temperature and that often data needs to be extrapolated to obtain data at operating temperature. Tim highlighted that his company's philosophy is to generate data at close to the actual temperature and pressures the catalysts would be employed at, sometimes as high as 1400° C and up to 100 bar, using a variety of complementary in situ techniques. The techniques used at Johnson Matthey included: high temperature and pressure XRD, XRD with evolved gas measurement by mass spectroscopy, XRD-TEM, Photo electron spectroscopy for depth profiling, XRD-NMR, XRD-TMA as well as SAXS, XAS and total scattering.

The second talk of the session was presented by **Axel Zeitler** from the Department of Chemical Engineering at the University of Cambridge. His talk was entitled: Terahertz Spectroscopy of Structure and Dynamics in Organic Molecular Crystals. Axel introduced the technique of terahertz spectroscopy, which is a vibrational spectroscopy in the far infrared region between IR and microwaves. He described how terahertz waves, a name that has changed over the years from ultra-red, sub millimetre and far IR, could be formed and detected using a GaAs substrate. Axel also described some potential uses for terahertz spectroscopy for polymorphism and pseudo polymorphism studies, both qualitative and quantitative. To finish, he then demonstrated some practical case studies: monitoring the phase transition of Carbamazepine Form III to I at 433 K which appears to go through an intermediate glassy state, and also the dehydration of Theophylline monohydrate which appears to be a two step process of phase change followed by evaporation of water.

The final talk of the session was by **Simon Watson**, a NMR specialist from GSK. His talk was entitled: Running Hot and Cold – Understanding Crystal Structure Phenomena with Variable Temperature Solid State NMR. Simon introduced the technique of SS NMR describing how the temperature could be varied from 153 – 400 K. He demonstrated how the peaks could be structurally assigned using an example of paracetamol in a tablet with MCC/starch, magnesium stearate and sodium bicarbonate. He showed how you could easily distinguish different polymorphs, hydrates and solvates as well as potentially gain information on how many molecules are in the unit cell. Finally Simon took us through three case studies where SS NMR had been used to troubleshoot issues in the pharmaceutical industry, including studies that could reveal whether additional peaks observed by XRPD were really phase impurities or just deviations in the crystal packing, where one group could flip positions from one orientation to another.

**Brett Cooper**

## CHEMICAL CRYSTALLOGRAPHY

The CCG sessions had a wide variety of speakers contributing to different areas of research. The first talk in the "Structure and Property Prediction" session was given by **Graeme Day** who is working on exploring lattice energy landscapes and ranking energies to try to predict whether solvates and inclusion compounds will form in particular systems. **Caroline Mellot-Draznieks** gave an interesting talk on the popular topic of metal organic frameworks (MOFs) from the point of view of using simulations to predict and design the formation of new MOFs. **Peter Galek** described his research using the CSD and certain descriptors to look at H-bonding structures because a lot can be found out about a structure depending on the dominant interactions. This knowledge can be used to predict whether polymorphism would be expected for a particular compound; this is important in the pharmaceutical industry.

### Dealing with Difficult Data
Chair **David Watkin**

In this session, the first on Wednesday morning, **Mathias Meyer** focused on how to optimize data collection strategies using new technology while **Arie van der Lee** presented the charge flipping algorithm for structure solution and comparing it with direct methods. Finally **Christopher Serpell** described some problems with obtaining the structures of large supramolecular assemblages, including crystallization difficulties, high levels of disorder, solvent inclusion and limited data quality resulting in the need for many restraints in the refinement.

### CCDC Prize Lecture
Chair **Andrew Bond**

The CCDC Prize this year was won by **Stephen Moggach** who gave a very enthusiastic and interesting talk entitled 'Putting

the squeeze on porous materials'. Stephen discussed the use of high pressure crystallography to investigate the effects of putting porous materials, for example zeolites and MOFs, under pressure. "Databases & Data Mining" drew attention to how databases, for example the CSD, can be used to make comparisons and form a basis for experimental and computational studies.

### Databases & Data Mining
Chair **Hazel Sparkes**

This session fitted in particularly well with the Spring Meeting's theme "Data Matters". The three talks focused on how information in databases, for example the CSD which now contains over half a million structures, can be used to extract information and draw comparisons as a basis for computational and experimental work. **Peter Wood** from the CCDC gave the session's first talk and highlighted problems with identifying structure-directing interactions involving hydrogen atoms by using van der Waals overlaps. Peter showed how data analysis using the CSD and theoretical energy calculations can complement each other to help study packing structures. The second talk was given by **Anna Stevenson** and focused on using the CSD for knowledge mining studies of gas storage materials. Porous structures, for example MOFs, can be used as gas storage materials because they provide tuneable frameworks that can be altered for specific usage. CSD searches were used to make structural comparisons and give insight into interactions between guest and host molecules in these structures. Finally she described some interesting preliminary experiments using an environmental gas cell to study how $SO_2$ and $CO_2$ can be stored in MOFs. **Mairi Haddow** gave the final talk of the session describing conformational analysis of $PEt_3$ and $P(OMe)_3$ in metal complexes. Steric bulk and electronic profile change with conformation, therefore knowing which conformer is favoured for different ligands and the interconversion pathways are important. $PEt_3$ and $P(OMe)_3$ conformers were ranked in order of popularity using the CSD and it appears this relates to the energy preference for the conformers. Overall this was an interesting, well attended and very informative session highlighting how databases and data mining can significantly enhance scientific research.

### Data & Structure Validation
Chair **Ross Harrington**

On the last day there were two important sessions. In the first talk of the first session **Anthony Linden** observed that as crystallography becomes increasingly automated and users less specialised, software such as CheckCIF is increasingly relied upon to validate structure. He warned that, invaluable though such measures are, the peculiarities of crystals and limitations of software's understanding mean they should not be relied on uncritically. He then described how recent efforts to validate structure factor listings against the corresponding CIF provide additional safeguards for identifying twinning and inconsistencies in the CIF due to the use of routines such as SQUEEZE and editing of files by hand. **Ian Bruno** of the CCDC introduced software which automatically processes structures for express publication on the web CSD. The talk provided a fascinating insight into the editorial process and was illustrated with interesting examples of systems which are genuinely hard to assign, as well as some obvious mistakes which can be overlooked by validation software or users. In the final talk of the session **Roy Copley** of GSK explained the importance of structure validation in industry, pointing out that you never know which data will suddenly become vitally important once it's published. He pointed out how easy mistakes can be avoided by precautions such as running Platon and Mogul before the last cycle of least squares and critically evaluating CIF error messages. The session was an excellent reminder of the importance of vigilance in checking structures; not least in case your structure ends up being used in such presentations as an example of what not to do.

### Unpublished Data & Almighty Blunders
Chairs **Richard Morris and Luca Russo**

The meeting ended with this light-hearted but nevertheless very important session. **William Clegg** showed some of the reasons why crystal structures do not get published. "Not fit for purpose", poor quality or outright incorrectness are good reasons. Less good reasons include "too many results", more experiments to be done, a desire for secrecy including commercial/legal confidentiality, or rejection by editors/referees. **Simon Coles** demonstrated how the eCrystals model could be used as a new approach for gathering, sharing and publishing crystallographic data. The final speaker was **Colin Groom** who rounded the meeting off nicely with an amusing talk showing some of the errors he has encountered. Among them were 2,2'-bipyridyl given as biphenyl, S and P atoms swapped, too few or too many atoms, a CN group that should be CO, confusion between °C and K for temperature (the CIF default is K). Despite the widespread publicity about the danger of getting "Marshed", even in 2009 some 10% of structures reported in P1 should have had higher symmetry. Colin concluded by the describing the perils of different polymorphs particularly in the pharmaceutical industry.

The speakers at the Unpublished Data and Almighty Blunders session

**Helen Mason and Jonathan Foster**
**Durham University**

# Young Crystallographers' Meeting 12-13th April 2010

**Although at first sight Warwick University can appear to be somewhat like a hospital placed in a field, it proved to be a great location for the Young Crystallographers meeting, and the sunny weather and the ducks waddling all over campus gave the place a charming atmosphere.**

Andrew Bond

The meeting kicked off with an interesting plenary talk given by **Andrew Bond**, a passionate crystal engineer, who discussed how inconsistencies in the way that crystal structures are interpreted, and pressure to find novel features which would increase chances of publication, can lead to very misleading descriptions in the literature. He showed that automated analysis of crystal structures could provide a solution.

**Eloisa Angeles Tactay** gave the first 'Young Crystallographer' presentation on predicting the formation of hydrates of pharmaceutical compounds. She described her use of crystal structure prediction to generate a large number of potential structures for a compound, from which structures with voids suitable for accommodating water molecules could be identified.

Then **Jonathan Foster** talked about gelators, molecules which can reversibly assemble into supramolecular networks. He demonstrated that crystallisation of pharmaceutical compounds, such as carbamazepine, within these networks can modify the size, habit and even polymorphic form of the crystals obtained.

Next up was **Bryan Boyle** who is investigating fluorination of DNA components for potential cancer treatments. By preparing cocrystals of fluorinated nucleic acids he showed that fluorination does not disrupt base pairing, but that fluorine-fluorine interactions are often present in the structures, affecting the overall crystal packing.

The following talk was on another planet, literally. **Helen Maynard-Casely** presented the structure of methane phase A, a polymorph stable in the high pressure conditions found within the planets Uranus and Neptune. She showed that the structure has a novel packing arrangement, and that this arrangement can also be formed by the related compounds $CF_4$ and $CCl_4$.

**Mark Warren** then introduced his work on photo-induced linkage isomerism. He was able to follow the conversion of $NO_2$ ligands from N-bound to O-bound both crystallographically and spectroscopically, while varying the temperature to maximise conversion.

The final talk of the first session was given by **Duncan Sneddon** on the work he is doing to develop the generic data acquisition software at Diamond. He described the diffraction viewer tool that can display diffraction patterns from the many beamlines and be used to measure intensity profiles and d-spacings.

**Andrew Goodwin** started the second session with a plenary lecture on diffuse scattering and his work with pair distribution function techniques. Using 2-dimensional ice as a model, he demonstrated that while Bragg scattering gives us an average structure, diffuse scattering can give us information about the disorder in a system.

**Nick Funnell**'s following presentation added a whole extra dimension, thanks to some special 3D glasses. Nick described his work to understand the conductivity changes in Krogmann's salt under different conditions of temperature and pressure.

**Areej Abuhammad** talked about the crystal structure of arylamine N-acetyltransferase, an enzyme found in tuberculosis, that she has solved, and use of docking software to understand what molecules could act as inhibitors in the active site.

In a last minute change to the schedule, **Clare McMullin** stepped in and gave a presentation on flexibility in complexed phosphorus ligands. She described her use of molecular modelling to calculate energy surfaces for the conformation of these groups, and how these energy surfaces change when the ligands are attached to various metals.

**David Brown** then set the room alight with his talk on matchbOx, a software package that he has developed. He talked about how MatchbOx enables matching between molecular structures and substructures, which can be imported into the software as either cif files or smile strings.

Lastly, **poster presenters** were given a mere 30 seconds to sell their interesting findings to the group, followed by a more relaxed opportunity to discuss their work, over food and wine, during the poster session itself. The final highlight of a very successful day was a pint or two of 'duck soup' at one of the campus bars.

**Elspeth Garman** began day two with a plenary lecture that covered a wide range of topics including the function of the flu virus and how obtaining crystal structures enabled the development of the treatment Relenza, the importance of cooling crystals to 100K during analysis, identifying and quantifying metals in proteins with microPIXE and even how better biological crystals can be grown in space (just don't tell the Daily Star!).

The lecturers and chairs from the YCs' conference

**Craig Wales** talked about the polymorphism of paracetamol and that while form II has a clear advantage over form I in that it can be easily compressed into tablets, it is form I that crystallises from solution. However, Craig then went on to describe how he has been able to prepare the elusive form II from solution by crystallising paracetamol in the presence of carboxylic acids.

The paracetamol theme was continued by **Mark Eddleston**, who demonstrated that transmission electron microscopy can be used to identify the polymorphic form present in different samples of this compound. Mark also used this technique to characterise defects in crystals of the pharmaceutical compound theophylline and showed that the crystals fracture along these defects.

After much mention of diamond anvil pressure cells during earlier talks, **Christopher Woodall** finally gave us a detailed description of how they work. His presentation also focused on the crystallography of dithienylethenes, compounds which undergo a reversible ring closure / opening, making them potentially useful as molecular switches or in molecular memory.

**Vicky Fawcett** then talked about using neural networks to determine the important factors for controlling polymorphism. She is using the outcomes of a wide range of experimental crystallisations, along with an extensive list of molecular descriptors, to train and test the neural network and determine which of the conditions and molecular properties have an influence on polymorphism.

The final presenter to (hedge)hog the limelight was **Simon Parsons**, who gave a talk in memory of **Andy Parkin**. He showed the importance of free energy in understanding why a particular crystal structure is observed, and how phase transformations occur to reduce the free energy of a system. Reminding us of the terms that make up the free energy, G = U + pV – TS, Simon pointed out that at high pressure the pV term usually becomes dominant. To decrease the free energy under such conditions, a phase change that reduces the volume is often favoured, even at the expense of raising the internal energy U. Progress has been made in calculating U and S.

After a day and a half of fun talks and interesting crystallography another hugely successful YC meeting had come to an end.

**Mark Eddleston**
**University of Cambridge**


Biological Crystallography
S3-MICROpix
Rigaku
X-RAY DIFFRACTION
CSD X-Press
Early access to newly published structures



SOME OF THE


# E EXHIBITORS

# CSD User Discussion Forum, BCA Spring Meeting 2010, University of Warwick

**THE first CSD User Discussion Forum was held immediately following the BCA Spring Meeting. Although numbers were curtailed somewhat by the activity of Eyjafjallajokull, 20 or so CSD users and 7 CCDC staff members contributed to a lively and wide-ranging discussion.**

Several enhancements or additions to the CSD were suggested. These included addition of ADPs, a sub-categorisation of the type of twinning, the Flack parameter (when reported with an ESD), bond length ESDs and face indexing information. Storing reflection data was a popular request and raises the challenge of how the CCDC would obtain such data: Does the author directly deposit with the CCDC or should journals make such data mandatory? Many of the suggestions made are already part of the plans for the 'Next Generation CSD', currently being developed.

The possibility of the CSD containing additional information on the quality of the structure was discussed. The issue that users may inadvertently filter out interesting structures on the basis of a "quality indicator" was raised. Among many suggestions to judge quality was the inclusion of a "why was this structure done?" field in CIFs. This could be useful, as in some cases the aim of a crystal structure determination is simply to establish connectivities, whilst in other cases the purpose may be to provide accurate charge density data. This difference may affect the value of structures to users.

CCDC were asked if they were open to editing of the CSD by external users? Indeed the CCDC is developing plans to encourage users to indicate any errors they have found or express opinions on the structures they have looked at. Users asked whether CCDC was interested in being a primary publisher or undertaking formal responsibility for refereeing structures? Other organisations already do this well, but CCDC will shortly begin issuing all CSD entries with a DOI, both to allow more effective citation of structures and to encourage more structures, not destined for publication elsewhere, to be "published" in the CSD.

Suggestions were made on how CCDC should best advertise new features to the community. Publications utilising these will, of course, continue and new features may well be highlighted in different colours or in a pop-up dialogue box.

Crystal morphologies, use of best representative lists, graphics quality and production of publication quality images were all discussed.

It was an enjoyable, worthwhile and challenging event, with attendees commenting that "The Forum was a refreshingly open event", stating that "I wish more organisations were prepared to stand up in front of their users" and "It was a good opportunity to hear the thoughts of the varied ...panel and also the rest of the audience".

The CCDC would like to thank all users who attended and will certainly host similar forums in future, encouraging users to help shape the future of the CSD.

# Prizes

**IN** a fitting tribute to the high quality of so many presentations the number of prizes plus Honourable Mentions exceeded my ability to photograph all of the recipients. **John McGeehan** was the first winner, receiving the much-admired Blue John trophy for Biological Crystallography. Next, **Amber Thompson** was awarded the Chemical Crystallography Prize. **Andras Kallay** and **James Holcroft** received Honourable Mentions. **Alan Martin** won the CrystEngComm Prize, **Alexander Graham** the CCG Poster Prize, while further Honourable Mentions went to **Edward Bilbé, Peter Byrne, Kirsten Christensen** and **Helen Mason.** Two Young Crystallographers were chosen by the Industrial Group to give Prize Lectures, the excellence of which fully justified their selection: first **Mark Eddleston** and then **Jonathan Foster. Lisa Simmons** received the Physical Crystallography Prize. As usual, there was a very strong field for the PANalytical PCG Thesis Prize. This highly significant prize, which rewards an entire thesis rather than a single piece of work, was awarded to **Helen Maynard-Casely.** Some of Helen's research has taken us "out of this world", elucidating high-pressure phases of methane that may exist in planetary interiors. On a more light-hearted note, **Andras Kallay** won the prize for the Young Crystallographers' quiz. The Cruickshank Prize went to **Kirsten Christensen,** and the Rigaku Prize for best theme poster to **Vicky Fawcett**, with Honourable Mentions to **Matthew Mold, Jenny Parker** and **Brian McMahon**. Prize-giving concluded with the PANalytical IPod competition, won by **Sarah Barnett.**

PANalytical PCG Thesis Prize

# Prize Winners

IG YC Talk Prize

IG YC Talk Prize

Rigaku Theme Prize

Cruickshank Prize

CCG Prize

PCG Prize

BSG Prize

CrystEngComm Prize

# News from the Groups

## YCG Update

**SINCE the BCA Spring Meeting in Warwick, only a few days have passed and the impressions from the conference on "Data Matters" are still fresh on every mind. The Young Crystallographers Satellite Meeting opened the proceedings, a tradition there to stay for hopefully many years to come, and again the presenters excelled with the professional delivery of their research. The variety of topics was truly astonishing making the Satellite a very attractive event for all generations. I would like to thank all contributors for their efforts, speakers, poster presenters and organizers alike! The BCA Spring Meetings always provide the opportunity to not only learn about exciting science but also to meet new fellow researchers and exchange thoughts on crystallography. It is this networking that I probably enjoy the most and that I believe is so important for Young Crystallographers. The financial support the YC Satellite gets from the BCA and this year also from EPSRC, is hence so important and valuable.**

In order to keep the YCG membership informed of any relevant business, I would like to summarise the most important proceedings in the following few paragraphs.

At this years YCG AGM six committee members retired due to reaching the end of their term of office. These are: **Susanne Coles** (née Huth) – Chairman, **Suzanne Buttar** – Deputy Chairman, **Graham Findlay** – Secretary, **Alex Hamilton** – CCG Representative, **John Kaniuka** – IG Representative, **Helena Shepherd** – Ordinary Member. Nominations were received prior to the AGM for the three Officer positions, the CCG Rep and one Ordinary Member. All nominations were unopposed and the new YCG committee is as follows: re-elected into post, **Susanne Coles** – Chairman, **Duncan Sneddon** – Deputy Chairman, **Anna Stevenson** – Secretary, **Arefeh Seyedarabi** – BSG Rep, **Peter Byrne** – CCG Rep, **Claire Murray** – IG Rep, **Samantha Callear** – PCG Rep, **William Lewis** and **Soshichiro Nagano**– Ordinary Members. However, the post of Webmaster could not be filled at the AGM and the committee is currently seeking possibilities to fill this vacancy. The details of the new Webmaster will be made available on the YCG website (*http://ycg.crystallography.org.uk*).

At present the YCG committee is engaged in defining the criteria for the Parkin Lecture, the first YCG Prize Lecture, created in recognition of the contributions of the late Dr **Andy Parkin** to the YCG. This year saw the inaugural Parkin Lecture given by Prof **Simon Parsons** and in future the lecture will be awarded to a Young Crystallographer. A call for nominations together with the criteria will be made in due course. Also on the agenda for committee activities is the securing of funds for the YC Satellite Meetings from sources outside the BCA. The BCA President, **Elspeth Garman**, set the scene this year with securing the contribution from EPSRC and it is hoped that other bodies will be equally approachable and supportive. If any YCG member would like to get involved in this process then please contact one of the committee members via the YCG website.

A final point I would like to raise is that of recruiting YCG members. If you are a student or within 5 years of having graduated from a degree then you are eligible for YCG membership irrespective of your interest group. You can join the YCG by ticking the YCG box on either the hardcopy or online membership form of the BCA. If your BCA membership is current then you can simply join by changing your membership details on the BCA website (*http://crystallography.org.uk*). And most importantly spread the news: If you know any crystallographer that should be a BCA YCG member but is not yet, then tell them all about it and make sure they join. In addition to the website the YCG can be found on facebook and on the X-Rayman xforum.

**Susanne Coles**
**YCG Chairman**

## Take Up The Challenge!

**IN November 2008 the EPSRC set up a process to develop "Grand Challenge Networks" to bring together groups of scientists from across the disciplines to discuss what the scientific Grand Challenges for the next 20 to 50 years would be and how they might be met. Since then, through a discussion process, three Challenge areas centred around Chemistry and Chemical Engineering, but interfacing with Biology, Materials Science and Physics have been identified, and in April this year three two-year network programmes started. The three Networks are:**

- Utilising $CO_2$ in synthesis and transforming the chemical industry
- Dial-a-molecule. 100% efficient synthesis
- Directed assembly of extended structures with targeted properties (DAESTP).

The third Network, DAESTP, may be of particular interest to readers of Crystallography News since it targets the solid state and its vision is to find ways to control the assembly of matter with sufficient certainty and precision to allow preparation of materials and molecular assemblies with far more sophisticated and tuneable properties and functions than are currently accessible.

The objectives of the Network over the next two years are:

1. To form new research communities that extend beyond Chemistry and Chemical Engineering, and which involve academia, industry and users.
2. Identify research priorities and the major barriers associated with these.
3. The development of community driven research agendas resulting in highly transformative research with long term scientific impact.
4. To generate a clear road map which identifies priorities, barriers and intermediate targets that will justify the Grand Challenge in an inclusive manner.
5. To address the major societal and economic issues associated with the Grand Challenge and demonstrate the positive impact that progress in the challenge will have on these areas.

The initial focus of the Network will be to "design" a condensed phase material with a desired function and then to "engineer" that material. With this in mind five focus areas have been proposed and, starting in the Autumn, a series of workshops will be organised so that the broad community can input into the development of the Network leading to the Challenge being met. The five focus areas are:

1. Controlling the assembly of designed molecular frameworks and hybrid materials with targeted properties.
2. Controlling nucleation and crystallisation processes leading to the design of physical forms of pharmaceuticals with pre-targeted properties.
3. Controlling the molecular self-assembly in biological and biomimetic systems.
4. Controlling surface-based molecular self-assembly for applications in interface science.
5. Developing self-optimised chemical systems through self-evolution.

A working group of 10 members, led by Paul Raithby, the past president of the BCA, has been assembled to coordinate the Network. Over the Summer this "core" team will be expanded to 15 members and an international advisory board will also be set up. The present team, covering aspects of Chemistry, Chemical Engineering, Materials Science and Biology, is:

- Prof Paul Raithby, University of Bath
- Dr Harris Makatsoris, Brunel University
- Prof Neil Hunter, University of Sheffield
- Prof George Jackson, Imperial College
- Prof Sally Price, UCL
- Prof Kevin Roberts, University of Leeds
- Prof Matthew Rosseinsky, University of Liverpool
- Prof Mike Ward, University of Sheffield
- Prof Chick Wilson, University of Glasgow
- Dr Sophia Yaliraki, Imperial College, London

The team will be busy over the next few months setting up an interactive website for the Network, organising an inaugural meeting, that will take place at some point over the Summer, setting up the themed workshops and developing an outreach programme.
The views of the community are vital to the success of the Network so that a "roadshow" programme will be set up where members of the team visit Universities and Industrial Centres to talk about the Grand Challenge and collect the views from the community. These visits are paid for by the Network so that the speakers come free! Please do invite the team members – initial contact can be made through Paul Raithby (p.r.raithby@bath.ac.uk).

Over the next two years the Network team wishes to construct a Roadmap for the development of directed assembly and correlate the structures with the material properties. Input from the community is essential if the Network is to be successful. The questions to which your answers are needed include:

- What are the challenging issues within the directed assembly area?
- What assembly processes would you like to be able to carry out that you cannot do now?
- What are the important properties that are needed in future materials?

To finishing on a very positive note at the same time as announcing the start of the DAESTP Network the EPSRC announced that "Directed assembly" would become a "signpost area". This means that research funds should be targeted at this area over the next couple of years, so it is a good time to join the Network and build interdisciplinary collaborations!

Paul Raithby, the Network leader, will be happy to provide additional information sand answer any questions that you have. He will also be happy to add you to the Network e-mailing list so that you will automatically be kept up to date with developments. He may be contacted via **p.r.raithby@bath.ac.uk**.

# Report on William (Bill) Clegg's "Retirement" Symposium

**IT must be at least two years ago that I first heard the rumour that Bill was considering retiring to join the cloth. My initial response was the same as everyone else: incredulity, "He's way too young!" However, last summer a formal announcement was made and his position at Newcastle was advertised. It turns out that Bill is really only retiring from the "bits he doesn't like" (i.e. the administration) and will still be involved in UK crystallography and research. So, in celebration, Bill's "Retirement" Symposium was held on a windy Thursday in Newcastle, in the middle of March.**

After coffee and cakes, the first session was introduced by **Mike Hursthouse** (Southampton). Reflecting Bill's particular interest in synchrotron radiation and involvement in Station 9.8 at Daresbury, the symposium was opened by **Paul Raithby** (Bath) talking about the impact synchrotron radiation has had on his research into linkage isomerism as well as the effect it has had on chemical crystallography as a whole. This was followed by **Steve Liddle** (Nottingham) discussing the difficulties associated with the extremes of lithium and uranium, which led into an interesting discussion of the merits of copper radiation in laboratory instrumentation. **Gary Nichol** (Arizona) closed the morning session with his view of synchrotron radiation in the USA and the challenges associated with getting his colleagues to accept that getting access was really worth it.

After an excellent lunch and much discussion concerning the unexpected outcome of National Service Tender, **John Helliwell** (Manchester) opened the afternoon session by outlining the extensive contribution Bill has made to editorial work for the IUCr, particularly as a founding Joint Section Editor of Acta Crystallographica Section E from 2000 to 2008. Following Bill's Personal Reflections (including a few additional interesting photos), **Simon Teat** added to the comparison of life on the other side of the pond with an interesting perspective on life as a beamline scientist at the ALS.
One of the great pleasures of attending the symposium was the wide range of speakers, reflecting the chemistry aspects of Bill's extensive career, many of whom I was not familiar with. **Rab Mulvey** (Strathclyde) was one such, who had previously worked with **Ken Wade** in Durham, and returned to the North East to present some of the work carried out during his long-standing collaboration with Bill into lithium chemistry and some of the fascinating structures the alkali metals can form. The meeting was closed by **Dietmar Stalke** (Göttingen) who successfully overpowered the best delaying tactics of planes, trains and automobiles to give us an insight into the bonding information obtainable from charge density.

Bill's "Retirement" symposium amply demonstrated his extensive contribution to chemical crystallography from his work at Göttingen where he achieved his "Habilitation", to the SRS at Daresbury, the National Synchrotron Service, Acta Crystallographica Section E, and his involvement in the Intensive Teaching School, all of which are reflected in his recent honorary membership of the BCA. The range of speakers and members of the audience clearly showed how widely respected Bill is in both crystallography and chemistry as a whole. Retirements are usually sad occasions for those of us left behind, but hopefully in this case the loss to administration will be a gain to crystallography.

**Amber Thompson**
**University of Oxford**

# CCG Autumn Meeting Wednesday 18th November 2009

**THE first CSD User Discussion Forum was held immediately following the BCA Spring Meeting. Although numbers were curtailed somewhat by the activity of Eyjafjallajokull, 20 or so CSD users and 7 CCDC staff members contributed to a lively and wide-ranging discussion.**

The CCG Autumn meeting 2009 entitled 'Methods Complementary to Crystallography' held in Oxford was highly successful thanks in part to the excellent local organisation of **Amber Thompson** and the kind sponsorship of Rigaku to whom we are very grateful.

The Autumn Meeting provided attendees with the chance to learn about a variety of techniques, many solid-state, that can be used to support crystallographic analyses. The meeting kicked off with **Kenneth Harris** giving us an insight into the use of solid state NMR to monitor crystallisation in-situ, with factors such as solvent deuteration affecting whether the initial polymorph formed in the crystallisation of glycine is metastable or the thermodynamically stable polymorph.

**Stewart Parker** then introduced neutron vibrational spectroscopy, which is complementary to more traditional Raman and infrared spectroscopy and has wide-ranging potential applications including the ability to study hydrogen storage using inelastic neutron scattering. The afternoon session began with **Moniek Tromp** explaining the potential of X-ray Absorption Spectroscopy to provide in-situ data, in a variety of sample environments, from amorphous samples inaccessible to crystallography.

This was followed by **Katharina Fucke** providing us with an overview of some of her PhD work, which demonstrated the information that crystallographers can gain from thermal analyses such as DSC and hot stage microscopy. The final session of the afternoon started with **Louis Farrugia** who discussed the type of information that is available from charge density analyses, and problems associated with obtaining a good charge density dataset before providing an example of charge density analyses of transition metal bonding. The final speaker of the day was **Matthew Tucker** who discussed the pair distribution function and the fact that local effects can have a major influence on structural properties despite the fact that the average structure does not change much. Overall, thanks to excellent speakers this meeting provided a fascinating and informative range of talks which provided attendees with a chance to gain insights into techniques which are complementary to normal crystallographic analyses.

**Hazel Sparkes**
**CCG Deputy Chair.**

# Crystallography Reviews discount still available for BCA members

**ALTHOUGH BCA members no longer receive the special "BCA Issue" of Crystallography Reviews by default, there is no need to miss out! Members are still entitled to the entire volume (Issues 1-4) of Crystallography Reviews for just £25 by taking up the greatly reduced 'Members' Subscription' rate. Please go to www.tandf.co.uk/journals/gcry and click on News & Offers for more details.**

In the picture taken at the recent BCA Spring Meeting the most recent issues are being displayed by **Katherine Eve**, Publishing Editor, Physical Sciences Chemistry at Taylor and Francis, and **Moreton Moore**, one of the Editors of Crystallography Reviews. Issue 2 of Volume 16 (2010) is the BCA Young Crystallographers' Special Issue. If I had browsed through this issue without looking at the authors' names, I would have expected that the authoritative coverage and clear writing must have come from long-established leaders rather than from authors who are relatively new to the field. The wisdom they have acquired, allied to their obvious enthusiasm, bodes well for the future.

**Carl Schwalbe**

# BCA Financial Summary

## The British Crystallographic Association
## Summary Financial Statements for year ended 31 December 2009

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

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

**INCOMING RESOURCES:**

| | 2009 | 2008 |
|---|---|---|
| Grants and sponsorship | 5,800 | 6,700 |
| Donations | 8,067 | 6,341 |
| Annual conference (5) | 99,572 | 93,431 |
| Meetings of groups | 21,254 | 9,406 |
| Crystallography News | 18,710 | 26,945 |
| Membership Subscriptions | 18,640 | 25,503 |
| Net income from trading | - | 15 |
| Investment income | 3,981 | 3,090 |
| Interest received | 851 | 5,243 |
| IUCr bursary | - | - |
| **TOTAL INCOME** | **176,875** | **176,674** |

**EXPENSES:**

| | 2009 | 2008 |
|---|---|---|
| Direct charitable expenditure (2) | 145,681 | 159,029 |
| Trading stock written off | 493 | - |
| Management and administration (3) | 34,233 | 31,675 |
| **TOTAL EXPENDITURE** | **180,407** | **190,704** |

| | 2009 | 2008 |
|---|---|---|
| **NET (EXPENDITURE):** | (3,532) | (14,030) |
| Unrealised gains (losses) on investment assets | 4,942 | (9,744) |
| **NET MOVEMENT IN FUNDS** | **1,410** | **(23,774)** |
| Balances brought forward at 1 January | 198,781 | 222,555 |
| Balances carried forward at 31 December | 200,191 | 198,781 |

**ASSETS:**

| **Fixed assets** | 2009 | 2008 |
|---|---|---|
| Tangible assets | 5 | 5 |
| Investments | 59,555 | 50,848 |
| **Total** | **59,560** | **50,853** |
| **Current assets** | | |
| Stock | - | 493 |
| Debtors | 5,446 | 1,758 |
| Cash at Bank | 154,277 | 169,491 |
| **Total** | **159,723** | **171,742** |
| **LIABILITIES:** amounts falling due within one year | (18,212) | (22,689) |
| **LIABILITIES:** amounts falling due after one year | (880) | (1,125) |
| **NET ASSETS** | **200,191** | **198,781** |

**INCOME FUNDS:**

| | 2009 | 2008 |
|---|---|---|
| Restricted funds (4) | 101,878 | 99,459 |
| Unrestricted funds (4) | 98,313 | 99,322 |
| **Total** | **200,191** | **198,781** |

**NOTES TO THE SUMMARY FINANCIAL STATEMENTS**

**1. ACCOUNTING POLICIES.**
These summary statements are based on financial statements which have been prepared under the historical cost convention, with the exception of investments which are included at market value. The financial statements have been prepared in accordance with the Statement of Recommended Practice, "Accounting and Reporting by Charities" published in March 2005 and applicable accounting standards.

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

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

**2. DIRECT CHARITABLE EXPENDITURE**

| | 2009 | 2008 |
|---|---|---|
| Subscription to International bodies | 9,875 | 6,912 |
| Annual conference (5) | 91,760 | 113,405 |
| Meetings of groups | 5,139 | 8,994 |
| Crystallography News + Newsletters | 18,129 | 22,236 |
| Course fees and accommodation | 15,558 | - |
| Grants and sponsorship | 720 | 2,982 |
| Awards & bursaries | 2,250 | - |
| Arnold Beevers Bursary Fund | 2,250 | 4,500 |
| **Total** | **145,681** | **159,029** |

**3. GOVERNANCE**

| | 2009 | 2008 |
|---|---|---|
| Administration fee | 18,167 | 18,021 |
| Administration expenses | 9,017 | 8,230 |
| Accounting fee | 4,113 | 3,967 |
| Insurance | 432 | 392 |
| Bank and security charges | 664 | 118 |
| Special Interest Group Administration | 637 | - |
| Council members' expenses | 1,203 | 947 |
| Depreciation- tangible fixed assets | - | - |
| **Total** | **34,233** | **31,675** |

**The full BCA accounts for 2009 are available as an e-mail attached file from the BCA administrative office.**

# The British Crystallographic Association
# Summary Financial Statements for year ended 31 December 2009

| 4. STATEMENT OF FUNDS | Brought Forward | Incoming Resources | Resources Expended | Gains (Losses) | Carried Forward |
|---|---|---|---|---|---|
| **UNRESTRICTED FUNDS** | | | | | |
| General Fund | **99,322** | **147,433** | **(153,384)** | **4,942** | **98,313** |
| **RESTRICTED FUNDS** | | | | | |
| IUCr bursary fund | 30,231 | - | - | - | 30,231 |
| Arnold Beevers bursary fund | 13,023 | 835 | (2,250) | | 11,608 |
| Dorothy Hodgkin prize fund | 8,080 | 562 | - | - | 8,642 |
| Chemical group teaching school | 17,650 | 18,518 | (18,159) | - | 18,009 |
| Chemical group fund | 2,192 | 2,912 | (1,313) | - | 3,791 |
| Industrial group fund | 12,483 | 1,444 | (2,568) | - | 11,359 |
| Biological Structures group fund | 15,800 | 3,171 | (2,483) | - | 16,488 |
| Durward Cruickshank fund | - | 2,000 | (250) | - | 1,750 |
| **Subtotal** | **99,459** | **29,442** | **(27,023)** | **-** | **101,878** |
| **Total of Funds** | **198,781** | **176,875** | **(180,407)** | **4,942** | **200,191** |

| 5. Spring Meeting 2009 Loughborough University | |
|---|---|
| **INCOME** | |
| Registration | 82,723 |
| Exhibition | 16,244 |
| Bursaries | 605 |
| **Total** | **99,572** |
| **EXPENDITURE** | |
| Accommodation & Meals | 29,049 |
| Facilities | 13,630 |
| Catering | 11,190 |
| Social Event | 5,834 |
| BCA Speakers Expenses | 1,941 |
| Refunds | 480 |
| Abstract Book | 5,233 |
| NNE Fee | 15,387 |
| Administration | 4,150 |
| Printing & Stationery | 2,738 |
| Young Crystallographers | 2,128 |
| **Total** | **91,760** |
| **TOTAL INCOME** | **99,572** |
| **TOTAL EXPENDITURE** | **91,760** |
| **MEETING SURPLUS** | **7,812** |

**All the transactions for the 2009 Spring Meeting were made through the BCA account, and consequently these detailed meeting accounts are reported as part of the BCA financial report**

**Treasurer's Report 2009**
This was a busy year for the BCA and its constituent groups. Overall we had a surplus of £1,410 during the year ended 31 December 2009, and the Association has no material guarantees or commitments which could affect its future solvency.

The general fund had a deficit of £1,009 after an increase of £4,942 in the value of the investments, but the reserve funds operated by the Groups and the School had an overall surplus of £2,419. The income from our investments brought in £4,832 this year.

The Association closed its bank accounts with HSBC in December. The major risks to which the Association is exposed are with regard to the cost of the Spring Meeting and its effects on the Association's major reserves. To mitigate those risks the Association has all its investments placed with an independent professional management company. Our investment portfolio was valued at £59,555. The Council's review of the reserves indicates that we should always be striving to generate more income to enable us to plan and encourage even higher levels of educational and scientific activity.

The Young Crystallographers' symposium before the Spring Meeting in Loughborough was well attended and appreciated, and sponsors were generous in their support too. Six Arnold Beevers bursaries were awarded to attendees at the Spring Meeting, and another four were awarded by commercial sponsors. We awarded a further three bursaries totalling £750 from the Arnold Beevers Bursary Fund to 3 people attending crystallographic meetings during the Summer. The Durward Cruickshank prize was awarded for the first time this year. The bursary fund for the IUCr was not required by the organisers of the meeting in Osaka, so the monies are accumulating in the reserve fund; they have been offered to the IUCr Congress in Madrid in 2011 but have not yet been accepted .

Crystallography News has made a small surplus this year from an income of £18,710. The BCA thanks its advertisers and sponsors who generously support our activities. There was a welcome surplus from the Spring Meeting.

Subscriptions to international bodies were £9,875, covering our membership of the IUCr at the five-vote level and two years' subscription to the European Crystallographic Association (covering both 2008 and 2009). Administration costs, including expenses, are £27,184. The online payment facility for Group meetings has been utilised by IG this year. The expertise and hard work of Northern Networking Events Ltd is very much appreciated.

Membership income is down by £6,863 this year; the reason for this has not been identified yet. Roughly half the members who pay by standing order have not amended their payment since the increase in dues; the option to pay this way will not be available in future. Nothing was received from the Inland Revenue in Gift Aid this year but this should amount to about £4,000 in 2010.

I would like to thank everyone who has helped me in my role this year, in particular the other Officers, members of Council, Gill, David and the team at Northern Networking Events, and our accountants Bob Young and Ray Philpott at The Young Company for all their help throughout the year.

**Harry Powell** **Treasurer**

**The full BCA accounts for 2009 are available as an e-mail attached file from the BCA administrative office.**

# Before Computers

## Crystallography Before Computers: How We Summed Our Fourier Series

**BEFORE computers became generally available to crystallographers after the Second World War, Fourier electron density calculations had to be carried out using desk adding machines (though some brave souls found that they could add mentally faster than they could enter numbers into the machines). In any case, evaluating the trigonometrical functions involved was very tedious until Arnold Beevers and Henry Lipson showed how the three-dimensional series for a 3D electron density distribution, or a two-dimensional series for an electron density projection, could be reduced to a sequence of one-dimensional series for evaluation with the aid of Beevers-Lipson strips. Their paper explaining the theory and describing the strips was published in the *Philosophical Magazine*, volume 17 (1934) 855-859. However, the practical sequence of operations in using the strips has hardly ever been described, apart from in a very informative article by Bob Gould in the December 1998 issue of *Crystallography News*. Even this omits one or two practical points that I felt should be mentioned before there were none of us left who actually used these strips. Since Bob's article is probably no longer available to most crystallographers, the whole method of calculation will be described.**

The essence of the method is the reduction of the standard formulae for electron density to separate products of cosine and sine terms. Then the strips give the values of these trigonometrical functions at regular intervals along one crystallographic direction, originally at 1/60th intervals but, in later boxes of strips, 1/60th intervals on one side of each strip and at the intervening 1/120ths on the other side (which could be ignored if 1/60ths provided sufficient resolution.). They thus obviated the need to look up a large number of sine and cosine values in tables. To allow a whole group of strips to be turned over at once, I arranged them between two sheets of glass hinged together with cellotape (figure 1).

The strips are in two hopper-shaped boxes, one giving values of $F\cos 2\pi(hX)$ (figure 2) and the other $F'\sin 2\pi(hX)$, where $F$ and $F'$ represent the amplitudes of the cosine and sine waves, respectively, h indicates the frequency of the wave and $X$ the distance along the wave in 1/60ths or 1/120ths of the unit cell length. The sum of the $F\cos$ or $F'\sin$ numbers on each strip is also noted in brackets (see figure 3) for the purpose of checking the arithmetic when the values on several strips are summed. The box is divided into sections, each corresponding to a given value of the frequency $h$, and the strips within each section have amplitudes –99 to +99, supplemented by –900, –800…–100 and + 100, +200, …..+900 (so for amplitudes between 100 and 999, two strips must be withdrawn from the same $h$ section). The hopper shaped boxes allow the strips to lean towards or away from the operator, making it easier to select the required strips and to save the places

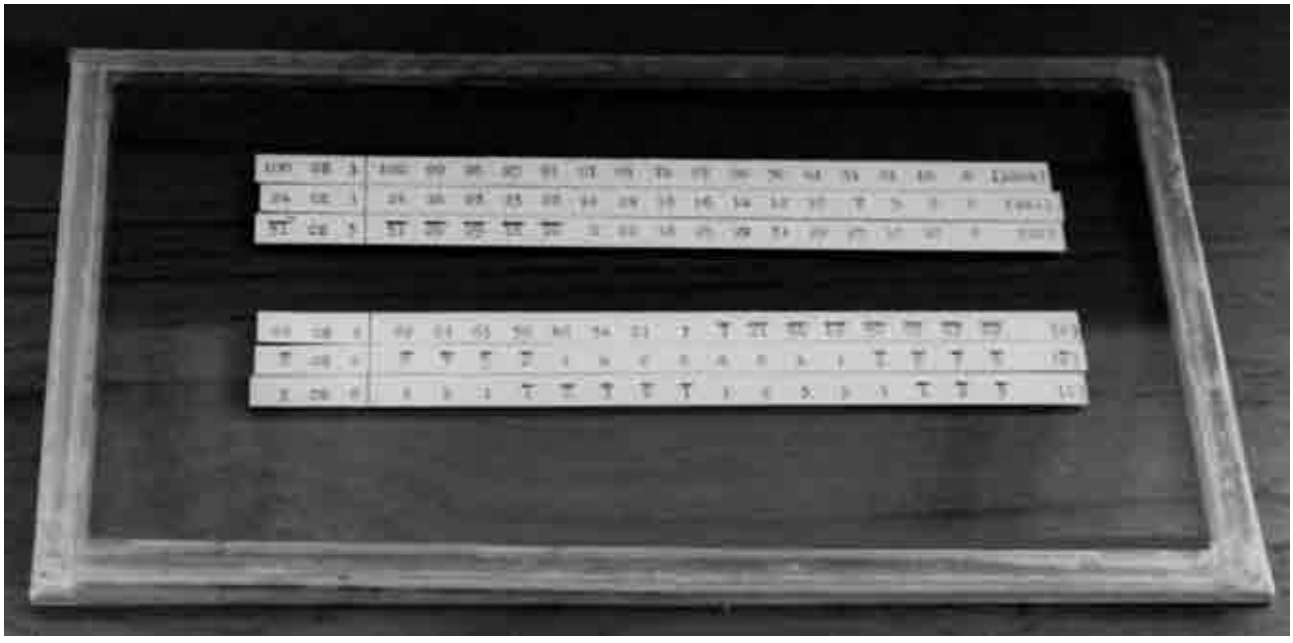

figure 1

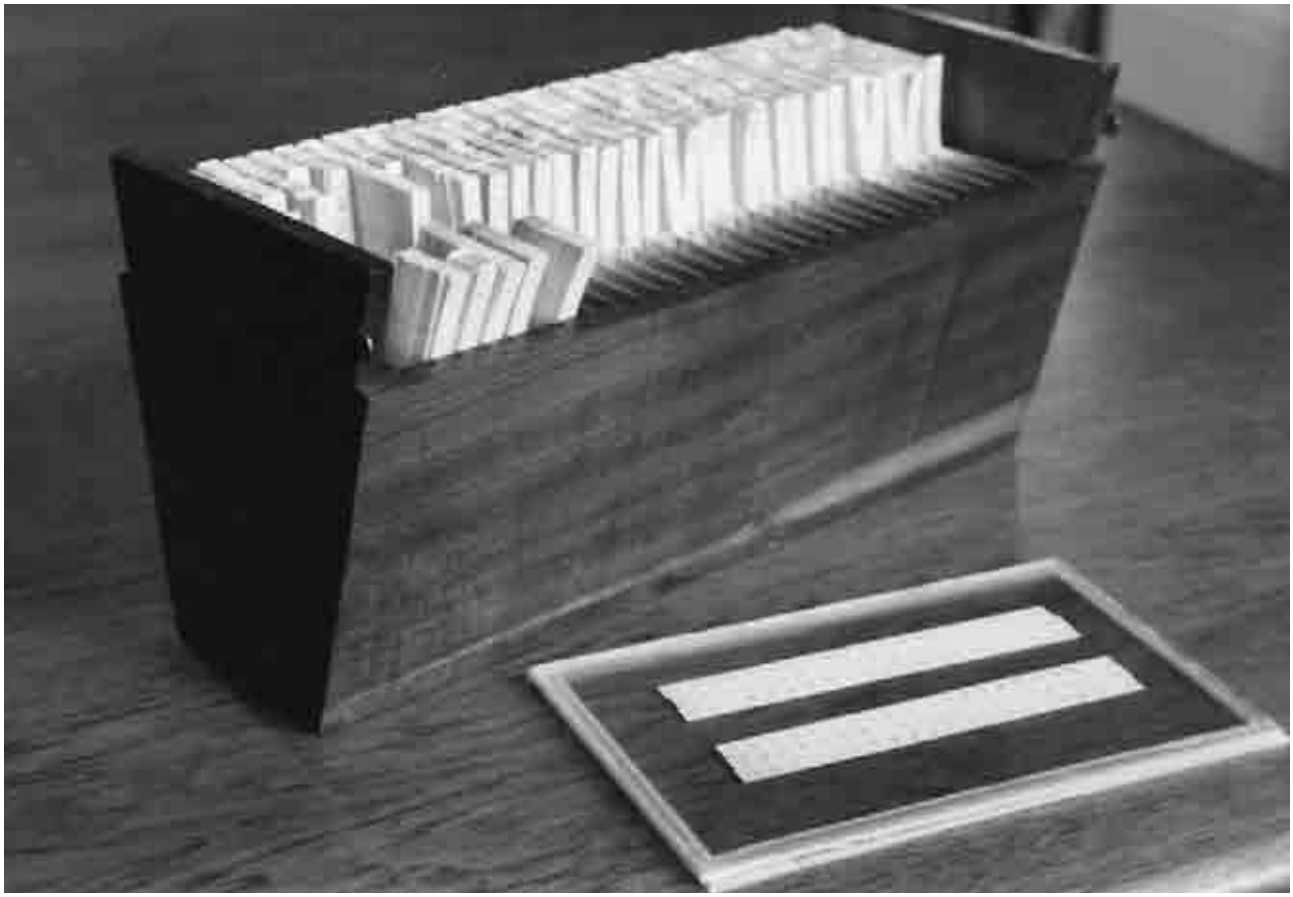

figure 2

of withdrawn strips for replacement. The frequencies range from 0 to 30 and the distances along each wave range from 0 to 15/60ths of the unit cell dimension, corresponding to a quarter of a revolution ($2\pi/4$) in angular terms. This distance range often needs to be extended to 30/60ths ($2\pi/2$) which is done by recognising that, for cosines of even frequency *h*, the values from 16/60ths to 30/60ths are a reflection of the values from 14/60ths down to 0/60ths and, for odd *h*, the cosines are a similar reflection but with a change of sign. For sine values, the odd *h* values reflect with no change of sign and the even *h* values change sign.

These complications, and the way they affect the calculation procedure are best illustrated by a particular hypothetical example in two dimensions, corresponding to generating an electron density map in projection along a cell axis. In the plane group p2, the electron density expression simplifies to:

$$\rho = \text{constant} \left[ \Sigma_h \Sigma_k \left[ (F\cos 2\pi(hX)\cos 2\pi(kY) - F'\sin 2\pi(hX)\sin 2\pi(kY) \right] \right]$$

where $F = (F_{hk} + F_{-hk})$ and $F' = (F_{hk} - F_{-hk})$. These combinations need only be made for half of the reciprocal lattice, since $F_{-h-k} = F_{hk}$ and $F_{h-k} = F_{-hk}$. In order to account for a multiplicity factor not shown in the above equation when including axial reflections in the summation, $F_{h0}$ and $F_{0k}$ must first be divided by 2.

The first stage, therefore, is to prepare a table of *F* values for the various values of *h* and *k* to use with the cosine strips and a corresponding table of F′ values to use with the sine strips. A decision must then be made as to whether to calculate first $\Sigma_h F\cos 2\pi(hX)$ for the various 1/60ths of *X* at each value of *k* or to calculate $\Sigma_k F\cos 2\pi(kY)$ for the various 1/60ths of *Y* at each value of *h*. The choice is made on the basis of which of these will result in the smallest number of strips to sum (the smaller the number of the *h* or *k* frequencies to calculate for, or the smaller the number of *X* or *Y* points at which to do each summation) in the subsequent second stage calculations. In the present hypothetical example, we decide to calculate $\Sigma_h F\cos 2\pi(hX)$ for columns of constant k first and for rows of constant *X* second.

Suppose the $k = 0$ row has *F* values on an arbitrary scale 124, 69, -31, -6, 9, 3 for h = 1 to 6. (Absolute scale and

Figure 3. Beevers-Lipson strips corresponding to *F* values in a hypothetical *k* = 0 column, ready for entry into a desk adding machine, as described in the text. CE indicates cosine values for even 1/120th intervals of the cell length (i.e. at 1/60ths).. The cosines for the odd 1/120ths are on the reverse and, if the strips are sandwiched between two pieces of glass, they are read, already in the correct arrangement, by turning over the glass sandwich.

| *F* cos *h* ↓ ↓ ↓ | *F*cos2π(*hX*) at *X* = 0/60 | 1/60 | 2/60 | ……etc. | ……15/60 | (check total) |
|---|---|---|---|---|---|---|
| 100 CE 1 | 100 | 99 | 98 | 95 | 91 | 87 | 81 | 74 | 67 | 59 | 50 | 41 | 31 | 21 | 10 | 0 | (1004) |
| 24 CE 1 | 24 | 24 | 23 | 23 | 22 | 21 | 19 | 18 | 16 | 14 | 12 | 10 | 7 | 5 | 3 | 0 | (241) |
| $\overline{31}$ CE 3 | $\overline{31}$ | $\overline{29}$ | $\overline{25}$ | $\overline{18}$ | $\overline{10}$ | 0 | 10 | 18 | 25 | 29 | 31 | 29 | 25 | 18 | 10 | 0 | (82) |
| sub-total, odd *h* | 93 | 94 | 96 | 100 | 103 | 108 | 110 | 110 | 108 | 102 | 93 | 80 | 63 | 44 | 23 | 0 | (1327) |
| 69 CE 2 | 69 | 67 | 63 | 56 | 46 | 34 | 21 | 7 | $\overline{7}$ | $\overline{21}$ | $\overline{34}$ | $\overline{46}$ | $\overline{56}$ | $\overline{63}$ | $\overline{67}$ | $\overline{69}$ | (0) |
| $\overline{6}$ CE 4 | 6 | $\overline{5}$ | $\overline{4}$ | $\overline{2}$ | $\overline{1}$ | 3 | 5 | 6 | 6 | 5 | 3 | 1 | $\overline{2}$ | $\overline{4}$ | $\overline{5}$ | $\overline{6}$ | $\overline{(4)}$ |
| 3 CE 6 | 3 | 2 | 1 | $\overline{1}$ | $\overline{2}$ | $\overline{3}$ | $\overline{2}$ | $\overline{1}$ | 1 | 2 | 3 | 2 | 1 | $\overline{1}$ | $\overline{2}$ | $\overline{3}$ | (0) |
| sub-total, odd+even *h* | 159 | 158 | 156 | 153 | 148 | 142 | 134 | 122 | 108 | 88 | 65 | 37 | 6 | $\overline{24}$ | $\overline{51}$ | $\overline{78}$ | (1323) |
| (odd+even) - odd - odd | $\overline{27}$ | $\overline{30}$ | $\overline{36}$ | $\overline{47}$ | $\overline{58}$ | $\overline{74}$ | $\overline{86}$ | $\overline{98}$ | $\overline{108}$ | $\overline{116}$ | $\overline{121}$ | $\overline{123}$ | $\overline{120}$ | $\overline{112}$ | $\overline{97}$ | $\overline{78}$ | $\overline{(1331)}$ |

addition of an $F_{000}$ value was often only introduced at the point of calculating at which arbitrary-scale ρ values to draw the contours on the final electron density map.) These *F* values determine which strips are to be withdrawn from the box of cosine strips so that the figures on them can be summed for each value of *X* (figure 3). Since the cosine values for odd values of h from *X* = 16 to 30 1/60ths are the negative of the values from 14/60 read backwards to 0/60, it is most convenient to arrange the corresponding strips above those for even h values which have no change in sign in obtaining the 16 to 30 1/60ths figures, as in the illustration. Note that the *F* value 124 has to be represented by two strips from the same section of the box, one for *F* = 100 and the other for *F* = 24. A bar over a number of course represents a negative number.

The summations for each value of *X* and the check totals in brackets can be carried out mentally but were usually done with the aid of a mechanical or electrical adding machine. I used an electrical dollar accounting machine (one for adding sterling would have had the complication of pounds, shillings and pence) that printed a paper record of every number and operation. It was most convenient, therefore, to obtain a printed subtotal of all the *F*cos values for odd *h*, then continue adding those for even h to obtain the subtotal for both odd and even *h* values for *X* = 0/60 to 15/60. Then finally subtract from this the odd h subtotal twice, to obtain the (even – odd) totals for *X* = 16/60 to 30/60. Repeating this for each value of k allows a table to be constructed of the 31 $\Sigma_h F\cos 2\pi(hX)$ values for each *k* value. Summation of the subtotals over all the *X* values should equal the corresponding subtotals of the check totals in brackets.

A similar table of the 31 $\Sigma_h F'\sin 2\pi(hX)$ values for each *X* value and for each value of *k* is then obtained by summing the numbers on sine strips with *F*′ values as the amplitudes and *h* values as the frequencies. This time the even *h* strips are summed first because they are the ones that change sign when extending the 0 to 15 1/60th calculations to 16 to 30 1/60ths of *X* by calculating the differences for odd – even *h*.

The next stage in the calculation uses the $\Sigma_h F\cos 2\pi(hX)$ values as the amplitudes in the selection of cosine strips for one value of $X$ at a time, for the different values of the frequency $k$. The successive numbers on the strips summed at each $X$ value give $\Sigma_h\Sigma_k F\cos 2\pi(hX)\cos 2\pi(kY)$ at the 31 1/60th values of $Y$. Again, odd and even $k$ strips are subtotalled separately to obtain first the cosine contribution to $\rho$ values from $Y$ = 0/60 to 15/60 and then from $Y$ = 16/60 to 30/60 by sign change. This completes the calculation of the contributions of cosine terms and they are listed in a 31 by 31 table of $X$ versus $Y$, preferably leaving alternate lines blank to receive later the sine contributions.

These sine contributions to $\rho$ are found in a second sine stage, similar to the second cosine stage. Strips are withdrawn for each of the 31 values of $X$ at a time, using as amplitudes at each X the $\Sigma_h F'\sin 2\pi(hX)$ found in the first sine stage, the values of $k$ being the frequencies.

As in the first sine stage, the even $k$ strips are summed first, since these are the ones that change sign in the range beyond 15/60ths, and the odd $k$ strips are added after. At each of the 31 1/60th values of $X$, the totals now give the value of $\Sigma_h\Sigma_k F'\sin 2\pi(hX)\sin 2\pi(kY)$ for 31 values of $Y$. These are then listed in either a second 31 by 31 table of $X$ versus $Y$ or, preferably, adjacent to the cosine terms in the same table as before. All that remains, to obtain the projected electron density map, is then to subtract the figure for each sine contribution from that for the cosine contribution at each $XY$ point and to draw contours at appropriate values of the resulting arbitrary scale $\rho$ values, calculated to show electron densities on an absolute scale. In spite of the simple nature of the operations when using Beevers-Lipson strips, it does not take much imagination to realise that a typical electron density projection would often take several days to compute.

**Stephen C. Wallwork**

# March Puzzle Answers

The winning answer was submitted by Jim Trotter: 10 lights on. It can be stated immediately that all the lights designated by prime numbers n between 2 and 100 will be "off" since only the first frog and the n-th frog will have jumped on their switches. Jim's reasoning continues:

think of the factors for each of the numbers, e.g. 12 = 1x12, 2x6, 3x4 (these occur in pairs, and hence these switches will be hit an even number of times, and so end up "off"), except when the number is a perfect square, e.g. 16 = 1x16, 2x8, 4 (squared), so those will be on (i.e.1, 4, 9, 16, 25, 36, 49, 64, 81, 100).

Jim adds a P.S. The instructions were a little unclear as to what "50 and 100, etc" meant. I have assumed that frog 51 hit only switch 51 etc.

# Meetings of interest

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

**21-24 June 2010**

IWPCPS12. Twelfth International Workshop on Physical Characterization of Pharmaceutical Solids, Lille, France.

**http://www.assainternational.com/workshops/iwpcps_12/iwpcps_12.cfm**

**21 June - 2 July 2010**

MathCryst Summer Schools: Topological Crystal Chemistry & Irreducible representations of space groups, Nancy, France.

**http://www.crystallography.fr/mathcryst/nancy2010.php**

**22-23 June 2010**

South West Structural Biology Consortium Meeting 2010, Cardiff.

**http://swsbc2010.chemy.cf.ac.uk/**

**26-28 June 2010**

ECRS-8 - the 8th European Congress on Residual Stresses, Riva del Garda, Italy

**http://events.unitn.it/en/ecrs8**

**4-8 July 2010**

First International Conference on Materials for Energy, Karlsruhe, Germany

**http://events.dechema.de/enmat2010**

**4-9 July 2010**

IZC16 and IMMS7. 6th International Zeolite Conference and 7th International Mesostructured Materials Symposium. Engineering of New Micro- and Meso-Structured Materials, Sorrento, Italy.

**http://www.izc-imms2010.org/index.php**

**5-8 July 2010**

MOLMAT2010. IVth International Conference on Molecular Materials, Montpellier, France.

**http://www.molmat2010.fr/**

**5-8 July 2010**

PNCMI2010: 8th international workshop on Polarised Neutrons in Condensed Matter Investigations, Delft, The Netherlands.

**http://www.tnw.tudelft.nl/live/pagina.jsp?id=3f2f14d1-c18b-4276-aa94-90d5d52fc337&lang=en**

**5-9 July 2010**

Combined Analysis Using X-ray and Neutron Scattering, Caen, France.

**http://www.iucr.org/news/notices/meetings/meeting_2009_222**

**11-14 July 2010**

7th International Conference on Synchrotron Radiation in Materials Science (SMRS-7) and 6th International Conference on Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation (MEDSI), Oxford.

**http://www.diamond.ac.uk/Home/Events/MEDSI.html**

**11-15 July 2010**

12th International Workshop on Radiation Imaging Detectors, Cambridge.

**http://iworid2010.mrc-lmb.cam.ac.uk/**

**11-16 July 2010**

MACRO2010. 43rd IUPAC World Polymer Congress: Polymer Science in the Service of Society, Glasgow.

**http://www.rsc.org/ConferencesAndEvents/RSCConferences/Macro2010/**

**11-16 July 2010**

Gordon Research Conference in 'Electron Distribution & Chemical Bonding', South Hadley, MA, USA

**http://www.grc.org/programs.aspx?year=2010&program=elecdist**

**13-17 July 2010**

SXNS11. Eleventh International Conference on Surface X-ray and Neutron Scattering Evanston, IL, USA.

**http://www.sxns11.northwestern.edu/**

**16-18 July 2010**

Celebrating 50 years of the British Biophysical Society, Robinson College, Cambridge.

**http://biophysics2010.org/**

**18-23 July 2010**

Gordon Research Conference in `Diffraction Methods in Structural Biology', at Bates College, Lewiston, Maine, USA. Chair: Andrew Leslie. Co-chair: Ana Gonzales.

**http://www.grc.org/programs.aspx?year=2010&program=diffrac**

**24-29 July 2010**

American Crystallographic Association Meeting, Chicago, Illinois, USA.

http://www.amercrystalassn.org//meetingspg_list/futuremeetings.html

**25-29 July 2010**

EHPRG Conference 2010. 48th European High Pressure Research Group Conference, Uppsala, Sweden

**http://ehprg2010.fysik.uu.se/**

**2-6 August 2010**

X-ray Science in the 21st Century, Santa Barbara, CA, USA.

**http://www.aps.org/meetings/meeting.cfm?name=XRS10**

**2-6 August 2010**

59th Annual Denver X-ray Conference, Denver, CO, USA.

**http://www.dxcicdd.com/**

**15-20 August 2010**

XRM2010. 10th International Conference on X-ray Microscopy, Argonne, IL, USA.

**http://xrm2010.aps.anl.gov/**

**15-20 August 2010**

Solid State Studies in Ceramics. Fundamental Phenomena in Energy Applications. Gordon Research Conference, New London, NH, USA.

**http://www.grc.org/programs.aspx?year=2010&program=ceramics**

**17-20 August 2010**

XXth International Symposium on the Jahn--Teller Effect, Fribourg, Switzerland.

**http://www.unifr.ch/jt2010/**

**21-27 August 2010**

20th General Meeting of the International Mineralogical Association, Budapest, Hungary.

**http://www.ima2010.org/**

**22-26 August 2010**

240th ACS National Meeting & Exposition, Boston, MA, USA.

**http://portal.acs.org/portal/acs/corg/content**

**23-27 August 2010**

FEL 2010. 32nd International Free-Electron Laser Conference, Malmö, Sweden.

**http://fel2010.maxlab.lu.se/**

**27-29 August 2010**

MaThCryst Satellite Conference of ECM26, Darmstadt, Germany.

**http://www.crystallography.fr/mathcryst/darmstadt2010.php**

**27-30 August 2010**

EPDIC12. 12th European Powder Diffraction Conference, Darmstadt, Germany.

**http://www.epdic12.org/**

**29 August - 2 September 2010**

26th European Crystallographic Meeting, Darmstadt, Germany.

**http://www.ecm26.org/**

**5-7 September 2010**

BACG 2010. British Association for Crystal Growth, Manchester.

**http://www.bacg2010.org/**

**5-9 September 2010**

Diamond 2010. 21st European Conference on Diamond, Diamond-Like Materials, Carbon Nanotubes, and Nitrides, Budapest, Hungary.

**http://www.diamond-conference.elsevier.com/**

**5-10 September 2010**

BCA/CCP4 Summer School XV, Oxford.

**http://crystallography.org.uk/bca-ccp4-summer-school-2010**

**9-11 September 2010**

4th International SAXS / GISAXS Workshop, Leoben, Austria.

**10-16 September 2010**

13th International Conference on the Crystallisation of Biological Macromolecules (ICCBM13), Dublin, Ireland.

**http://www.iccbm13.ie/**

**13-17 September 2010**

E-MRS 2010 Fall Meeting, Warsaw, Poland.

**http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=334&Itemid=1**

**14-16 September 2010**

BCA Industrial Group PANalytical Tube Factory Visit, Netherlands

**http://sites.google.com/site/bcaindgrp/meetings/14-16-sept-2010**

**19-23 September 2010**

Structure Under Extreme Conditions of Pressure and Temperature Gatlinburg, TN

**http://neutrons.ornl.gov/conf/IUCr2010/**

**19-24 September 2010**

IWN2010. International Workshop on Nitride Semiconductors, Tampa, FL, USA.

**http://www.iwn2010.org/**

**20-22 September 2010**

17th Bruker Users' Group Meetings 2010 Single Crystal X-ray Diffraction, Karlsruhe, Germany.

**20-23 September 2010**

XTOP2010, the International Conference on High-resolution X-ray Diffraction and Imaging. University of Warwick, UK.

**http://www2.warwick.ac.uk/go/XTOP2010**

**20-24 September 2010**

10th International Symposium on Ferroic Domains and Micro- to Nanoscopic Structures, Prague, Czech Republic.

**http://palata.fzu.cz/isfd10/**

**26-29 September 2010**

Neutrons for Global Energy Solutions, Gustav-Streseman Institute, Bonn, Germany.

**http://www.iucr.org/news/notices/meetings/meeting_2009_270**

**26 September - 2 October 2010**

International School on Aperiodic Crystals, Carqueiranne, France.

**http://www-xray.fzu.cz/sgip/isac2010/isac2010.html**

**27 September - 2 October 2010**

HSC12: Synchrotron Radiation and Neutron for Extreme Conditions Studies, Grenoble, France.

**http://www.esrf.eu/events/conferences/HSC/HSC12**

**28-29 September 2010**

2010 Annual Meeting of the Mineralogical Society. Nuclear Waste Management: Research Challenges for the Future, Cambridge.

**http://www.minersoc.org/pages/meetings/nuclear/nuclear.html**

**4-7 October 2010**

Nuclear Materials 2010, Karlsruhe, Germany.

**http://www.nuclearmaterials2010.com/**

**11-14 October 2010**

IXS2010. 7th International Conference on Inelastic X-ray Scattering, Grenoble, France.

**http://www.esrf.eu/events/conferences/ixs2010**

**11-26 October 2010**

X-ray Methods in Structural Biology, Cold Spring Harbor, NY, USA.

**http://meetings.cshl.edu/courses/c-crys10.shtml**

**12-14 October 2010**

Specimen Preparation for X-ray Fluorescence, ICDD Headquarters, Newtown Square, PA, USA.

**http://www.icdd.com/education/spec-xrf-workshop.htm**

**13-16 October 2010**

Murnau Conference on Structural Biology – The modern RNA world, Murnau, Germany.

**http://www.murnauconference.de/2010/**

**18-20 October 2010**

Basic Rietveld Refinement & Indexing, ICDD Headquarters, Newtown Square, PA, USA.

**http://www.icdd.com/education/rietveld-workshop.htm**

**21-22 October 2010**

Advanced Rietveld Refinement & Indexing, ICDD Headquarters, Newtown Square, PA, USA.

**http://www.icdd.com/education/rietveld-workshop.htm**

**21-23 October 2010**

SENSE 2010 Superconductivity explored by Neutron Scattering Experiments, ILL, Grenoble, France.

**http://www.ill.eu/news-events/events/sense2010**

**27-29 October 2010**

68th Annual Pittsburgh Diffraction Conference, Pittsburgh, PA, USA.

**http://www.pittdifsoc.org/PDC_2010/index.htm**

**3-4 November 2010**

BCA Industrial Group Autumn Meeting, Diamond Light Source, Harwell.

**http://sites.google.com/site/bcaindgrp/meetings/3-4-nov-2010**

**10-11 November 2010**

Synchrotron radiation in Earth, Space & Planetary Science - Exploiting the UK's newest facility, Didcot.

**http://www.diamond.ac.uk/Home/Events/EE_village_workshop.html**

**29 November - 3 December 2010**

MRS Fall Meeting, Boston, MA, USA.

**http://www.mrs.org/s_mrs/sec.asp?CID=16777&DID=216967**

**8-10 December 2010**

8th International Conference on X-ray Investigations of Polymer Structure, XIPS 2010, Wroclaw, Poland.

**http://www.xips2010.ath.bielsko.pl/**

**26 March - 3 April 2011**

13th Intensive Teaching School in X-ray Structure Analysis Durham.

**http://www.dur.ac.uk/durham.x-ray-school/**

**11-14 April 2011**

BCA Spring Meeting, Keele University.

**http://crystallography.org.uk/spring-meeting-2011**

**10-14 May 2011**

ICSG 2011 International Conference on Structural Genomics, Toronto ON, Canada.

**http://www.sgc.utoronto.ca/ICSG2011/**

**21-26 May 2011**

American Crystallographic Association Meeting, New Orleans, LA, USA.

**http://www.amercrystalassn.org/content/pages/main-annual-meetings**

**2-12 June 2011**

The Power of Powder Diffraction, Erice, Italy.

**http://www.crystalerice.org/Erice2011/2011pd.htm**

**2-12 June 2011**

Electron Crystallography: New Methods to Explore Structure and Properties of the Nano World, Erice, Italy.

**http://www.crystalerice.org/Erice2011/2011ec.htm**

**22-29 August 2011**

IUCr2011. XXII Congress and General Assembly, Madrid, Spain.

**http://www.iucr2011madrid.es/**

**25-29 August 2013**

28th European Crystallographic Meeting, University of Warwick.

**http://www.crystallography.org.uk/**

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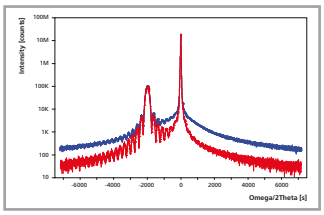

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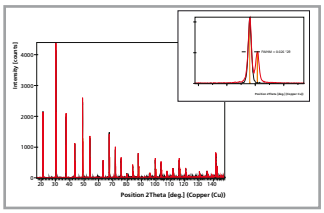

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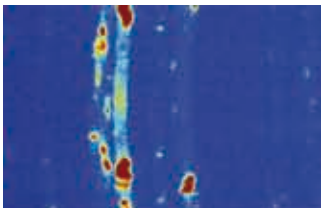

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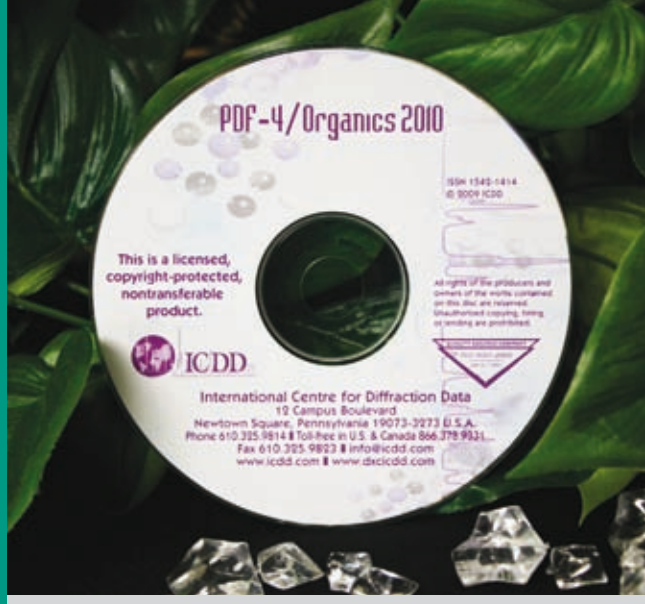


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