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British Crystallographic Association

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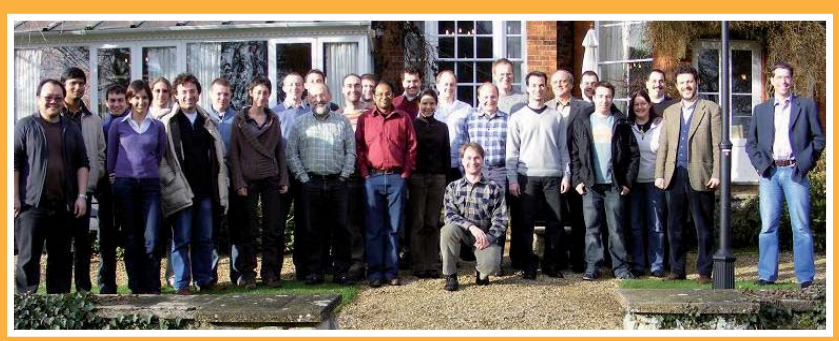
BCA Spring Meeting 2008 - York p14-23



Crystallography News March 2008

Contents

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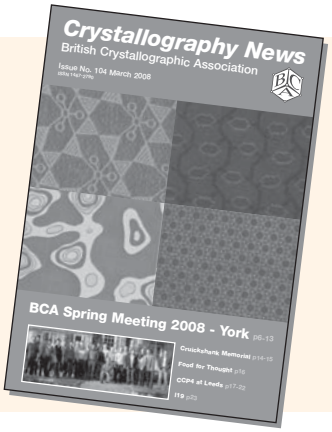
This month's cover:

Fabrics based on crystal structures - see page 26 (Pictures courtesy of Victoria and Albert Museum). Insert shows keen students of magnetism!



From the President

TIME has been flying again and by the time this is published the York Spring Meeting will be upon us. The Meeting commences with the Young Crystallographers session on Monday 7th April and the main Meeting starts on Tuesday, 8th April, and runs through to the afternoon of Thursday, 10th April.

John and **Ivana Evans**, and the Programme Committee, have done an excellent job and, as you will see in the full programme published in this issue, they have assembled a wide ranging and exciting programme that will appeal to the whole community. York University has proved a very popular and successful venue in the past and I am sure it will be so again this year. I look forward to seeing you all there.

Thinking further ahead, we have the XXI Congress and General Assembly of the International Union of Crystallography at Osaka, coming up between 23-31st August. The website has been open for registration and abstract submission since mid-January and the details of the programme are available. The programme looks very extensive, covering all aspects of crystallography and there is a series of excellent keynote lectures, coupled with an extensive social programme including tours and options to visit other regions of Japan at the end of the meeting. Perhaps this would be a good opportunity for a late summer holiday with mountains to climb? From glancing down the list of microsymposia there is a very good representation from the BCA community which is pleasing to see. It is, of course, an expensive trip from the UK but there are a small number of bursaries available from the Royal Society and the BCA will provide some financial help to students wishing to attend through our own bursary scheme.

I am delighted to report that after the receipt of a number of top quality nominations the BCA Officers, in consultation with the Council, have recommended the election of two new Honorary Members of the BCA, **Paul Fewster** and **Bob Gould**, in recognition of their outstanding services to BCA and crystallography. They will receive their letters of election at the York Meeting.

As you may also know Bob Gould is stepping down as Editor of Crystallography News after this edition. Bob has put in sterling service for the past six years and will be sadly missed. I am sure that we would all agree that he has done a splendid job and the fact that Crystallography News is recognised as a highly professional and informative journal is due, in no small measure, to his efforts. So let me take this opportunity to thank him most sincerely on behalf of the BCA for all his hard work and enthusiasm. As President, I would also like to express my personal thanks to Bob for all his help and support, for always reminding me of what I needed to do in the most gentle of ways and for correcting all my spelling mistakes. (Bob - you're not allowed to edit this paragraph!).

Not only is Bob retiring but **Sheila Gould** is also standing down as Treasurer at the end of her term of office. Our sincere thanks go out to her as well. Over a number of years, having been treasurer of the 1999 IUCr and three years as our Treasurer, Sheila has kept the BCA in a financially healthy state and we are most grateful to her for her untiring efforts. Bob and Sheila are a great team and have supported the BCA throughout their careers. The community owes them a great deal and we wish them all the very best for the future. We do, of course, very much hope to see them at the Spring Meeting in 2009!

Therefore, at the AGM at the Spring Meeting, we need to elect a new Treasurer. The Council officers and I look forward to receiving nominations for this key post.

Finally, it is a great pleasure to welcome **Carl Schwalbe** as the new Editor of Crystallography News who will be taking over from Bob over the next few months. The Officers are extremely grateful to him for agreeing to take on this important job within the BCA and look forward to seeing his first issue in the summer.

Paul Raithby

BCA Council 2006-07

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

From the Editor

THE main point - and the centrepiece - of this edition is, of course, getting our readers to come to the Spring Meeting in York. You will find an almost complete programme and details in the middle of the issue. As Editor, I must express special gratitude to John and Ivana Evans and their Programme Committee for the excellent work in getting material to me in good time and good order. It should be an excellent meeting in a very fine place.

There is more from **Lesley Jackson** about the forthcoming exhibition (24 April - 10 August at the Wellcome Collection) of the remarkable things designed from crystal structures and diffraction patterns for the Festival of Britain back in 1951. The various fabrics illustrated on the cover are courtesy of the Victoria and Albert Museum and were supplied by **Mike Findlay** at Wellcome. Slightly sad is the sentence in Lesley's article: "Science enjoyed great popular appeal during the early post-war period, and X-ray crystallography was one of the most exciting fields of science at the time." Those past tenses should spur us to have a revival!

Biological Crystallography is well represented in this issue, with accounts from up and down the country of the BSG Winter Meeting in London, CCP4 at Leeds, and the Northern Protein Group in Carlisle. I am particulalry grateful to CCP4 for the full accounts of their meetings that the send us each year.

This is my last issue as Editor. It is the 25th that I have edited, and I have greatly enjoyed this position. Being an editor is about the only job which gives one a chance for a 100% success rate in publication! It is, though, time to pass on the baton or whatever it is. As the years go by, it becomes more evident to me that some fresh ideas are required, and I'm very happy that **Carl Schwalbe** has agreed to take on this post. I can certainly say that you, our readers and contributors, are fun to work with.

In my time, I have had only a few disappointments. The main one is the small number of replies to "Puzzle Corner". Despite this, I have carried on, as I enjoy setting things, and people often tell me that they work on them but simply don't send anything in. Of the more faithful, I should mention **Tim Weakley**, who often replies before my own copy has arrived!

There are many, many people that I could thank for their help during my time. Three Presidents: **Chris Gilmore**, **Chick Wilson** and **Paul Raithby** have all been most patient and faithful at getting in their "pastoral letters" with a minimum of nagging. Programme Committees of successive Spring Meetings and Group Secretaries have been very co-operative, but there are two people who really must have special mention. I have had very helpful assistance from one of my predecessors **Kate Crennell**, who has discovered all sorts of interesting things that I would have missed, and deserves much credit for what has appeared. And then there is **Professor Dolding-Beadle**, of whose more conventional identity I shall give no clue, except that (s)he is very definitely not I! I trust that (s)he will continue to send my successor his/her animadversions!

I will end with a little plea. I am not disappearing entirely, as I am now responsible for the IUCr's on-line lists of jobs and meetings. It is a great help to us if people will let us know about anything of interest to crystallographers when they plan it - just send a note, with a website, to news.online@iucr.org

Many thanks!
Bob Gould

Letter to the Editor

FROM FRANCES BERNSTEIN

I found pages 34 and 35 of the December 2007 Crystallography News very difficult to read. The pale green against dark green is hard to read in any case and especially on shiny paper. My husband, Herbert, also gets the newsletter and he is red-green color-blind and he had even more trouble with it. The title of a meeting is the primary information that someone reading the Newsletter would be looking at and that is the hardest to read on these pages. After deciding that the title looks interesting then one might be concerned with the dates to determine if one might be able to attend.

In general black on white is the easiest to read. If color is needed it should be used sparingly to make something stand out or to distinguish different sections (as in the blocks of the program). Light print on a dark background is the most difficult to read.

Dear Frances,
I have to admit that I am delighted to learn that someone is actually trying to read these meeting notices, but I'm sorry that they were difficult in the last issue. We try to make *Crystallography News* attractive, but it is, of course, more important to make it legible! We currently have eight feature colours, which we alternate over a two-year period. They range from a yellow (the colour of this issue) to a dark brown, and the way they can be used inside the issue clearly varies. This is my swan song, but I'll suggest to my successor that these lists should always be in white or black type.

Puzzle Corner

FOR my last entry in this space, I'll return to what is clearly our readers' favourite - the substitution cryptogram. The text below occurs, unencrypted, elsewhere in this issue. To make it a little more difficult, all punctuation has been omitted. A usual prize of a £20 Book Token for the best entry before the Spring Meeting, including the page reference!

jyjvmsrm cvpslguf sjgpvrujs eauw cruujvif zrfjs pi gvmfurd fuvlgulvjf rvj uwj flztjgu pb uwaf aiipyruayj fwpe ewagw zvaihf uphjuwjv ri jgdjguag rvvrm pb ujxuadjf erddcrcjvf brfwapi blviaulvj dmairujf grvcjuf ris urzdjervj svreaihf pb rupnag fuvlgulvjf eadd fau rdpihfasj uwj sjfahif uwjm aifcavjs vjbdjguaih uwj liaklj gpddrzpvruapi zjuejji zvauraif djrsaih cpfuerv fgajiuafuf ris nrilbrgulvjvf

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Oh dear, last month's puzzle, despite being in keeping with the season, got no entries at all except the artist's own! The prize had better go to him, **Luke Yates**, a summer student with **Jon Cooper** at Southampton.

SDPD Round Robin - 2008

THE Commission on Powder Diffraction (CPD) of the International Union of Crystallography (IUCr) is sponsoring a round robin on structure determination by powder diffractometry (SDPD). The purpose is to compare different methods of structure solution on the identical sets of measurements.The results will be published in the open literature. This initiative follows the 1998 and 2002 previous SDPD Round Robins of which the short conclusions were published in CPD Newsletters 25 & 29. There are a dozen different methods that can yield the desired result (atomic coordinates) from a powder pattern, the most recent being charge flipping. And that excludes prediction, which does not need diffraction data! Information can be found in previous CPD Newsletters, including the recent issue N°35. http://www.iucr-cpd.org/. Two weeks into the trial, there have already been 65 downloads, and one solution has already been submitted.

More details and the data for two samples are available at: http://sdpd.univ-lemans.fr/SDPDRR3/
Deadline: Wednesday 30 April 2008

Best wishes !
Armel Le Bail & Lachlan Cranswick

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:

- Up to 10 free BCA memberships for your employees.
- A 10% discount on exhibition stands on the annual BCA Spring Meeting, OR - A promotional poster at the annual BCA Spring Meeting.
- Free insert in the annual Spring Meeting delegate bag.
- Two free full registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly BCA Newsletter.
- Corporate Members will be listed in every BCA Newsletter and on the BCA Web Site with links to your corporate site.

The cost of this membership is **£750.00** per annum

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Cruickshank Memorial

Mini-Symposium at Manchester University

A MEMORIAL and celebratory mini-symposium for the life and achievements of Durward W J Cruickshank, FRS (1924-2007), was held at Manchester on 26 November 2007. By courtesy of the University President, the meeting took place in the fabulous Whitworth Hall. With the organ played by Dr James Garrett, the event began with the hymn "To be a Pilgrim" and a prayer by the Rev. Dr Terry Biddington. Among about 100 speakers and participants from Canada, USA, Hungary, Italy and all over the UK, Farid Ahmed, co-author of Cruickshank papers separated by half a century, had travelled specially with his wife Jean from Ottawa. It was touching that he, from a different faith, recalled Durward's unselfconscious Christian evening prayers.

Many relatives of Durward were present, some perhaps not fully aware of his scientific distinction. **John Cruickshank** welcomed participants and also closed the proceedings after some spontaneous recollections by individuals. Summarising Durward's activities in genealogy, which included several visits to Salt Lake City, his daughter **Helen Stuckey** described family history searches. Durward's parents met as young medical doctors at Charing Cross Hospital, but his father's family was from Aberdeenshire. His mother, née Meek, who, incidentally, started to read mathematics at Cambridge before switching to natural sciences and medicine, had family origins in the Macclesfield/Prestbury area, close to Durward's house in Alderley Edge. Maternal family links had been established with William Wordsworth, John Hymers, FRS (a 19th century mathematician who founded a college in Hull), and a Whitby whaling captain (one reason for Durward's two Arctic cruises). Helen showed Durward's photographs of several Penguin species taken on one of his Antarctic voyages which included South Georgia and crystallographer R W James's Elephant Island. Cruickshank was not one of the crystallographers' names commemorated by an Antarctic geological feature, but **Chick Wilson** (Glasgow University), described the opening of the Cruickshank Laboratory in Chemistry at Glasgow. The photograph fronting the mini-symposium booklet was of Durward, happily quizzical and with inclined bow-tie, at his Hon. D.Sc. signing at Glasgow in 2004 [and also appeared on the front cover of our December edition - Ed.].

John Helliwell (Manchester University), co-organiser of the symposium with **Bob Munn** (who praised Durward's wisdom in financial management of UMIST and in coping with idiosyncratic principals) surveyed the immense range of Durward's scientific interests and achievements. Outside science and the family, his interests included golf, travelling, genealogy, history and biography. His scientific activities encompassed the use of diffraction data from electrons and monochromatic and polychromatic X-rays, quantum chemistry, structure determination and refinement (inorganic, organic and protein), accuracy, and thermal vibrational analysis. After formal retirement he had contributed appreciably to the emergence of dynamic crystallography through the interpretation of Laue photographs. It wasn't so much the date span and number of publications (they peaked around 1964 and included 80 in Acta Crvst. alone) that was so impressive, but the high average citation per publication of 64, dominated by the 1949 and 1956 Acta papers and the 1958 benzene paper.

Polycyclic hydrocarbons and their aromaticity and distortions, which Durward studied from the 1950s to the 1990s, figured in almost one-third of the papers (J.Mol. Struct. **130** 1/2, Aug 1985) after the 1984 Cruickshank Symposium. Although less evident here, they were alluded to by both **Guiseppe Filippini** (Milan University), who was a post-doc at UMIST in the 1970s, and **Alajos Kalman** (Budapest University). 'Luigi' enlarged on his own and collaborative work on tetrahedral oxyanions. Structure determinations of 2nd row oxyanions such as the aminedisulphonates with George Jeffrey at Leeds led to a much wider investigation and reconsideration (Durward self-critical as ever) of the contribution of $d\pi$ - $p\pi$ bonding.

Keith Moffat (Chicago University) described the remarkable Daresbury collaboration from 1986 between himself, Helliwell (at York) and 'irreverent post-doc' Cruickshank on the Laue X-ray method. Crystals of haemoglobin had been studied even before X-ray diffraction was devised while Laue photography, despite multiple contributions to single spots, was the technique of the Braggs and of Pauling and Wyckoff in the 1920s until Polanyi, Bernal and others

developed monochromatic photographic techniques. The Laue method was resuscitated when the availability of powerful polychromatic X-ray sources raised the possibility of tackling the structural kinetics of biochemical reactions. Thanks to what Keith called the 'fun' interaction of the argumentative trio, many of the overlap problems were solved. With enhanced time-resolution, Keith hinted at applications to new systems such as photoreceptors from bacteria and the molecular basis of signalling. **Dame Louise Johnson** (Biophysics, Oxford, and Diamond Light Source) described the contribution to enzymology that time-resolved Laue studies of light-activated reactions had made, especially with freeze-trapping. Some of the work is described in the 1992 publication of the Royal Society meeting on time-resolved macromolecular crystallography edited by Cruickshank, Helliwell and Johnson.

For the International Union of Crystallography, **Mike Dacombe** (IUCr) said that, on becoming the first Treasurer in 1966, Durward had set about establishing the incorporated status of the Union secured in 1972. **Robert Gould** (BCA) noted Durward's election as Honorary member in 2003 and, on behalf of the President, announced the establishment of the Cruickshank Prize for conference travel for young crystallographers.

The highlight of the symposium was a series of excerpts from a videoed interview, conducted by **Martyn Clark** (Leeds Computer Society), of Durward's reminisces made only days before Durward died. His wartime education in Mechanical Engineering at Loughborough and directed service at the Welwyn Research Station (including testing a midget submarine) and in Whitehall were recalled. Soon after Durward's arrival in 1946 as a temporary research assistant in Gordon Cox's department at Leeds, George Jeffrey showed him A D Booth's papers on novel methods of structure refinement and accuracy estimation. Encouraged by Cox, Durward moved from instrument development to the mathematics of refinement and accuracy and so to methods of computation, then involving punched cards. Returning to Leeds from Cambridge as a mathematics wrangler, Durward made extensive overnight use (1952-57) of the Ferranti Mk I electronic computer at Manchester and was a prime mover in securing the allocation to Leeds of one of the handful of University Pegasus computers.

Garib Murshadov (York University and CCP 4) referred to REFMAC for protein refinement and summarised the utility in macromolecular crystallography of the Cruickshank dispersion precision indicator. In a telling reflection on Durward's contribution to our science, Garib suggested that the Cruickshank papers, not least those of 50 years ago, should be required reading for new entrants into crystallography as examples of insight and concise clarity - a compliment their author would have appreciated. At the 1984 Symposium Dinner, the toast to Durward was as 'international scientist and crystallographer in the Manchester tradition'.

In this 2007 celebration, Manchester has again honoured itself and Durward.

Derry W Jones

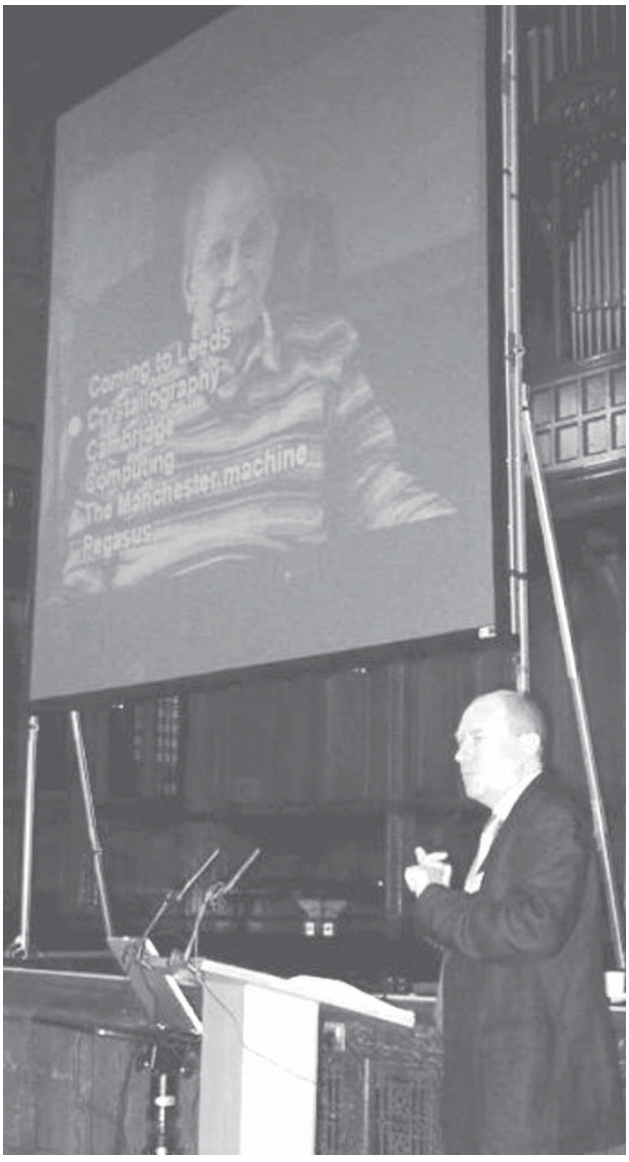
The Cruickshank Prize

THANKS to an extremely generous bequest from the estate of Professor Durward Cruickshank, the BCA Officers are pleased to announce the establishment of the "Durward Cruickshank Young Crystallographers' Prize" to be awarded on an annual basis to a Young Crystallographer (normally with less than 3 years of post doctoral experience) who has made an outstanding contribution in any area of crystallography.

The contribution will be judged on poster and oral presentations and all-round contributions during the BCA Spring Meetings by designated members of the Young Crystallographers Group who will nominate the Prize Winner to the BCA Officers for ratification.

In the first instance a sum of £250 will be associated with the Prize and should be used by the recipient to assist them in attending a national or international conference.

Paul Raithby



CCP4 at Carlisle and Leeds

Seeds Sown In 'Carla' Provide Food For Thought

THE 14th Northern Universities Protein Crystallography Meeting (5th - 7th September 2007) - sponsored by CCP4 and AstraZeneca, as well as contributions from other Life Sciences companies - found itself in the uncharted territories of Carlisle (Carla) in 2007, with the University of Cumbria providing the venue; as the more familiar Galashiels venue had been demolished. However, despite the change of scenery, intrepid crystallographers turned out in force, resulting in a meet that was full to capacity.

The theme for 2007 was Crystallisation, and attendees were very lucky to witness outstanding presentations from two of the top scientists in this field - **Allan D'Arcy** from Novartis, Switzerland, and **Terese Bergfors** from Uppsala University, Sweden. Both provided interesting, stimulating talks (discussion on them was overheard well into the twilight hours in venue No2; the pub!), in an attempt to shed some light on to a process that some have previously considered a 'Black Art'. Both speakers left us all with a definitive take-home message; SEED YOUR CRYSTALS.

The bulk of the Meeting was concerned with student talks, all of which were of the highest quality, and sparked new relationships and interactions between participants. A major attraction of this meeting is the emphasis on student participation, giving the opportunity for most of the attending students to present their work to a sizeable audience, which may not arise at some of the larger Conferences. These talks covered not only the topic of Crystallisation, but also encompassed all the associated processes; from cloning, expression and protein purification, through Crystallisation to structure determination, as well as covering related subjects including biochemistry and functional studies.

Congratulations are also extended to **Stefan Schmelz** from the University of St. Andrews, winner of the prize for Best Student Talk over the three days for his presentation 'AcsD Co-Complex Structure of an NRPS-Independent Siderophore Synthetase'. A first year PhD Student, Stefan has already solved this structure to 2.2Å in its Native form, as he described in his presentation; he then went on to explain that immediately preceding the Meeting he had obtained 2Å data for an ATP-bound form, thus giving him a lot more work to do upon returning to University!

Once the nerves of giving talks were over (or hangovers from the previous night's conference dinner and karaoke had been dispelled) students were able to relax and enjoy the final slot of presentations given by senior scientists, post-docs, and researchers to try and pick-up some thoughts and ideas from their experiences.

Also present at the Meeting were representatives from the various Sponsor Companies -including GE Healthcare, Merck, Genomic Solutions, Molecular Dimensions, Oxford Diffraction, and others- who had the chance to ply their wares and show off latest products during the multitude of coffee-breaks which we all know that scientists need in order to survive!!

The 2007 Northern Universities Protein Crystallography Meeting was a successful one, from which everybody benefited - be it the experience of giving a presentation, developing new contacts, finding a new idea to try, or perhaps being persuaded to retry a technique with which they had no luck previously. But that was 2007. Next year: MEMBRANE PROTEINS!

Matt Horsham, Claire Waterston, Gillian Young, Frank Kroner
University of Glasgow

Annual Meeting - Leeds

THE annual Collaborative Computational Project in Macromolecular Crystallography (CCP4) Study Weekend returned once again to the University of Leeds for a stimulating meeting on January 3-5, 2008. The meeting, "Low Resolution Structure Determination and Validation", included a range of talks covering different strategies for obtaining structures from low resolution data and a variety of methodologies for assessing the quality of those structures. Also there were examples demonstrating successes and failures of modeling structures based upon low resolution data. The stimulating scientific programme was organised by Randy Read (University of Cambridge, UK) and Gerard Kleywegt (Uppsala University, Sweden). The popular meeting, attracting 444 delegates, was attended by individuals from Europe, Asia and North and South America.

The chairman of CCP4 Working Group 1, **Jim Naismith** (University of St. Andrews, UK), welcomed the attendees as usual, and reminded them of the open and collaborative nature of CCP4. He stressed the importance of the study weekend format as a training feature on the young crystallographers' calendar, and encouraged everyone to participate in all CCP4 activities and developments. Session 1, "Introduction" began with a talk by **Wayne**

Hendrickson (Columbia University, USA), who explored 'What Structure Tells Us at Different Resolutions'. Simple equations were used to set the frame. When resolution is doubled, the number of observations is increased 8-fold, due to the volume correlation. Resolution of 1Å or higher usually gives enough observations to describe the model completely. But historically, the first macromolecular structures were all completed at much lower resolutions. These were meaningful exercises, proven with later higher resolution work, because the observations were matched to the parameters used to describe the model: At 5-6Å, torsional angles were capable of adjusting the secondary structural elements of myoglobin and haemoglobin; at 4.5-3.5Å, rigid features, such as Fe-S or Fe-His boxes, could be modelled accurately; between 3.5 and 2.7Å, enough observations became available for individual x,y,z atomic refinement, depending on the solvent content. Examples of maps and models at such resolutions were reviewed, and the methods have been updated to apply to modern structures that afford only modest resolution between 3 and 4Å. These are usually large molecular assemblies of a number of proteins, where models of some components are known at reasonable resolution individually, but the assembly showed the packing arrangement and revealed the structure of other unknown components necessary for the assemblies.

'Resolution, Resolution, Resolution: Starting at the Bottom and Moving Up' was the theme the talk **Thomas Steitz** (Yale University, USA), where he argued that it is sometimes useful to start working with low resolution maps in order to gain important information. Phasing the ribosome 50S particle needed large heavy atom clusters, looking like a single anomalous scattering centre at 16 Å, thus giving very useful phases, used in ever increasing resolution data sets at 12 Å then at 9 Å. The particle shape was clearly resolved, and when 6.8Å data became available, certain RNA features could be fitted into the map as rigid bodies. The usual solvent flattening and density modification methods made it possible to locate protein helix and sheet features. But heroic effort was needed, eventually, to achieve the resolution necessary for locating substrates and antibiotics at 2.4-2.7 Å resolution. Essential in all this work was multi-crystal averaging to sharpen the maps sufficiently for correct interpretation. Similar multi-crystal averaging of 70S ribosome particle data sets, even though at 3.7-4Å, revealed that the peptidyl-transferase centres are very similar in both 50S and 70S. Similar low resolution strategies are now being used in work on a number of other large assemblies such as gamma-delta resolvase and fatty acid synthase.

Session 2, "Biological Insights at Low Resolution", opened with **Piet Gros** (Utrecht University, The Netherlands) who described the crystal structure determinations of different forms of the human C3 complement component, a large protein (1641 residues) which plays a central role in mammalian immune defense against micro-organisms. In particular, his work has focused upon the crystallographic determination of active and inactive forms of C3 using medium to high resolution data to yield an improved understanding of the central steps of complement activation. Comparison of the different structures demonstrated how conformational changes between the different forms of C3 are related to their respective roles in the activation and regulation of this important biochemical pathway.

Simon Jenni (ETH Zurich, Switzerland) followed with a presentation describing crystallographic determination of the 2.6MDa fatty acid synthase complex, which assembles as a heterododecamer yielding a 27nm barrel-shaped particle composed of approximately 23,000 amino acid residues. Interestingly, crystals of the enormous complex were reported 40 years ago. Solution of the structures from fungal and mammalian sources benefited from data collection at the Swiss Light Source (SLS) and considerable computational efforts which led to successful phasing to yield interpretable electron density maps at approximately 5Å resolution. More recent work was reported on the crystallographic determination of the fungal enzyme at higher resolution which again suggested that conformational changes are critical for the shuttling of substrates between different active sites within this complex.

Florian Brückner (University of Munich, Germany) then presented a series of studies which provided both structural and functional insight into the RNA polymerase II (Pol II) elongation complex which is plays a key role in the production of messenger RNA as part of the transcription cycle in eukaryotic cells. Of particular interest were the descriptions of the crystallographic determinations of Pol II, composed of 12 different protein subunits (514 kDa) which was determined at 3.8Å resolution; the complete Pol II elongation complex which contains the addition of DNA and RNA which was determined at 4.0Å resolution; and the complete Pol II elongation complexes containing different thymine-thymine photodimers at 3.8 to 4.0Å resolution. These structure provided insights into the structural organization of the nucleic acids, mechanisms involving strand separation and recognition of "lesions" (errors) in nucleic acids. It was particularly interesting to note that the software used for data processing had, in some cases, a significant influence on the ability to obtain a final structure.

The final talk of the session was by **Jens Preben Morth** (Aarhus University, Denmark) who provided a detailed description of the crystallographic determination of the sodium-potassium pump at 3.5Å resolution. The structure reveals key molecular features important for subunit assembly and sodium ion binding. The project was clearly challenging and the successful determination of this crystal structure utilised a range of methods which included the use of litholoops enabling the very thin crystals obtained to remain flat when cryo-cooled, data collection with a brilliant light source (SLS), as well as careful density modification using two non-isomorphous datasets which ultimately enabled phase extension of the original MIRAS phases at 7.0Å to the 3.5Å resolution structure presented.

Session 3, "Model Building and Refinement at Low Resolution", opened with **Manfred Weiss** (EMBL, Hamburg, Germany) who described how the combination of various

factors, such as completeness, redundancy, the shape of the Wilson plot, R_{merge} and $I/\sigma(I)$ affect the nominal resolution of our X-ray diffraction data. He also spent some time on the ever recurring discussion topic, the misleading property of R_{merge} and was arguing for the use of the redundancy independent merging *R*-factor.

Nick Furnham (Cambridge University, UK) described how the numerous challenges are dealt with in the program RAPPER to interpret low resolution electron density maps to generate an atomic model. Experimental data are combined with prior knowledge from homologous structures and a set of restraints applied on the protein stereochemistry. This knowledge-based conformational sampling algorithm usually provides useful information that would otherwise be discarded because of the uncertainty in the interpretation.

Axel Brunger (Stanford University, USA) presented their recent development in low resolution phasing and refinement. Their approach combined the phasing information from known fragments, molecular replacement and SeMet data. Modification and enhancement of the bulk solvent model and B-factor sharpening of electron density maps were essential for successful refinement. Reasonable R_{free} values were achieved at the very modest 4-5Å resolution range, where the data are often noisy and the observable to parameter ratio is very low.

Session 4, "Validating Proteins and Nucleic Acids", or rather 'the session after the night before' focussed on validation of protein structures. In spite of the gruelling slot (9am, Saturday morning) **Gerard Kleywegt** (Uppsala University, Sweden) drew a large audience for his summary of "Applied common sense, the 'Why, What and How' of validation". Perhaps a morbid fascination in who was going to be exposed and for what? The talk began with a discussion of precision versus accuracy, the 'Gospel according to Kleywegt' (Anastassis Perrakis CCP4BB, 17/12/07), and was as entertaining as everyone had anticipated. He discussed what is a good model: one that makes sense in every respect: chemically (bond lengths, angles, planarity etc.); physical contacts, statistically the best model to explain the data; biologically a model that explains other independent observations. Since models of biological molecules are necessarily determined with some subjectivity (map interpretation, model parameterisation, refinement protocol) there is a need to validate the model to ensure that it is on the whole reliable, and preferably to ensure that the bits of interest (active sites, ligands etc) are also correctly interpreted. He presented a selection of examples from the PDB that exemplified why we should all try harder to make sure that our models are as good as possible, and closed by emphasizing the importance of independent data for quality assurance: independent observations (R_{free}) and other prior knowledge including chemical information, Ramachandran plot, biochemical evidence.

Randy Read (Cambridge University, UK) then described the application of 'case-controlled validation' to explore which factors might influence the quality of a structure. A structure of interest is matched against a control structure that has similar values for all relevant factors - such as size of the structure, size of unit cell, year of deposition, to enable a fair comparison. This approach was used to ask the question whether structures derived from structural genomics consortia reach the same level of quality as structures from traditional sources - at the time the analysis was done (2004) there was no evidence of any significant difference in quality, perhaps contrary to popular expectations. The approach was also used to tackle another piece of dogma - that the quality of structures published in the high-impact journals, *Nature, Science* and *Cell*, are of lower quality than structures published elsewhere, perhaps because of the pressure to publish high impact science quickly. The case controlled approach here was particularly appropriate since it compares like with like and the 'average' structure published in Nature has quite different protein size, diffraction limit, and unit cell size to the 'average' structure published in a lower impact journal. The analysis demonstrated that low resolution/large structures are difficult to determine and more likely to have errors than small/high resolution structures, irrespective of where they are published. Analysing structure quality as a function of time, there was significant improvement up until the introduction of Procheck, but since then there has been little progress, presumably because a structure that satisfies Procheck is generally considered to be 'done'. There was an interesting discussion after his presentation about how we might communicate the uncertainty in certain parts of the structure to the outside world - a question to which there is not yet a clear answer.

Prof. Jane Richardson (Duke University, USA) concluded the session with an introduction to MolProbity [1], accessible via a website to the general community. She suggested that a strength of the approach used in MolProbity is the inclusion of hydrogen atoms in the calculation of close contacts, which can be used to correctly assign side-chain conformations even in lower resolution data (3-3.5 Å) where the density is not well enough defined to distinguish. She concluded by outlining a vision for the future where it is possible to derive quite accurate structures from good but low-resolution data, by careful application of robust outside information about what is and is not structurally possible. The session provoked in the listener a useful awareness of some of the pitfalls of over interpretation (or incorrect interpretation) of data, along with some useful suggestions about how to avoid being the next on the list for shaming on a future occasion.

The penultimate session, Session 5, "Validating Other Molecules", was opened by **Ton Spek** (Utrecht University, The Netherlands) reviewing structure validation in chemical crystallography. Structure determination of 'small molecules' is less time consuming which is reflected in the number of entries in the Cambridge Structural Database and the number of papers published each year. However, a number of these structures have been found to contain errors. Most of the errors are related to incorrect space group assignments and wrong atom type assignments. The high volume of structures and papers has required an automatic validation system to be implemented. This produces a report upon submission which is sent to the author and referees, to aid the detection of problems and reduce the number of

problematic structures. Although this system is proving to be successful, the process must be continually reviewed to enable a greater coverage of problems to be detected.

Alexander Schüttelkopf (University of Dundee, UK) gave an overview on the validation of ligand structures in complexes with biomacromolecules. Although high quality restraint definitions are available for proteins, which has simplified model refinement and validation, such definitions are not available for many heterocomponds. This results in this class of molecule being poorly defined and often not validated fully leading to 'unchemical' ligand structures in the PDB. The problems associated with getting accurate restraints for these molecules were discussed together with the sources for obtaining accurate data and associated problem of each method. Finally ValLigURL was discussed. This is a web based tool that compares the conformation and quality of a submitted ligands with all instances of that ligand in the PDB.

This session was rounded off by **Thomas Lütteke** (Utrecht University, The Netherlands) with a description of the quality checks for carbohydrate structures in the PDB. Due to the complexity of carbohydrates and the lack of validation tools designed for carbohydrate structures, 30% of entries within the PDB that contain carbohydrates contain at least one error in the carbohydrate moiety. Several recently developed programs that aid the validation of carbohydrate structures were discussed. These included 'pdb-care', a tool for checking the correct carbohydrate content within a PDB file, and 'carp' and 'glycomapsdb' which check the torsion angles in the carbohydrate chain and compare them with known bonds of that type.

The sixth and last session, "Looking Backwards and Forwards", opened with **Rhiju Das** from David Baker's group (University of Washington, USA) who presented a very exciting *ab initio* protein structure prediction using the Rosetta method. What has impressed the protein crystallography community is that for the first time they have met the 'Petsko test'. They have predicted a truly unknown structure well enough to solve it by molecular replacement albeit only one of 112 amino acids. The method has also improved NMR structures enough to make them better molecular replacement models. The Rosetta method was (perhaps modestly) presented more or less as a triumph of brute force. Using intensive computing including downloadable programs for home PCs to use idle CPU, they have found that just occasionally a very low energy structure is found, and this really is closer to the true structure. However, this is not a random walk for the backbone (which would take far more power to find minima) but judicious mixing of protein fragments, which are combined and minimised in a simpler force field and then a full energy minimisation is done on the best of these.

Next **Gert Vriend** (Radboud University, Nijmegen, The Netherlands), a brave NMR spectroscopist, stood up and told us about the millions of errors he has identified in the PDB using his program Whatcheck. The most severe are 6 space group errors, although one of these is only detectable as there is a hydrogen bond between the NH and the O of an Asn across a crystallographic two fold which means that this side chain does not obey two-fold symmetry. He recalculates the refinement of all structures in the PDB he can from deposited data and has improved R_{free} for 11,355 of the 17,117 he is able to refine. He made the excellent point that careful refining of the uninteresting residues allows correct and unbiased placing of the interesting residues.

The final two talks covered the inspiration for the topic of the whole meeting, the retraction of 5 high profile structures by Geoffrey Chang's group at Scripps just before Christmas 2006. The cause was some homemade software that flipped the sign of his delta anomalous. This then led to his map being a mirror image, which he then built into with normal L-amino acids. First **Chris Tate** (MRC Laboratory of Molecular Biology, Cambridge, UK) presented his 7Å resolution 2D-electron crystallography structures of EmrE, one of the two systems that Chang had published, explaining how the MRC group were confident of their work as they had high (wild type) affinity for a substrate in their 2D crystals. Their already published projection structure was simply not compatible with Chang's. The MRC group were also involved in a second controversy as they find that the EmrE protein is in a dimer in the active form with rotational symmetry in the plane of the membrane, meaning that half the protein is in the membrane one way round and half the other. This is an unusual phenomenon which has not been accepted by all in the field. About 12 months after the retraction Chang has published a corrected structure which agrees well with the MRC work.

Finally, **Phil Jeffrey** (Princeton University, USA) presented his analysis of Chang's mistake (Chang had declined an invitation to speak). Phil showed that indeed you do get a superficially reasonable map if you use inverted anomalous differences with inverted anamolous scattering sites. Indeed this solution was not distinguishable from the true solution by SHELX correlation coefficient. He also showed that you had to have a pretty low resolution for the hand of the helices not to be clear - part of Chang's problem was that his resolution was worse than 4 Å. Chang's more serious mistake, however, was his refinement, where he used multicopy refinement to get R and R_{free} down to 'publishable' levels. At a resolution where there were not enough data to refine a single model properly, to include several models is clearly overfitting. Although in allowing this method, some fault must lie with reviewers (or with editors' interpretation of their comments), the incompatibility with the biology should have been enough for the structures to be queried.

Finally, the success of the meeting was again ensured by excellent support team provided by the CCP4 organisation (Daresbury, UK) which includes **Maeri Howard**, **Shirley Miller**, **Damian Jones**, **Tracey Kelly**, **Nina Woodall** and **Laura Johnstone**. We again thank **Stuart Eyres** who is responsible for the meeting photos and the web streaming of the meeting.

Kate Brown

[1] Davis et al. (2007) Nucleic Acids Res **35**: W375-W383

I19 - at Diamond

I19 - The New Small-Molecule Single-Crystal Diffraction Beamline at Diamond

SINCE the successful bid, in 2003, for a dedicated small-molecule single-crystal X-ray diffraction beamline at the Diamond Light Source (the new synchrotron facility at the Harwell Science and Innovation Campus), the design and development of the beamline, designated I19, has been moving apace. The project has been lead by the Principal Beamline Scientist, initially **Simon Teat**, and for the last 16 months by **Dave Allan**, very ably supported by **Harriott Nowell**, the Beamline Scientist, and a Working Group made up of members of the "small molecule" community. Recently, the beamline team has welcomed **Sarah Barnett** as Support Scientist. The design and building of the station is now nearing completion with commissioning scheduled to take place over the summer. It is confidently predicted that a limited amount of user beam will be available for experiments from October this year, with the station expected to become fully operational a few months later. The main point of this article, therefore, is to let potential academic users know that it will soon be possible to submit proposals for beamtime for the October 2008 - March 2009 period through the on-line submission process accessed through the Diamond website. The closing date for these initial submissions is 1st April 2008. Access for industrial users is expected to begin in late 2009. Any enquiries about industrial access should be addressed to **Elizabeth Shotton** (industry@diamond.ac.uk).

Initially, because aspects of the beamline will still be at the commissioning stage, for this first application round, it would be advisable to put in fairly modest requests for experiments that require only an open flow nitrogen stream in terms of sample environment equipment, and a fixed wavelength close to 0.7 Å. However, do not be put off; by mid-2009 you will be able to do more complex crystallography experiments on very small samples, and to collect the data very quickly!

The station has been designed to have two hutches, set up in series one behind the other. The first hutch, which will be operational from October 2008, will have a diffractometer with a conventional CCD detector and a robotic sample changer allowing a higher throughput of samples. The robot will become available after the first I19 allocation period (after March 2009); as will the possibility for high pressure studies in the first hutch, using a diamond anvil cell. An open flow helium device is expected to be available in either hutch from the second allocation period. The second hutch will have a larger diffractometer and will be available during the second allocation period (from April 2009). This will be equipped with a CCD and a purpose-built fast detector will be provided as a later upgrade. This diffractometer will take a range of environmental cells and a closed circuit cryostat. Equipment for excited state crystallography experiments is currently being designed for commissioning in this larger hutch next year. The two hutch system will allow complex experiments to be set up in the second hutch while allowing the beam to be used in the first hutch, thus optimising beamtime allocations. Thus, a whole range of new exciting experiments can now be envisaged. So get planning!

The synchrotron component of the EPSRC-funded National Crystallography Service, which is run by **Bill Clegg** and his team in Newcastle with support from the Southampton group, will transfer its operation from SRS to Diamond from the commencement of the operation of I19, subject to the usual constraints of beam time allocation. Access to the facility via this service is an efficient and effective way of obtaining synchrotron data sets and/or complete crystal structure results without having to go through the full beamtime application procedure or carry out the data collection experiments yourself. For further information about the service please contact Bill (w.clegg@ncl.ac.uk) or see www.ncl.ac.ak/xraycry

Diamond runs on a three 8-hour shift system per day. The intention is that beamtime on I19, initially at least, will be allocated in periods of whole days (i.e. three slots). Efficiency on I19, once it is optimised, will mean that a large number of samples will be processed in a day. Beamtime proposals can be discussed in advance with the Principal Beamline Scientist (david.allan@diamond.ac.uk) or Beamline Scientist (harriott.nowell@diamond.ac.uk).

Paul Raithby, User Group Chair
David Allan, Principal Beamline Scientist

Beamline inside and outside at 1 February 2008

Bars and Overlay

THE ever active Rietveld site has been buzzing again about the problem of bars - the ones that go over numbers and letters in crystallography, that is, not the ones that feature in the après-talk programme at the Spring Meeting. I've omitted the names to protect the innocent, but I felt that this is a subject that interests more than Rietvelders, so I have arranged the question with the answers that came in. Editor

The Question:
I have heard that there are several ways to create a 3 with an over-bar symbol (as would be used for space group R-3c, for example) in Micro$oft Word, but none are convenient. I know how to do this with the equation editor. Can anyone contribute any better choices?

Answer 1:
I still maintain ditching the evil empire for LaTeX is the best ;-), but, in all seriousness, equation editor is the only way to go. See:
http://helpdesk.princeton.edu/kb/display.plx?id=4558

Answer 2:
Try: Insert -> Field EQ \s \up 6 (\f (,3))
Using Alt-F9 you can toggle between field view and "source code" for modifications (e.g. when you use something else than 12 point font size and need to change the parameter for \up). I then select the resulting 3bar symbol and use Tools -> Auto Correct Options to create an autocorrect code (like "3bar"). With that, each time I type 3bar, Word converts it to the symbol I generated. No LaTeX quality, but no equation editor required either.

Answer 3:
Here is the link to crystallographic font that has 1,2,3,4,6 with bars and other useful symbols:
http://x-seed.net/crystallography.ttf

The disadvantage to use this is that others who open the file Must have the font installed.

Answer 4:
I use word bar symbol which is 20th symbol after "z" when you choose "Insert symbol". You could create shortcut to this bar and insert it before 1"P¯1"but also you need to select this bar and make font condensed by about 6 pt. The crystallographic 1bar looks like this: 1 *(Sorry, yes that's what happens when you send it for publication! - Ed.)*

Answer 5:
Try the font Arial Overlined, but make sure to install it on any computer you use. I once gave a talk with the title "1 bar", written in Arial Overlined. Of course, the computer in the lecture hall did not have that font, which turned the title into "1". Not very clever, if you want to give a talk on inversion symmetry, ... I think there is an option to embed fonts into a powerpoint document that would help with the latter situation, but has some other drawbacks with respect to editing or such...

Answer 6:
If you are a Mac user - there is a program called LaTeXiT which allows you to simply write out equations in LaTeX and then you can drag and drop the output into a program such as powerpoint. There will be no need to play around with fonts.
http://ktd.club.fr/programmation/latexit_en.php

Shorly after that came another discussion of general interest.

The Question:
Does anyone know a free program capable of overlaying crystal structures?

Answer1:
The only program I am aware of that can do this graphically is CrystMol http://www.crystmol.com/features.html
Structure overlay and comparison. It is not free but the cost is reasonable. I would be interested to hear of other programs that can do this graphically as well as give numerical output.

Answer 2:
In mercury
http://www.ccdc.cam.ac.uk/products/mercury/
there is an option for a manual graphical structure overlay, but this option is only available when the CSD database is installed.

Answer 3:
Try Jmol http://icsd.ill.fr/icsd/help/CIF-help.html
Click "Demo" and "Reload" if necessary. You can upload your own CIF files. Just put two or more structures in the same file to flip the drawing between them with Jmol. You can also try pyMOL: http://pymol.sourceforge.net/
It's intended for "biostructures" actually, but also works with pdb-files as well as mol-files and many other formats. So you have to convert your structures, but I think it's worth a trial because of the nice graphics and animations you can create with pyMOL.

Answer4:
The DRAWxtl program has some capabilities for this - see the frame command:
http://home.att.net/~larry.finger/drawxtl/

York

Plenary Lectures

BSG Plenary and BCA Prize Lecture: Tuesday 11:30
Tony Crowther (MRC LMB Cambridge) *From Molecular Replacement to the Structure of Viruses: a Tale of Two Careers*
PCG Plenary: Wednesday 09:00
Paul Attfield (Edinburgh) *Charge Order in Oxides - Putting the Fun into Functional Materials*
IG Plenary: Wednesday 17:15
Rob Delhez (Delft) *X-ray Diffraction on Mars?*
CCG Teaching Plenary - Controlling Difficult Refinements: Thursday 09:00
Peter Muller (MIT) *Dead End Highway 13 - the Carriage of No Return*

Prize Lectures

CCDC Chemical Crystallography Younger Scientist Award 2008: Tuesday 15:30
Kirsty Anderson (Durham) *Crystal Structures with Z' > 1*

Physical Crystallography Prize: Tuesday 16:15
Winner to be announced at the meeting

Industrial Group Prize: Wednesday 10.15
Winner chosen at Young Crystallographers' Meeting.

Description of Sessions and Confirmed Speakers

Local Structure and Disorder in Crystalline Materials (Tuesday 8th April, 13:30-15:00)

THIS session will focus on total scattering methods which aim to obtain information on both long and short range order. For many functional materials structural knowledge on a range of length scales is vital for understanding their properties.

13:30-14:00: **Thomas Proffen** (Los Alamos Neutron Science Center): *Total Scattering: the Key to Understanding the Local- and Medium-Range Structure of Materials*

14:00-14:30: **Sharon Ashbrook** (St Andrews): *Investigating Local Structure and Disorder by MAS NMR*

14:30-14:45: **Simon Hibble** (Reading): *Not So Simple: The Structures and Dynamics of Simple Transition-Metal Cyanides from Total Diffraction*

14:45-15:00: **Alex Hannon** (ISIS): *Polyhedral Distortion in Glasses and Crystals*

Crystal Chemistry of Functional Extended Solids (Wednesday 9th April, 10:15-11:45)

PROPERTIES of solid state materials and their functionalities are inherently related to their crystal structures. This session will highlight examples of structure-property relationship studies in extended solids, such as inorganic oxides and chalcogenides.
10:15-10:45: **Peter Slater** (Surrey): *Relationship between Structure and Conductivity in New Ionic Conductors*

10:45-11:15: **Edmund Cussen** (Strathclyde): *Switching on Fast Lithium Ion Conductivity: Structure and Transport Properties of the Garnet Structure*

11:15-11:45: **Ian Reaney** (Sheffield): *Crystal Chemistry of Dielectric Ceramics*

Functional Molecular Materials I (Wednesday 9th April, 13:30-15:00)

THE field of molecule-based materials has seen a very rapid progress since the discovery of compounds with a variety of technologically important properties such as conductivity, superconductivity and ferromagnetism. One of the major opportunities offered by this area is the possibility of designing building blocks which combine properties allowing the preparation of multifunctional materials. These sessions will focus on the new discoveries and achievements in the field.

13:30-14:00: **Peter Skabara** (Strathclyde): *Controlling the Conformation of Conjugated Molecules through Non-Covalent Interactions*

14:00-14:30: **Jeremy Rawson** (Cambridge): *Sulfur-Nitrogen Radicals: Systematic Design of Spin-Transition Materials*

14:30-15:00: **Guillermo Mínguez Espallargas** (Sheffield): *Non-Porous Materials Can Also Take Up Gases*

Parallel Sessions

Symposium Title	Chairperson	Contact
Local Structure and Disorder in Crystalline Materials	**Matt Tucker**	m.g.tucker@rl.ac.uk
Crystal Chemistry of Functional Extended Solids	**Ivana Evans**	ivana.radosavljevic@dur.ac.uk
Functional Molecular Materials I	**Andrew Bond**	adb@ifk.sdu.dk
Functional Molecular Materials II	**Serena Margadonna**	serena.margadonna@ed.ac.uk
Strongly Correlated Electron Systems I	**Paolo Radaelli**	p.g.radaelli@rl.ac.uk
Strongly Correlated Electron Systems II	**Peter Hatton**	p.d.hatton@durham.ac.uk
Calculating Properties from Structure	**Simon Coles**	s.j.coles@soton.ac.uk
Design of Functional Materials	**Neil Champness**	neil.champness@nottingham.ac.uk
Structures from Pharmaceutical Powders	**Kenneth Shankland**	k.shankland@rl.ac.uk
Jekyll and Hydrate	**Roy Copley**	royston.c.copley@gsk.com
Applied Crystallography Showcase	**Chris Staddon**	chris.staddon@nottingham.ac.uk
Small Is Smart	**Judith Shackleton**	judith.shackleton@manchester.ac.uk
Big Is Beautiful	**Judith Shackleton**	judith.shackleton@manchester.ac.uk
Membrane Proteins I	**Neil Isaacs**	n.isaacs@chem.gla.ac.uk
Membrane Proteins II	**Neil Isaacs**	n.isaacs@chem.gla.ac.uk
Neutrons in Biology	**Garry McIntyre**	mcintyre@ill.fr
Probing Fast Biological Reactions	**David Leys**	david.leys@manchester.ac.uk
Complementary Methods in Structural Biology	**Helen Saibil**	h.saibil@mail.cryst.bbk.ac.uk
Ligand Binding and Drug Design I	**Rod Hubbard**	rod@ysbl.york.ac.uk
Ligand Binding and Drug Design II	**Rod Hubbard**	rod@ysbl.york.ac.uk

Functional Molecular Materials II (Wednesday 9th April, 15:30-17:00)

15:30-16:00: **Kosmas Prassides** (Durham): *Fullerene Superconductivity: Are There Any Surprises Left?*

16:00-16:30: **Darren Bradshaw** (Liverpool): *Pressure-Dependent Hysteretic Sorption Behaviour in a Flexible Metal-Organic Framework*

16:30-17:00: **Alessandro Prescimone** (Edinburgh): *High Pressure And Magneto-Structural Correlations in Single Molecule Magnets*

Strongly Correlated Electron Systems I (Thursday 10th April, 10:15-11:45)

STRONGLY correlated systems where changes in structural properties are intimately linked with changes in electronic/ magnetic properties remain an extremely topical area in condensed matter physics. These sessions will cover various aspects of this field such as multiferroics, materials displaying charge ordering, materials with electronic and or magnetic phase transitions and GMR materials.

10:15-10:45: **Des McMorrow** (UCL): *XRS Study of the Electric Control of Chiral Magnetic Domains in Multiferroic $TbMnO_3$*

10:45-11:15: **Claudio Mazzol**i (ESRF): *New Magnetic Spin State Evidenced by XRS in a Frustrated Spin System*

11:15-11:45: **Martin Lees** (Warwick): *Magnetic Order in $Ca_3Co_2O_6$*

Strongly Correlated Electron Systems II (Thursday 10th April, 12:00-13:30)

12:00-12:30: **Radu Coldea** (Bristol): *Charge Order to Remove Orbital Degeneracy in Triangular Antiferromagnet $AgNiO_2$*

12:30-13:00: **Neil Mathur** (Cambridge): *Limited Local Electron-Lattice Coupling in Manganites*

13:00-13:30: **Alan Tennant** (Hahn-Meitner Institut): *Patterning of Sodium Ions and the Control of Electrons in Sodium Cobaltate*

Calculating Properties from Structure (Thursday 10th April, 12:00-13:30)

THIS session will demonstrate the wide diversity in current approaches to the derivation of physical properties from crystal structure. Talks will be presented from the areas of computational drug delivery, cheminformatics, charge density determination and solid state quantum chemistry.

12:00-12:30: **Jamshed Anwa**r (Bradford): *Phase Transition Phenomena from Molecular Simulation*

12:30-13:00: J**ohn Mitchel**l (Cambridge): *Informed by Informatics?*

13:00-13:15: **Chick Wilson** (Glasgow): *Computing the Solid State: Complementing Experiment with Plane-Wave DFT Approaches to Understanding Hydrogen Bonding and Associated Physical Effects*

13:15-13:30: **Michael Probert** (Durham): *Electrostatic Molecular Properties of Non Steroidal Anti-Inflammatory Drugs from Studies of their Charge Density Distributions*

Design of Functional Materials (Thursday 10th April, 10:15-11:45)

IN keeping with the structure, property, function theme of the meeting, this session will contain talks on the topic of material design (crystal engineering) and its application to obtain materials with desired properties.

10:15-10:45: **Stuart James** (Belfast): *Solvent-Free Synthesis and Some 'Design' Aspects of Metal-Organic Frameworks*

10:45-11:00: **Charles Mason** (Sheffield): *The Design and Synthesis Of Homochiral Metal Organic Frameworks Using Diols*

11:00-11:15: **Colin Seaton** (Bradford): *Charge Transfer and Hydrogen Bonding: Creating Ternary Complexes*

11:15-11:45: **Xiang Lin** (Nottingham): *Metal-Organic Framework Materials: Porosity and Storage*

Structures from Pharmaceutical Powders (Tuesday 8th April, 13:30-15:00)

THIS session will present some applied examples of structure determination of molecular materials by powder diffraction. Practical methods, common problems and software tools will be exemplified in talks by users of this technique.

13:30-14:00: **Alastair Florence** (Strathclyde): *Challenges and Opportunities for Structure Determination from Laboratory Powder Data in Physical Form Discovery*

14:00-14:30: **Vincent Favre-Nicolin** (ESRF): *Solving Structures Using Fox and Flexible Modelling*

14:30-15:00: **Matthew Johnson** (GSK): *A Pharmaceutical Industry Perspective on SDPD*

Jekyll and Hydrate (Tuesday 8th April, 15:30-17:00)

HYDRATED solid-state forms are commonly found in the pharmaceutical industry and their discovery can be both a benefit and a hindrance. This session will concentrate on the characterisation, properties and behaviour of hydrates.

15:30-16:00: **Gérard Coquerel** (Rouen): *The Different Roles of Water Molecules in Chiral Discrimination in the Solid State*

16:00-16:30: **Alan Kennedy** (Strathclyde): *Mony a Meickel Maks a Muckel: Systematic Investigations of Crystal Structures of Organic Salt Hydrates*

16:30-17:00: **Roy Copley** (GSK): *The Complex Solid-State Structure of Carvedilol Phosphate: a Case Study of a Pharmaceutical Hydrate*

Applied Crystallography Showcase (Wednesday 9th April, 10:15-11:45)

A range of talks will be presented from all areas of the BCA describing how X-rays are used in commercial/ industrial applications. The speakers will be asked to give a tutorial-like overview of their work for a non-specialized audience. Where possible, talks from young crystallographers starting out in industry will be selected.

10:15-10:30: *Industrial Group Young Crystallographer Prize Talk*

10:30-10:45: **Alison Burke** (Huntsman Pigments): *Application of XRD within the Pigments Industry*

10:45-11:00: **Judit Debreczeni** (AstraZeneca): *Protein Structures in Drug Discovery*

11:00-11:15: **Mark Farnworth** (Pilkington Group Ltd): *Application of XRD within the Glass Industry Including 2D Mapping*

11:15-11:30: **Suzanne Harte** (Pharmorphix Ltd): *Application of XRD and other Analytical Techniques to Pharmaceuticals*

11:30-11:45: **David Rendle** (ICDD): *Application of XRD within Forensic Science*

Small Is Smart (Wednesday 9th April, 13:30-15:00)

SUB-MICRON crystallites can present peculiar challenges to X-ray powder diffraction; as the crystallite size decreases the reflections broaden and can become difficult to detect. However, nanotechnology is an area of great interest to both industry and academia. X-ray diffraction can give a useful insight into the structure and

subsequent behaviour of these novel materials. In this session we will look at these challenges, how they can be overcome and what type of information can be obtained.

13:30-14:00: **Steve Norval** (Intertek MSG): *Powder Diffraction of Nanomaterials*

14:00-14:30: **Chris Staddon** (Nottingham): *In Plane Scattering from GaN Nanorods*

14:30-15:00: **Chris Gilmore** (Glasgow): *Solving Crystal Structures of Zeolites using Powder Diffraction and Electron Crystallography*

Big Is Beautiful (Wednesday 9th April, 15:30-17:00)

LARGE objects can be just as much of a challenge to diffractionists as very small crystallites. Do you take the sample to the diffractometer, or the diffractometer to the sample? In either case, how do you get an accurate diffraction pattern? There may also be problems with the microstructure, for example large grains or preferred orientation. This session will focus on samples which are inconvenient to handle, usually through their size, shape or micro structure.

15:30-16:00: **Supriyo Ganguly** (Open University): *Measurement of Weld Residual Stresses in Design Geometry Engineering Components and Structures using Pulsed Neutron Diffraction*

16:00-16:30: **George Bibby** (Rolls-Royce): *TBA*

16:30-17:00: **Michael Drakopoulos** (Diamond): *JEEP: The Joint Engineering, Environmental and Processing Beamline at Diamond Light Source*

Membrane Proteins I (Tuesday 8th April, 13:30-15:00)

MEMBRANE proteins remain one of the most under-represented groups in the PDB. These sessions will focus on advances in membrane protein expression, purification and crystallization as well as highlighting recent exciting membrane protein structures.

13:30-14:10: **Chris Tate** (MRC LMB): *Thermostabilisation and Structure Determination of the β1 Adrenergic Receptor*

14:10-14:35: **Karen McLuskey** (Glasgow): *Back to Basics: Developing High Throughput Methods*

14:35-15:00: **Liz Carpenter** (Imperial/Diamond): *High Throughput Crystallisation of Membrane Proteins in the Membrane Protein Labs at Diamond*

Membrane Proteins II (Tuesday 8th April, 15:30-17:00)

15:30-16:10: **Roger Dawson** (Zurich): *Structure and Mechanism of ATP-binding Cassette (ABC) Transporter Proteins*

16:10-16:35: **Thomas Sorenson** (Diamond): *Ion Pump Structures - the Ca^{2+}-ATPase and the Na^{+}/K^{+}-ATPase*

16:35-17:00: **Per Bullough** (Sheffield): *Visualising Membrane Protein Assemblies*

Neutrons in Biology (Wednesday 9th April, 10:15-11:45)

THE recent upgrade at the ILL of LADI-I to LADI-III gave a three- to five-fold gain in detection efficiency, to extend the range of biological problems that can be tackled by neutron diffraction. A dedicated biological diffractometer, LMX, is also proposed for target station II at ISIS. This session will outline the new instrumental capabilities and limitations for biological neutron diffraction, present some recent highlights, and explore the problems that we might consider with the new instruments.

10:15-10:30: **Matthew Blakeley** (ILL): *Neutron Protein Crystallography using LADI-III*

10:30-10:45: **Lee Brammer** (Sheffield): *LMX - Large Molecule Crystallography on ISIS Target Station 2*

10:45-11:00: **Susana Teixeira** (Keele): *The Deuteration Laboratory Platform at the Grenoble Partnership in Structural Biology (PSB)*

11:00-11:15: **John Helliwell** (Manchester): *The Determination of Protonation States in Proteins*

11:15-11:30: **Stephen Prince** (Manchester): *Crystallography of Membrane Proteins with Contrast Matching at Lower Resolution*

11:30-11:45: *Questions to all speakers*

Probing Fast Biological Reactions (Wednesday 9th April, 13:30-15:00)

This session will focus on time resolved crystallography, reaction intermediate trapping and other emergent techniques as a means of probing fast biological reactions.

13:30-14:00: **Dominique Bourgeois** (ESRF/IBS): *Kinetic Protein Crystallography: a Tool to Watch Proteins in Action*

14:00-14:30: **Ylva Lindqvist** (Karolinska Institutet): *Snapshots of Enzymatic Oxalate Degradation in Oxalobacter Formigenes*
14:30-15:00: **Arwen Pearson** (Leeds): *Further Insights into*

the Mechanism of Tryptophan Tryptophylquinone Catalyzed Amine Dehydrogenase Reactions

Complementary Methods in Structural Biology (Wednesday 9th April, 15:30-17:00)

UNDERSTANDING biological functions requires the study of large and dynamic macromolecular complexes. Such assemblies may contain dozens of different components and are usually flexible and heterogeneous, making them intractable to structure determination by X-ray crystallography. This session will cover three approaches that can address such problems in combination with X-ray crystallography. Low and intermediate resolution maps of large assemblies can be determined by single particle electron microscopy and tomography yields low resolution 3D maps of unique structures. Advances in NMR spectroscopy methods enable the determination of dynamic information in the context of large complexes. Finally, current methods in mass spectrometry make it possible to analyse and dissect large assemblies in the intact state to determine their topology.

15:30-16:00: **Justin Benesch** (Cambridge): *Mass Spectrometry for Functional Genomics? Structure and Dynamics of the Small Heat Shock Proteins*

16:00-16:30: **John Christodoulou** (Cambridge): *Structure and Dynamics of Ribosome-Bound Nascent Chains by NMR Spectroscopy*

16:30-17:00: **Helen Saibil** (Birkbeck): *Understanding Molecular Machines by Combining Cryo EM and Crystallography*

Ligand Binding and Drug Design I (Thursday 10th April, 10:15-11:45)

THERE has been much excitement in recent years in using high throughput crystallography in drug discovery, both in identifying new hit compounds (virtual screening and fragment-based discovery) and in structure-guided drug design. However, even with such large datasets of structures, we are still fairly poor at predicting the strength of protein-ligand interactions. As well as helping predictive drug discovery, an improved understanding of the thermodynamics and kinetics of these interactions would enrich our appreciation of molecular recognition events. These sessions will explore how the recent explosion in the use of high throughput crystal structures has been linked to various biophysical and modelling approaches and how these have informed our views on ligand binding.

10:15-10:30: **Rod Hubbard** (York): *Introduction*

10:30-11:05: **Tom Davies** (Astex Therapeutics): *Fragments, Structures and Drug Discovery*

11:05-11:40: **Nicolas Foloppe** (Vernalis R&D Ltd): *Exploiting Crystal Structures for Ligand Discovery and Design*

Ligand Binding and Drug Design II (Thursday 10th April, 12:00-13:30)

12:10-12:30: **Matthew Higgins** (Cambridge): *The Structure of a Chondrotin Sulphate. A Binding Domain in Placental Malaria*

12:30-13:05: **Chris Phillips** (Pfizer): *HIV-1 Reverse Transcriptase: Crystals to Clinic*

13:05-13:30: **Stephen Curry** (Imperial): *Crystallographic Analysis of Metabolite and Drug Binding to Human Serum Albumin*

Workshops

PDF Workshop: (Monday 13:00-18:30 and Tuesday 09:00-10:30)

Shedding Light on the Local Structure and Disorder in Crystalline Materials
Organisers: Matt Tucker (ISIS) & **Ivana Evans** (Durham)

Matt Tucker (ISIS) and **Thomas Proffen** (LANSCE) will run a full day hands-on PDF workshop. The importance of local structure and disorder in crystalline materials is increasingly being recognised as a key property of many functional materials. From negative thermal expansion to solid state amorphisation and the 'nanoscale' problem to improved fuel cell technology, a clear picture of the local atomic structure is essential to understanding these phenomena and solving the associated problems. A powerful technique for exploring the local structure of materials is total scattering, also known at the PDF method. Synchrotron X-ray and/or neutron powder diffraction data can be used to obtain information on the local, medium and long range atomic structure simultaneously. To gain the maximum information from the data, specialised refinement methods are required. Two of the most powerful methods currently available for refining this type of data are RMCProfile and PDFFIT. The aim of this workshop is to provide an overview of the methods and the opportunity to gain some hands-on experience of applying them to total scattering data. No previous experience is required. For more information about the PDF workshop please email **Matt Tucker** (m.g.tucker@rl.ac.uk) or **Ivana Evans** (ivana.radosavljevic@durham.ac.uk).

DASH Workshop (Tuesday 17:15-18:30)

Organisers: **Richard Cooper** (Oxray) & **Kenneth Shankland** (ISIS)

Kenneth Shankland will be running a hands-on workshop in the computing lab, using the DASH software. DASH is a program for crystal structure determination from powder diffraction data. This workshop is aimed at students and researchers who have no previous experience using DASH and who are interested in structure determination from powders.

For more information please email **Richard Cooper** (richard.cooper@oxray.com) or contact **Kenneth Shankland**.

Olex2 Workshop (Thursday)

Organisers: **Horst Puschmann** and **Oleg Dolomanov** (Durham)

Immediately following the main BCA Spring Meeting, an Olex2 Workshop will be held on the afternoon of Thursday 10th April, 2008. Olex2 is free software which is developed in collaboration between Oxford and Durham Universities. It is aimed at making working with molecular crystal structures easy and intuitive while giving experienced crystallographers access to powerful new modelling and refinement tools (http://www.olex2.org).

The workshop is suitable for crystallographers of all levels of experience. For further information and registration, please contact us at horst.puschmann@durham.ac.uk.

Young Crystallographers at York: 7-8 April 2007

Monday 7th April: 12:00-13:00: Registration

13:00 Welcome: **Simon Coles** (University of Southampton)

SESSION 1: 13:00-15:30: *Chair:* **Susanne Huth**

13:00-13:30: Plenary: **Ehmke Pohl** (Durham University) *Why is macromolecular crystallization so difficult, and why do we still obtain suitable crystals?*

13:30-13:45: **Gordon Cunningham** (University of Glasgow) *Application of High-Throughput Cluster Analysis to Multiple Data Types - Differential Scanning Calorimetry and Infrared Data*

13:45-14:00: **Alexandra Bowyer** (University of Southampton) *DAD - A Possible Enzyme for Safely Degrading Pollutant Hydrocarbons*

14:00-14:15: **Shaun Evans** (University of Edinburgh) *Structures and transitions in light lanthanides at high pressure*

14:15-14:30: **Anthony Reilly** (University of Edinburgh) *A molecular dynamics approach to equilibrium structures in crystals*

14:30-14:45: **Marc Schmidtmann** (University of Glasgow) *H-transfer and polymorphism in IN2-OA*

14:45-15:00: **Richard Gildea** (Durham University) *Olex2: The New Molecular Tool*

15:00-15:30: Tea & Coffee

SESSION 2: 15:10-17:00 Chair: **Duncan Sneddon**

15:30-16:00: Plenary: **David Allan** (Diamond) *Beamline I19: A Facility for Small-Molecule Single-Crystal Diffraction at Diamond*

16:00-16:15: **Leo Chavas** (University of Manchester) *Structural studies on vesicle trafficking: atomic model of Rab27a:Exophilin4/Slp2-a complex*

16:15-16:30: **Stefanie Schiffers** (University of Bath) *Solid state reactions with photocrystallography*

16:30-16:45: **Helen Maynard** (University of Edinburgh) *Evidence for a new phase of Methane*

16:45-17:00: **Graham Stinton** (University of Edinburgh) *The Structure of Molecular Nitrogen at High Pressure using X-ray Diffraction and Maximum Entropy Maps*

17:00-17:30: Break

SESSION 3: 17:30-19:00: Chair: **Alex Griffin**

17:30-18:00: Annual General Meeting - Elections

18:00-19:00: Flash Presentations - 1 minute presentations for Poster Contributors

19:00-21:00: Buffet Dinner and Poster Session with wine!

Tuesday 8th April:

SESSION 4: 09:00-11:00: Chair: **Mike Probert**

09:00-09:30: Plenary: **David Beveridge** (HARMAN technology Ltd.) *Crystals, Grots and X-rays*

09:30-09:45: **Mark Warren** (University of Bath) *Time-resolved photocrystallgraphic investigation of metastable species*

09:45-10:00: **Riccardo Montis** (University of Southampton) *A Simple Salt with a Complex Structure; 4-Aminopyridine Hydrochloride with Z' = 30*!

10:00-10:15: **Lorreta Lawton** (University of Glasgow) *Magnetic Coupling in model cubic V, Ni and Cu structures comprised of interlinking HF_2^-, HCl_2^- and $HFCl^-$ ligands*

10:15-10:30: **Iain Oswald** (University of Edinburgh) *High pressure structural studies of energetic materials*

10:30-10:45: **Susanne Huth** (University of Southampton) *Crystal Chemistry of Functionalised Organic Molecules. A Structural Systematics Approach*

10:45-11:00: **Andy ONeill** (University of Glasgow) *Nucleation studies of substituted aromatic compounds*

11:00-11:05: Closing Remarks

11:05-11:30: *Registration for main meeting*

BCA 2008 Spring Meeting -

	Monday, 7th April		Tuesday, 8th April		
9:00			**YC 4**	**PDF workshop**	
9:15					
9:30					
9:45					
10:00					
10:15					
10:30			Registration/exhibition 10.30-11.30		
10:45					
11:00					
11:15					
11:30			BCA Prize Lecture and BSG Plenary 11.30-12.30 From Molecular Replacement to the Structure of Viruses: a Tale of Two Careers		
11:45					
12:00					
12:15					
12:30			Lunch/Exhibition/Registration 12.30-13.30		
12:45					
13:00	**YC 1**	PDF workshop	Sessions 13.30-15.00		
13:15					
13:30					
13:45			Local structure	Membrane proteins	Pharmaceutical powder diffraction
14:00					
14:15					
14:30					
14:45					
15:00	**Coffee 15.00-15.30**		Coffee 15.00-15.30		
15:15					
15:30	**YC 2**	PDF workshop	Sessions 15.30-17.00		
15:45					
16:00			CCG Prize PCG Prize	Membrane proteins	Hydration of pharmaceutical materials
16:15					
16:30					
16:45					
17:00	**Break**	Break	Break 15 minutes		
17:15			Exhibitors Forum 17.15-18.45		DASH workshop
17:30	**YC 3**	PDF workshop			
17:45					
18:00					
18:15					
18:30					
18:45	**Break**	Break	Dinner, exhibition and posters		
19:00	**YC dinner**	Dinner			
19:15					
19:30					
19:45					
20:00					
20:15					
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20:45					
21:00					

Timetable

<table>
<tr><th colspan="3">Wednesday, 9th April</th><th colspan="3">Thursday, 10th April</th></tr>
<tr><td colspan="3">PCG Plenary 9.00-9.45
Charge Order in Oxides:
Putting the Fun into Functional Materials</td><td colspan="3">Teaching Plenary 9.00-9.45
Controlling Difficult Refinements</td></tr>
<tr><td colspan="3">Coffee 9.45-10.15</td><td colspan="3">Coffee 9.45-10.15</td></tr>
<tr><td colspan="3">Parallel sessions 10.15-11.45</td><td colspan="3">Sessions 10.15-11.45</td></tr>
<tr><td>Functional extended solids</td><td>Neutrons in biology</td><td>Applied crystallography</td><td>Strongly correlated systems</td><td>Ligand binding and drug design</td><td>Design of functional materials</td></tr>
<tr><td>PCG AGM
11.45-12.30</td><td>BSG AGM
11.45-12.30</td><td>IG AGM
11.45-12.30</td><td colspan="3">Break 15 minutes
Sessions 12.00-13.30</td></tr>
<tr><td colspan="3">Lunch, Exhibition 11.45-13.30</td><td rowspan="2">Strongly correlated systems</td><td rowspan="2">Ligand binding and drug design</td><td rowspan="2">Calculating properties from structure</td></tr>
<tr><td colspan="2"></td><td>CCG AGM
12.45-13.30</td></tr>
<tr><td colspan="3">Sessions 13.30-15.00</td><td colspan="3">Close 13.30</td></tr>
<tr><td>Functional molecular materials</td><td>Probing fast biological reactions</td><td>Small is smart</td><td colspan="3" rowspan="8">Olex2 Workshop</td></tr>
<tr><td colspan="3">Coffee 15.00-15.30</td></tr>
<tr><td colspan="3">Sessions 15.30-17.00</td></tr>
<tr><td>Functional molecular materials</td><td>Complementary methods in structural biology</td><td>Big is beautiful</td></tr>
<tr><td colspan="3">Break 15 minutes</td></tr>
<tr><td colspan="3">IG Plenary 17.15-18.00
IG: X-Ray Diffraction on Mars</td></tr>
<tr><td colspan="3">BCA AGM 18.00-19.00</td></tr>
<tr><td colspan="3">Comfort time</td></tr>
<tr><td colspan="3">Conference dinner 19.30 for 20.00</td></tr>
</table>

2008 Annual General Meeting of the BCA

THE Annual General Meeting of the British Crystallographic Association will be held on Wednesday 9th April 2008 at 6.00 p.m. in the University of York.

At this meeting we will elect a new Treasurer.

Draft Agenda

1. Approval of Agenda
2. Apologies for absence
3. Minutes of the last AGM (published in Crystallography News)
4. President's Report
5. Secretary's Annual Report
6. Northern Networking Events' Report
7. Report of the Treasurer to include Presentation of the Accounts for 2007 and the Examining Accountant's Report
8. Acceptance of the Accounts
9. Election to Council
10. Appointment of Examining Accountant for 2008
11. Any other business

Georgina Rosair (Secretary)

From the Secretary

Announcement of elections to Council

AT the 2008 Annual Meeting in Canterbury we will elect a new Treasurer of Council as the present incumbent has reached the end of her term. There are no other vacancies on Council this year. Nominations for this post is invited. Each nomination requires a proposer and seconder, and, should you wish to nominate someone, please obtain their consent first. Properly seconded nominations will be received up till two weeks before the date of the AGM which is on 9th April 2008. They may be sent by email to secretary@crystallography.org.uk

Georgina Rosair
Secretary to Council

Minutes of Annual General Meeting held on Wednesday, 18th April 2007 at 17.00 in The University of Kent

The President (Paul Raithby) in the Chair

95 VOTING MEMBERS WERE PRESENT

1. Approval of agenda
The agenda was approved.

2. Apologies for absence
There were no apologies for absence.

3. The Minutes of the last meeting were approved
(proposed: Simon Parsons, seconded: Lindsay Sawyer)

4. President's Report
The President said that this has been a successful year for the BCA with all the groups being very active through the year and this meeting being attended by 370 people. He welcomed the XRF group to this Spring Meeting and thanked Lindsay Sawyer for his excellent programme, as well as the organisers and sponsors.

The Young Crystallographers were also welcomed, over 70 of them; they are forming their own Group which has the approval of Council. A "Brains Trust" is being set up to "preach the good news" of crystallography to universities and schools. He reported that a new post (Education Coordinator) has been created, who would be co-opted on to Council, in post for 3 years but open to election considering the importance of the role to the BCA. He announced that we had online registration for the meeting for the first time and that the website development was ongoing.

The President recorded that after a tendering process the Northern Networking Events contract had been renewed for a further five years.

He led a minute's silence to honour the memory of Glen Smith.

Officers approved the election of Prof Mike Hursthouse to honorary membership of the BCA. There are now 16 honorary members of the BCA .

He thanked the Secretary and Vice President for their hard work. He also recorded that Bob Gould would like to retire as Newsletter Editor. Finally he said that the poster prizes would be announced at dinner.

There were no questions.

5. The Secretary's Report had already been distributed, and appears in the June 2007 issue of Crystallography News.

6. An election was held for the position of Vice-President, and after a secret ballot, Sandy Blake was deemed elected. Georgina Rosair was elected unopposed as the new Secretary. Chick Wilson was elected unopposed as Education Officer; nominated by Alex Griffin, seconded by Andy Parkin.

7. Northern Networking report
Gill Moore reported that there were 370 delegates with 74 Young crystallographers. 67 delegates were attending the Sam Motherwell event.

There were 99 posters, and for the first time the abstracts had been handled by Northern Networking. Although there had been a few technical problems these would addressed by next year. The exhibition had attracted 27 companies with a waiting list of 6. Gill thanked each of the exhibitors and Lindsay Sawyer and Elaine Fulton.

BCA membership stands at 743 (704 in 2006), by group there are 210 biological, 249 chemical, 92 physical, 78 inorganic, 114 not specified members. The 100th edition of Crystallography News was produced; she thanked Bob Gould for his editorship and the sponsors of CN. There are 16 Corporate members, 2 less than last year, due to budgetary constraints.

Questions raised:
Jeremy Cockcroft asked if the registration desk could be open the day before the meeting starts from lunchtime. Gill replied that it was open until quite late in the evening. He also raised the issue of lectures and exhibition being located too far from each other, and she replied that the lecture rooms booked were not what the BCA were eventually given, she apologised that the wireless network did not work for many people, these issues will be taken up with Kent University.

More detailed signage, room numbers in the conference book synopsis, and location map with registration documentation were also requested.

8. Treasurer's report.
Sheila Gould presented the Treasurer's report, which was distributed separately, and appears in the June 2007 issue of Crystallography News.

John Finney proposed that the accounts be accepted, seconded by Georgina Rosair.

Jeremy Cockcroft asked how many members paid Gift Aid. Sheila answered that about 300 out of 700 did so and encouraged more members to sign up for this. It was proposed that R. Young be retained as accountants; proposed Nick Keep and seconded by Georgina Rosair.

There being no further business, the meeting closed at 17.45.

Christine Cardin
Hon. Secretary

Bursary Report 2007 from the Treasurer

THE BCA is always pleased to fulfil its duties to further the education of crystallographers by supporting them financially to attend meetings relevant to their research activities, and we do appreciate the generous donations to the Arnold Beevers Bursary Fund which enable these bursaries to be awarded. This year the BSG donated £829.38, the interest from its reserves, to the fund and the Gift Aid refund of £1,558.30 on the membership subscriptions was also placed in the fund. Other membership donations amounted to £136.50, and there was an individual donation of £600.00.

There were 30 bursaries worth £175 awarded to students attending the Spring meeting at the University of Kent in Canterbury. 10 of these Bursaries had commercial sponsors, and we are very grateful to ICDD (3), Incoatec (1), PANalytical (4) and Rigaku (2) for this valuable support.

During the rest of the year, there were 6 Arnold Beevers Bursaries awarded, totalling £1,050. Many of the bursars' reports of these meetings have been incorporated into the articles which have been printed in Crystallography News.

ECM-24 Marrakech
Stephen Cairns (University of Glasgow)

Workshop on XD2006, Martina Franca, Italy
Peter Byrne (St Andrews' University)

15th International Conference on Crystal Growth, Salt Lake City
Michael Orley (University of Leeds)
Spoorthi Dharmayat (University of Leeds)

ETOX13 European Workshop on Bacterial Protein Toxins, San Martino al Cimino
David Albesa-Jove (Imperial College)

Gordon Conference on Electron Distribution and Chemical Bonding, Mount Holyoke, USA
Michael Probert (Durham University)

The BCA also donated £2000 to the 11th BCA/CCG Intensive Course in X-Ray Structural Analysis, Durham.

IUCr Congress Bursary Fund
The BCA Council offered the money in this fund on loan to the organising committee of the XXI Congress in Osaka, Japan in 2008, but the offer was not taken up this time.

Sheila Gould

Crystal Growth

The 15th International Conference on Crystal Growth, Salt Lake City, Utah August 12-17 2007

THE 15th International Conference on Crystal Growth (ICCG), held in conjunction with the 13th International Conference on Vapour Growth and Epitaxy (ICVGE) and the 13th Biennial Workshop on Organometallic Vapour Phase Epitaxy (OMVPE) was attended by over 700 delegates from more than twenty different countries. Salt Lake City, USA, nestled between the Great Salt Lake and the steep, glacially carved Oquirrh and Wasatch mountain ranges on the edge of the Rocky Mountains played host to the conference, providing breath-taking scenic views worthy of a second visit.

The conference itself was held in the luxurious 24-story Grand America Hotel that was built especially for the 2002 Winter Olympics.

The meeting was excellently organised by the American Association of Crystal Growth (AACG) and included topics such as the fundamentals of crystal growth, thin film growth and epitaxy, crystal growth under applied external fields, bulk crystal growth, growth of quantum dots, wires and nanocrystals, novel materials, crystal growth technology, *in-situ* measurements and characterisation of crystal growth, and also extensive sessions on the biological control of crystallisation - a topic not usually included in an ICCG programme.

The programme consisted of a total of six plenary lectures and three prize lectures over the course of the meeting and a choice of six parallel sessions every day.

The plenary lectures covered talks by notable speakers from each of the main sessions. **Jim DeYoreo** from the Lawrence Livermore National Laboratories introduced the Biological Control of Crystallisation session in his talk entitled *Biomolecular Controls over Templated Nucleation and Growth of Crystals*. Here he highlighted the control exerted on the growth of crystals from solution in many biomineral structures ranging from kidney stones to ice crystals found in the blood of arctic fish. The challenge in this particular field was linking the surface energetics of growing crystal, in particular the biomolecule-crystal interactions, with the physical landscape of the crystal surfaces manifested in the growth morphology and kinetics. A combination of *in-situ* Atomic Force Microscopy (AFM) and molecular modelling was used to modify the crystal interactions to alter the energy barrier and free energy minima which are related to the growth kinetics and crystal morphology, respectively. The Bulk Crystal Growth and Crystal Growth Technology session was covered by **Takamoto Sasaki** from Osaka University where a wide range of solution grown materials were reviewed from NLO crystals to crystals in electro-optical applications, most notably caesium lithium borate grown from high temperature fluxes. The work highlighted the importance of crystal perfection in terms of laser dominance threshold. The importance of achieving efficient mixing of the high viscosity solution fluxes was stressed in terms of obtaining good crystals.

Lars Samuelson of Lund University, **George Craford** of Phillips-Lumileds and **Peter Rudolph** from the Institute for Crystal Growth in Berlin led the plenary sessions on the Growth of Quantum Dots, Wires and Nanocrystals, Novel Materials and Crystal Growth under Applied External Fields. Lars Samuelson reviewed the nanowire technology aiming at producing structures of 10nm size from the current capability at 50nm and the development of III-V compound devices operating with nanowire configuration. Metal organic chemical vapour deposition (MOCVD) method was used to prepare the nanowires using Au nanoparticles as catalyst and the wires were found to preferentially align along <111>. The work showed the development of stacking faults with different packing arrangements and stressed that the challenge in this field is to control growth process and guide the development of the wire structure at an atomic scale.

The development of high power LED's was reviewed by George Craford where the work highlighted the major challenge as being able to set full performance across the visible spectra, notably in green, thus achieving full colour capabilities via spectral mixing. The importance of not just one spectral generation but also the maximising of light extraction via fabrication methods to reduce light re-absorption was highlighted. Finally, a brief overview of the growing application of white LED's in specialist home lighting, mobile phone/camera flash, car lighting etc was given. The current cost base of this technology is, however, along with thermal management issues, the major barrier to wide implementation. Peter Rudolph's talk focused on the crystal growth from melt and the use of magnetic fields to enhance mixing and prevent temperature fluctuations in the melt. Applications to organic crystals were also shown and the work highlighted the demand for accurate 3D modelling studies of turbulence in melts.

The last, and perhaps one of the most enjoyable plenary sessions, was **Greg H Olsen**'s (GHO Ventures) account as a crystal grower in space which encompassed over 900 hours of

training including physical and survival training, learning about the International Space Station (ISS) Systems, fire fighting, zero gravity training and also Russian. Greg, with interests in growing III-V components for Infra-red/remote sensing, was able to fund his own trip through his company and spent 7 days as a private citizen on board the Soyuz spacecraft. However, no crystals were grown during this trip and the future prognosis for crystal science in space does not look very promising, as the planned shuttle flights are mostly mission oriented.

Among the many different parallel sessions attended throughout the conference, the most notable and enlightening talks were **Peter Vekilov**'s (University of Houston) *Nucleation of sickle-cell haemoglobin polymers and sickle-cell anaemia: a new outlook* and **Marcel Rost**'s (University of Leiden) *Polycrystalline film growth observed in real-time using in-situ Scanning Tunnelling Microscopy* (STM).

Peter Vekilov gave a brief overview of sickle-cell anaemia, a chronic and lifelong genetic disorder that considerably shortens the life expectancy of sufferers and is thought to be caused by red blood cells undergoing changes in shape upon de-oxygenation due to the polymerisation of the sickle-cell haemoglobin (HbS). This causes the HbS to stick together, making the cell rigid and sickle shaped leading to the blocking of blood vessels, thus depriving downstream tissues of oxygen. The HbS polymerisation follows a first order transition which starts with nucleation, heteronucleation in particular, and leads to the thickening of polymers. The work speculated on the possibility of stopping polymerisation of HbS to stop sickle-cell anaemia and found that the incorporation of HbS molecule into fibres has high transition-state entropy and that nucleation follows a two-step mechanism where the fibres were found to nucleate in highly viscous droplets within 100-1000nm size range. Both these observations suggest a novel control mechanism which can lead to the development of novel treatment strategies.

Marcel Rost's talk followed on from his colleague's talk which had highlighted the challenges faced in the development of a new Laser Confocal Microscope (LCM) capable of video-rate imaging during film growth with 10 frames per second compared to the older technology with a rate of 10 seconds per frame. Its application was demonstrated in Marcel Rost's talk where real observation of film growth was carried out on a crystal surface with very good resolution that showed the nucleation and progression of 2D islands. The talk focused on the growth kinetics and impurity effects observed in gel solutions and it was found that the 2D nucleation rate is enhanced in both cases due to the gel fibres acting as heteronucleation sites and as an impurity filter.

Despite a heavily scheduled conference programme, the social aspect was not compromised in any way. Those of us who arrived early took advantage of a visit to the regular Sunday morning concert given by the world famous Mormon Tabernacle Choir. This concert series, broadcast live on TV/radio, has continued uninterrupted for the last 78 years.

The conference social activities were excellent and included a welcome reception and conference dinner, providing the perfect opportunity to meet and socialize with the many delegates.

The social program also offered a choice of three excursions to explore the most famous places of interest around Salt Lake City: Utah Olympic Park and Park City, Snowbird Mountain Resort and the Great Salt Lake and Kennecott Copper Mine. We took the coach trip to the Snowbird Mountain resort in the Wasatch Mountain region where a short but thrilling aerial tram ride took us to the 'Roof of the Rockies' with breathtaking vistas unfolding in every direction. With a storm close to our heels, or rather faces, at 11000ft up, hiking some of the way back, the descent from the top of the mountain was certainly interesting. The mountain resort was followed by a heritage visit to the historic theme park which re-created 19th century Mormon pioneer life and included supper and country music.

With whatever reservations one might have approached the setting of the ICCG conference in Salt Lake City, the whole experience exceeded our expectations and we are grateful to the **BCA Arnold Beevers Bursary** for helping us fund the travel. We found the conference to be thoroughly enjoyable and the setting to be pleasantly cosmopolitan with many good restaurants, bars and their own local brewery that makes decent beer. And with names such as 'Capitan Bastard's Oatmeal Stout' and 'Polygamy Porter' the humour can be certainly appreciated. The next ICCG-16 conference will be held in Beijing, China in 2010 followed by ICCG-17 in Warsaw, Poland in 2013.

Spoorthi Dharmayat and Mike Orley
University of Leeds

Ewald Prize for David Sayre

THE IUCr is pleased to announce that Dr D. Sayre (Department of Physics, State University of New York, Stony Brook, NY 11794, USA) has been awarded the eighth Ewald Prize for the unique breadth of his contributions to crystallography, which range from seminal contributions to the solving of the phase problem to the complex physics of imaging generic objects by X-ray diffraction and microscopy, and for never losing touch with the physical reality of the processes involved.

The presentation of the Ewald Prize will be made during the Osaka Congress Opening Ceremony on 23 August 2008.

Mike Dacombe, IUCr

From Atoms to Patterns

From Atoms to Patterns: Crystal Structure Designs from the 1951 Festival of Britain

HAEMOGLOBIN dress fabrics…aluminium hydroxide ties…insulin wallpapers…quartz carpets... pentaerythritol ashtrays…apophyllite window glass… afwillite curtains….

A groundbreaking exhibition created by London's Wellcome Collection will, for the first time, bring together the unique and stylish materials designed by the Festival Pattern Group for the 1951 Festival of Britain.

Everyday products decorated with patterns based on crystal structures are the subject of this innovative show, which brings together an eclectic array of textiles, wallpapers, fashion, furniture, laminates, carpets and tableware. Drawings of atomic structures will sit alongside the designs they inspired reflecting the unique collaboration between Britain's leading post-war scientists and manufacturers.

From Atoms to Patterns:
24 April - 10 August 2008
Press Preview:
23 April 2008 (Contact Mike Findlay for details)
Venue:
Wellcome Collection,
183 Euston Road,
London NW1 2BE
www.wellcomecollection.org.uk
Admission FREE
Gallery opening times:
Tues-Wed, Fri-Sat: 10.00-18.00 / Thurs: 10.00-22.00
Sun: 11.00-18.00; Closed Mon (except Bank Holidays: 10.00-18.00)

The 1951 Festival of Britain provided an extraordinary platform for British ingenuity and creativity in science and the arts. One of the boldest initiatives within the Festival was the Festival Pattern Group, which brought together adventurous manufacturers with cutting edge crystallographers to create a collection of quirky furnishing designs.

Inspired by the intricate patterns of crystal structures, Dr **Helen Megaw** came up with the novel idea of using them for textiles. As scientific consultant to the Festival Pattern Group, she collated crystal structure diagrams from eminent colleagues and ensured that they were interpreted in an accurate and authentic way. The project was spearheaded by the Council of Industrial Design: they enlisted the manufacturers, vetted the designs and organised special displays at the Festival of Britain - notably in the Regatta Restaurant on the South Bank, which was kitted out with crystal structure furnishings, and the Exhibition of Science at South Kensington.

The Festival Pattern Group's products included ICI 'leathercloth', Dunlop pvc, Wedgwood china, Chance glass, John Line wallpapers, Warerite laminates and Warner fabrics. Other crystallographers involved in the project included **Lawrence Bragg**, **Dorothy Hodgkin**, **John Kendrew** and **Max Perutz** .

Science enjoyed great popular appeal during the early post-war period, and X-ray crystallography was one of the most exciting fields of science at the time, when **Rosalind Franklin**'s X-ray diffraction photographs, taken at King's College London, provided crucial visual evidence for **Francis Crick** and **James Watson**'s landmark discovery of the double helix structure of DNA in 1953.

Hidden away for over 50 years in the vaults of the Victoria & Albert Museum and the Science Museum, the Festival Pattern Group's creations have been reunited *en masse,* for the first time since 1951. Significantly too, From Atoms to Patterns provides the first ever opportunity to view these products alongside their original source material - dyeline drawings of crystal structures. The displays will also elucidate the mysteries of X-ray crystallography to non-specialists, and trace the process from diagram to design.

The exhibition features a diverse and eclectic range of exhibits, including:

- Rayon dress fabrics and nitrocellulose-coated 'leathercloth' printed with the molecular structure of haemoglobin.
- Tie silks woven with ball-and-spoke atomic structures of chalk and china clay.
- Plastic laminates and wallpapers adorned with intricate insulin motifs.
- Lace embroidered with the crystal structures of beryl (emerald) and aluminium hydroxide (hydrargillite).
- Carpets emblazoned with patterns derived from the chemical compound resorcinol.
- Relief-patterned window glass evoking the atomic structure of the mineral apophyllite.
- Fluid abstract-patterned curtains based on diagrams of afwillite, a hydrated calcium silicate formed during the setting of cement.

Guest curator: **Lesley Jackson** (Writer, Curator and Design Historian specialising in post-war design)
Co-Curator: **Emily Jo Sargent** (Curator, Wellcome Trust)

Accompanying publication:

From Atoms to Patterns - Crystal Structure Designs from the 1951 Festival of Britain
by **Lesley Jackso**n, published by **Richard Dennis** Publications in association with the Wellcome Trust.

- Tells the fascinating story of the Festival Pattern Group and how it came about.
- Provides background information about the 28 manufacturers involved in the scheme and documents all the products they created.
- Illustrates pages from the original Souvenir Book of Crystal Designs and archive photographs from the Festival of Britain.
- An A-Z of Crystal Structures provides a glossary of materials and traces the scientific sources of the diagrams.
- Also includes biographical information about the crystallographers and excerpts from **Helen Megaw**'s notes.

Event details

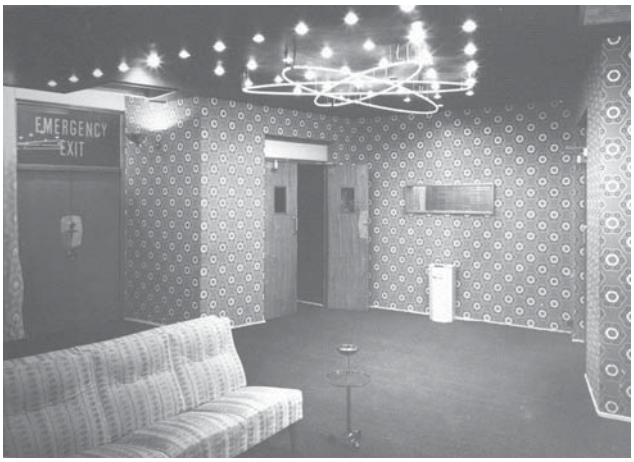
From Atoms to Patterns
24 April - 10 August 2008
Thursday 15 or 22 May
Women in science
A discussion evening in the Forum of Wellcome Collection on the role of women in science from the Festival of Britain to today. What is the position of women in science in the UK and abroad, what challenges do they face and what has been done to improve the situation? Speakers to be confirmed.

Timorous Beasties in Conversation
Saturday 21 June or Saturday 28 June

Alistair McAuley and **Paul Simmons**, textile and wallpaper designers at Timorous Beasties will discuss the role of science and medicine in their work. In 2006 Timorous Beasties created a window display for the Gibbs Building. The display of oversized lampshades and lace curtain featured scientific images from the Wellcome Library.

The Wellcome Trust is the largest charity in the UK. It funds innovative biomedical research, in the UK and internationally, spending around £500 million each year to support the brightest scientists with the best ideas. The Wellcome Trust supports public debate about biomedical research and its impact on health and wellbeing. http://www.wellcome.ac.uk

The Wellcome Trust's former headquarters, the Wellcome Building on London's Euston Road, has been redesigned by Hopkins Architects to become a new £30 million public venue. Free to all, the Wellcome Collection explores the connections between medicine, life and art in the past, present and future. The building comprises three galleries, a public events space, the Wellcome Library, a café, a bookshop, conference facilities and a members' club. http://www.wellcomecollection.org



Festival Pattern Group furnishings in cinema foyer at the Exhibition of Science, South Kensington, Festival of Britain, 1951. Interior includes Myoglobin upholstery designed by Charles C. Garnier for ICI Leathercloth on benches (crystallographer Dr John Kendrew) and Insulin wallpaper designed by Robert Sevant for John Line & Sons (crystallographer Dr Dorothy Hodgkin).
Photo credit: The National Archives

Printed bone china plate based on the crystal structure of beryl, designed by Peter Wall for Wedgwood (crystallographer Sir Lawrence Bragg), part of the Festival Pattern Group, Festival of Britain, 1951.
Photo credit: V&A Images / Victoria and Albert Museum, London

Plastic laminate based on the crystal structure of insulin, designed by Martyn O. Rowlands for Warerite (crystallographer Dr Dorothy Hodgkin), part of the Festival Pattern Group, Festival of Britain, 1951.
Photo credit: V&A Images / Victoria and Albert Museum, London

News from the Groups

News from the Biological Structure Group

Biological Structures Group Sessions at BCA Spring Meeting

A strong Biological programme has been coordinated for the 2008 BCA spring meeting. Tony Crowther will be presenting the plenary lecture entitled 'From Molecular Replacement to the Structure of Viruses: a Tale of Two Careers'. There will also be sessions covering membrane proteins, neutrons in biology, probing fast biological reactions, complementary methods in structural biology, and ligand binding and drug design.

Biological Structure Group AGM.

This was held at the BSG Winter meeting. The full minutes will be published elsewhere. Elections were held for the posts of Treasurer, Secretary and a vacant committee member position. The current committee comprises **Andrea Hadfield** (Chairman, University of Bristol); **Vilmos Fulop** (Vice-chairman, University of Warwick); **Nick Keep** (Treasurer; Birkbeck College); **Darren Thompson** (Secretary, University of Sussex); **Kate Brown** (Imperial College); **Jon Cooper** (Webmaster, Southampton University); **Pierre Rizkallah** (Daresbury Laboratory); Dr. **Neera Borkakoti** (Medevir); **Sheila Gover** and **Snezana Djordjevic** (School of Pharmacy, University of London).

Biological Structures Group Winter Meeting 2008

The BSG winter meeting will be held at the University of Newcastle in 2008, and will be organised by **Richard Lewis**.

Darren Thompson, Secretary
(D.Thompson@sussex.ac.uk)

Structural Investigations of Gene Regulation - BSG winter meeting

Organisers: **Snezana Djordjevic** (UCL) and **Gary Parkinson** (SOP)

On Tuesday December 18th (2008) a well-attended BSG winter meeting took place in the heart of Bloomsbury, a district of London famous for its architecture, gardened squares and literary connections, not to mention hospitals, museums, libraries and academic institutions.

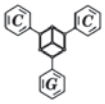
The first speaker, **Laurence Pearl** (ICR, London), eloquently described the range and role of post-translational modifications affecting histone proteins and their involvement in regulating gene expression. He then described the structure of CARM1 (Co-activator Associated aRginine Methyltransferase), a protein involved in the formation of a multi-protein complex that methylates the histone tails of nucleosomes. He also described how his group had made a chimaeric protein comprised of CARM1 and part of histone H3 in order to define the binding of the substrate arginine residue to the enzyme. Next, **Udo Oppermann** (SGC, Oxford) described a class of nuclear enzyme that catalyses the demethylation of histone lysine residues in an oxoglutarate- and iron-dependent manner. The structure of the histone demethylase (JMJD2A), which possesses a 'jumunji' domain, was solved with various lysine-containing peptides bound to it, revealing much about the enzyme's specificity and the mechanism of iron-dependent oxo-ferryl attack on the substrate. **Maria Jose Sanchez-Barrena** (MRC-LMB, Cambridge) then described the structure of an elegant complex involving 'Pygo' PHD and HD1 domains. This complex recognises methylated histone tails and is involved in the 'Wnt' signalling pathway. Last, but not least, of the morning speakers was **Daniela Rhodes** (MRC-LMB, Cambridge) who described the stalwart efforts by her group to define the structure of the 30nm chromatin fibre using cryo-electron microscopy. Success hinged on the use of reconstituted nucleosomes formed from a DNA sequence repeat with high affinity for core-particles. End-on views of short fibres captured on ice allowed a model of the arrangement of histone core particles to be devised. The data are most consistent with an 'interdigitated one-start helix model'.

After lunch and posters in the exhibition area, participants were enticed back to the lecture theatre where **Tracey Barrett** (Birkbeck, London) described the role of the NF-kappaB pathway in the control of apoptosis. One cellular anti-apoptotic protein, known colloquially as FLIP, possesses a (subtly named) death-effector domain (or DED for short) and has a harmful homologue in the Kaposi sarcoma tumor virus. The structure of a vFLIP - kinase complex was described suggesting how the NF-kappaB pathway is activated. Next, **Stefan Knapp** (SGC, Oxford) presented a review of the structure and function of members of the 'kinome' - enzymes better known as protein kinases, along

with recent contributions from his group to the field. Stefan emphasised the role of a key loop in dimerisation of the enzyme which is important for its activation and is enhanced by phosphorylation. **Rick Lewis** (Newcastle) then gave a vivid presentation of molecular stress-management in *B. subtilis* as facilitated by the RsbR-RsbS-RsbT complex. EM has shown that this forms icosahedral structures or 'stressosomes' with symmetry that Rick likened to transverse sections of quinces and eucalyptus pods.

After much needed coffee, **Stephen Curry** (Imperial, London) described the X-ray and NMR structures of a nuclear protein, known as La, which binds the 5' untranslated region of RNA transcripts, initiating their processing and translation. The complexes with various oligonucleotides bound to La were described. Next, **Jon Hadden** (Leeds) outlined painstaking efforts to crystallise a complex of the phage T7 endonuclease with a synthetic Holliday junction. Over 100 crystals were screened to find one which allowed the structure to be solved to 3.1 Å resolution showing how this domain-swapped, dimeric protein grips the DNA junction. **Xiaodong Zhang** (Imperial, London) then described work involving X-ray crystallographic and EM reconstruction studies of sigma54-factor complexed with RNA polymerase. In the 'closed' complex, the sigma factor was found to block the channel through which the template strand would normally reach the RNA polymerase active site. Last, but not least, **Alona Sosinsky** (Birkbeck, London) elegantly presented an analysis of the DNA recognition motif of 'homeo-box' recognition or Hox proteins. Binding of arginine into the minor groove and compression of the latter are common features of these DNA binding proteins. This concluded a very memorable meeting and the organisers are thanked for putting together an excellent programme.

Jon Cooper
University of Southampton



CCG Autumn Meeting 2007

INTRODUCTION

This year's autumn meeting was held on the 14th of November at the UK's new synchrotron, Diamond Light Source, with an appropriate subject of 'Chemical Crystallography at Diamond'.

The journey from Edinburgh to Oxford is always an arduous one, especially when four fully grown men are confined to one small car on the M6 for the best part of ten hours. This is what happened when we made our first visit to Diamond back in August for the user meeting. This time, however, the group decided that I would have to get over my fear of flying and take the plane. The journey was thankfully a lot shorter than the previous trip and when we arrived, we were once again awestruck by Diamond's exceptionally futuristic appearance. To have the meeting held in such a place as this was an enormous privilege. It was indeed to be an interesting day.

Despite the fairly specialised theme the turnout of crystallographers at this years CCG autumn meeting was as good as in previous years. Undoubtedly, the opportunity to take a guided tour of the new synchrotron laboratories was part of the attraction for many people that were first time visitors to the newly built facility.

The meeting started off with an inspiring lecture by Prof **Peter Luger** of the Free University of Berlin during which he demonstrated how synchrotron radiation is utilised in charge density studies. Very impressive was the number of quality high-resolution data sets that had been obtained at the synchrotron sources HASYLAB and SLS and that were used to resolve the electron density distribution of small molecules like thymidine as well as bigger systems such as Vitamin B12. In the second part of his talk, he presented the results of charge density studies on oligopeptides, work that is concerned with the construction of an electron density database and the concept of INVARIOMS.

Dr **Dave Allan** gave an extremely interesting account of Diamond's new small-molecule single-crystal diffraction beam line I19. The talk gave a detailed description of the layout of the two new diffractometer systems, the first being a user friendly high-throughput assembly with an automated sample changer, and the second, a larger diffractometer used for bulky samples with a cooling system, capable of reaching temperatures as low as 4K. Particularly interesting was the new PILATUS 300K detector which has the ability to count photons, meaning real time frames and the promise of much faster data collection.

Paul Raithby (University of Bath) showed us how, with the rapid advances in modern technology, the ability to monitor solid-state reactions as they occur has become much more commonplace. He introduced us to the fascinating technique of photocrystallography, amusing us with his liberal use of pond-liner and enthralling us with the characterization of exciting new metastable states of SO_2 and NO_2 complexes, which undergo linkage isomerism upon photoactivation. Paul ended his talk by illustrating the point that station I19 at Diamond will provide the

photocrystallographic techniques necessary to develop *time resolved crystallography* in the UK.

Stephen Moggach (University of Edinburgh) continued the series presenting his work on a novel design of Beryllium-free Diamond Anvil cells using Tungsten carbide. He showed that synchrotron radiation improves the data by resolving problems that arise in high pressure studies such as data completeness and 3D peak resolution. Concluding his talk, he elaborated on the vast amount of time that can be saved using synchrotron radiation, *e.g.* the collection of 122 high-pressure data sets takes approximately 12 weeks with a standard laboratory source but only 2 weeks at the SRS - imagine how much faster this will be done at Diamond in the future!

Peter Byrne (PhD student, University of St. Andrews) sparked a lot of interest with his talk on the investigation of ionic liquids as potential templates and solvents for the synthesis of zeolites. A user of the beamlines 9.8 and 16.2 at the SRS, he demonstrated how PXRD is used to monitor material composition during ionothermal expansion of the metal organic frameworks in the zeotypes $GaPO_4$ and $AlPO_4$. He finished by presenting first studies of the charge density of the templating molecules as they reside in the framework pores.

Professor **Bill Clegg** (University of Newcastle) gave an almost nostalgic finale to this year's meeting, starting with a brief history of the ground-breaking station 9.8 at Daresbury SRS. Bill acknowledged the success that it has seen over the ten years that it has been a full user facility, highlighting some of the particularly interesting results. He then recognised the completion of the first six years of the provision of a national synchrotron crystallography service and discussed the prospects for the transfer of service operation to beamline I19. He finished with several publication highlights where he showed that the work of a synchrotron scientist is mainly focused on difficult samples. Thanks to them, highly disordered systems or Z' >1 crystal structures are made available to every chemist.

All together it was a very interesting event and thanks should go to the committee for organising yet another successful autumn meeting.

Russell Johnstone
University of Edinburgh

Susanne Huth
University of Southampton

CCG - Prizes

The CCDC Chemical Crystallography Prize for Younger Scientists 2008 has been awarded to Dr **Kirsty Anderson** from the University of Durham for her research into the phenomenon of structures with more than one molecule in the asymmetric unit (Z' > 1). She will be presented with the prize and will give a lecture entitled "Structures with Z' > 1" at the BCA Spring Meeting at York (Tuesday 8th April, 3.30pm).

"The CCG will be awarding two poster prizes this year: a cash prize for the best poster, and a copy of Volume A of International Tables for the best student poster kindly sponsored by the IUCr."

News from the industrial Group

The 25th ANNUAL GENERAL MEETING of the Industrial Group will be held at York on 9th April 2008 at 11:45

NOMINATIONS are sought to fill vacancies for two committee members to serve for three years from April 2008.

Nominations, which shall be proposed by not less than two members of the Group and shall be accompanied by the written consent of the nominee, shall be sent to reach the Honorary Secretary of the Group not later than seven days before the Annual General Meeting.

Secretary/Treasurer - Dr David Beveridge
HARMAN Technology Limited (ILFORD Photo),
Ilford Way, Mobberley, Knutsford, Cheshire. WA16 7JL
Tel: 01565 650000 Fax: 01565 872734
Email: david.beveridge@harmantechnology.com

The proposed constitutional changes can be found on the Industrial Group's web site:-

http://bca.cryst.bbk.ac.uk/bca/ig/news/n08-1text.htm#const

Forthcoming Meetings:

MINERALS and much more! - 14th May 2008, British Geological Survey (BGS), Keyworth, Nottingham.

http://bca.cryst.bbk.ac.uk/bca/ig/XRF/Meetings/meet08.htm

XRD and Minerals - 15th May 2008 , British Geological Survey (BGS), Keyworth, Nottingham.

http://bca.cryst.bbk.ac.uk/bca/ig/meet08MIN.htm

IG Autumn Meeting - 8th November 2007

http://bca.cryst.bbk.ac.uk/bca/ig/reps07AM.htm#a

The Industrial Group Autumn Meeting was held at the AstraZeneca Silk Road Business Park site in the outskirts of Macclesfield. The morning session focussed on Rietveld refinement and its applications; the afternoon session focussed on Crystallography in Industry.

The meeting was opened with a welcome from **Anne Kavanagh** (AstraZeneca) and **Steve Norval** (Intertek MSG). **Jeremy Cockcroft** (UCL) started the programme with a brief introduction to the Rietveld method, followed by a discussion of the pitfalls it can provide for the unwary user. Hugo Rietveld's original paper in 1969 referred to neutron diffraction, and recognised that peak positions are determined by the unit cell and may be affected by instrument set-up; peak area intensities are determined by the contents of the unit cell i.e. crystal structure; peak width is determined by the measurement resolution and is a fundamental parameter factor derivation, and peak shape is a convolution of many symmetric functions - in reality it is often very close to Gaussian.

Tony Bell (Daresbury) continued, looking at the transformation of waste iron oxide into commercially useful materials, using the bacterium *Geobacter sulferreducens*. He described how the bacterium can produce nanoparticulate magnetite (Fe_3O_4) by the reduction of amorphous Fe(III) oxyhydroxide. Synchrotron X-ray powder diffraction gave high-quality data. Topas Rietveld Refinement and Pair Distribution Function (PDF) software have been used to characterise the materials.

Steve Norval (Intertek MSG) spoke on application of Rietveld refinement in the real world. A basic and common limitation for many laboratories, especially in industry, is the reality of non-ideal materials. Real world materials often contain several phases, some of which can be of variable or uncertain composition. For example, boehmite (AlOOH) bio-protein carrier has been found to be a less effective carrier after freeze/thaw cycling. The aqueous gel was dried onto a silicon crystal surface. Rietveld refinement showed it to be very oriented.

Michela Brunelli (ESRF, Grenoble) has investigated hydrogen-bond patterns in organics and looked into temperature effects. A particular focus has been the analysis of new nitro-S proligands which have applications in Biometrics. The role played by water in the crystal structure of amino-acids has been found to be diverse.

Stuart Turner (Birkbeck College) described the experimental methods that have been used with the Rapid2 detector which is located at station 6.2 of the Synchrotron Radiation Source (SRS). Research undertaken has included studies of the dehydration of gypsum; and investigations of cement kiln feedstocks. He also talked about the different refinement methods in the Fullprof suite. He stressed the need for good initial models before undertaking batch refinements.

After an excellent lunch, the afternoon session - chaired by **Judith Shackleton** - was begun by **Ian Ferguson** (formerly UKAEA), who discussed what inverse pole figures are and how they can be used to obtain a detailed understanding of anomalous intensity and line positions in X-ray Powder Diffraction. They are produced by the projection of a pole figure onto an equatorial plane. A Nelson-Riley function is used. The figures reveal information about texture and cell-edge variations. He placed specific emphasis on their use in the metals industry.

Moataz Attallah (Materials Science Centre, University of Manchester) spoke next, on the use of synchrotron X-ray diffraction for characterising stresses in two-phase titanium linear friction welds. Linear Friction Welding (LFW) is a novel welding technology, which combines frictional heating and plastic deformation to join difficult-to-weld materials. He discussed the welding of the Ti-6246 two phase alloy used in the construction of parts of aeroengines. High pressures and temperatures are generated, and the materials are not melted - only softened. The material usage is much more efficient than with other welding methods.

Andrew Winn (Materials Testing and Analysis Unit, Manchester Materials Science Centre) described the study of residual stresses by XRPD. In XRPD it is strain that is measured and from this stress is calculated. The lattice planes are used as a strain gauge. Andrew uses the $\sin^2\psi$ method to calculate stress.

Robert Hammond (Leeds University) described how in-line XRPD had been applied to a flow-through cell for the quantitative analysis of a phase transformation, within a slurry during crystallisation, that converted the metastable α-form of L-glutamic acid to the stable β-form. Crystallisation involves nucleation (3D formation and assembly of molecular clusters) and growth (2D growth of clusters to crystals). The crystals need to match the specification with respect to their size and shape.

James Chisholm (CCDC) showed how the new Materials module of the Mercury software for the Cambridge Structural Database (CSD) can be used to study the packing patterns of polymorphs, hydrates and solvates. The Mercury CSD Visualizer program can compare crystal structures and identify similarities between polymorphs and specific regions that are similar. It can investigate packing to provide insights into the forces that direct crystal growth. Other new features in Mercury allow searching of the CSD for specific interaction motifs or more general packing features.

Overall, it was a very interesting meeting. Both sessions were well-attended, and the venue was excellent. We are grateful to AstraZeneca for their sponsorship of the meeting.

Mark Farnworth and John Kaniuka

PDF versions of the full Autumn meeting reports can be downloaded from the Industrial Group's web site at:-

http://bca.cryst.bbk.ac.uk/bca/ig/ig.htm

For the Young Crystallographers' meeting, the Industrial Group is again offering a prize of £100 plus a bottle of bubbly for the best talk which has some relevance to industry. The standard last year was very high, and we expect no less this year, so we look forward to interesting talks and difficult judging. The winner will be invited to present the talk again at the Industrial Group session at 1015 on the Wednesday.

Pharmaceutical Special Interest Group 7th November 2007

http://bca.cryst.bbk.ac.uk/bca/ig/reps07AM.htm

This meeting was held at AstraZeneca's excellent conference facilities at their Macclesfield site, and attracted seventy delegates. The morning consisted of talks of general pharmaceutical interest, with considerable time devoted to polymorphism.

Roger Davey (Manchester University) opened the meeting with a personal perspective on *Polymorphism - what have we learnt?* Examples from over 100 years of the scientific literature were given, illustrating, for example, the different solubilities of polymorphs, the solution-mediated transformation of the metastable to the stable form, the methods of discovering new forms. Roger questioned the use of high throughput methods with thousands of experiments and huge quantities of data.

Gordon Barr (Glasgow University) spoke on the use of automated cluster analysis of XRPD and Raman data for use in solid form screens in a talk with a thought-provoking title: *Is PXRD the Gold Standard in High Throughput Experiments?* Gordon described the benefits and disadvantages of XRPD and Raman spectroscopy: preferred orientation and degree of crystallinity are two disadvantages which can affect the cluster analysis of XRPD data, while Raman data can suffer from relatively small differences between polymorphs, variability in background level, and cosmic ray spikes.

Talbir Austin (AstraZeneca) gave a talk titled, *Understanding relative polymorph stability through structure and thermodynamics*. She described the process of polymorph selection of a pharmaceutical and explained how it is essential to understand which polymorphs can form since their different physical properties may affect bioavailability, and hence efficacy, of the drug. Having identified which polymorphs exist, it is then necessary to understand the stability relationships between them.

Bill Jones (Cambridge University) described the use of grinding to produce new forms in his talk *Screening for New Crystal forms Based on Mechanical Activation of Mixtures.* Grinding together of components, particularly in the presence of a drop of solvent, can produce novel co-crystals, salts, polymorphs and solvates, which solution experiments may (at least initially) fail to produce. Many examples of new solid forms produced by grinding were given.

Jerry Heng (Imperial College) considered the importance of surface functional groups to the behaviour of pharmaceuticals in his talk, *Crystal Engineering: Importance of Surface Properties*. Jerry described the use of macroscopic crystals of paracetamol, aspirin and ibuprofen to enable physical and chemical measurements to be made on individual faces. Jerry used a combination of methods: contact angle measurement, XPS, and approximations from knowledge of the crystal structure to understand how wetting properties are affected by the chemistry of different crystal facets.

After (a very tasty) lunch, the afternoon session concentrated on structure solution and refinement. Two themes ran through all the talks: a sense of confidence that good quality powder data can be used for structure solution from powders and a requirement that complementary techniques are used to confirm structures and avoid pitfalls.

Fred Vogt (GSK) spoke on *X-ray diffraction, Computational Chemistry and NMR: A Multi-disciplinary Approach to Understanding the Pharmaceutical Solid State*. He demonstrated the use of the combined approach to maximise the understanding of the structure, dynamics and properties of pharmaceutical compounds. Fred described the use of ssNMR in the determination of the crystal structure of a pharmaceutical compound for which single crystals were not available.

Jonathan Burley (Nottingham University) gave an introductory lecture - *Cocrystals and Other Complex Pharmaceutical Materials: Structure Solution from Powder Diffraction.* He described the process of data collection and strongly recommended the use of the Debye-Scherrer (i.e. capillary) over Bragg-Brentano (flat plate) geometry. This was to avoid or reduce the errors associated with the latter: preferred orientation, X-ray absorption by the sample and sample height effects. Jonathan then described how the structure could be obtained in three stages: indexing, obtaining an approximate structure solution, and refinement to obtain an accurate structure.

Jacco van de Streek (Frankfurt University) spoke on *Semi-automated Rietveld Refinement of Molecular Crystal Structures with DASH and TOPAS*. Jacco described the use of DASH to direct a Rietveld refinement in TOPAS, by generating input files, then taking the output files from TOPAS and adapting them to be used as new input files. This removes the need for tedious manual intervention, and going back and forth between DASH and TOPAS, and speeds up the process so that high-quality Rietveld refinements can be carried out routinely in a matter of minutes.

Maryjane Tremayne (Birmingham University) speaking on *Powders and Peer-Pressure: Pitfalls and Progress.*

Maryjane described her work on the development of the Cultural Differential Evolution (CDE) technique for structure solution from powder data. The 'biological' evolutionary approach to the generation of trial structures is enhanced with the addition of a 'cultural' driving force, or 'peer pressure' in which the distribution in values of structural parameters in each generation is used to guide and enhance the optimisation process. This enables a more rapid convergence to the global minimum.

I would like to extend my thanks to the speakers for making this such a fine meeting, with very high quality and informative talks.

Anne Kavanagh

Magnetic Structure Determination Workshop,

14-17 January 2008

THE challenge faced by researchers, both new and experienced, to studies of magnetism and magnetic structures are considerable. The drive to ordering can lead to unexpected structures that lie at the heart of a material's magnetic properties. Many are captivated by systems that possess competing interactions, these are said to be *frustrated*, or the coupling between magnetic and electric dipole ordering in multiferroics. Such delicate plays between energies may be first evidenced and characterised by phase diagrams decorated with equally subtle magnetic structure.

The biannual PCG/ISIS workshop on magnetic structure determination provided a rare opportunity to go through the basics of what magnetic structures are, their different types, how they can be described and determined. The language follows that of the physicist because descriptions built from the relevant physics lead to an underlying elegance of the mathematics, and the clearest reflection of the physical processes involved. There could be no apology for the sessions being filled with terms such as Bloch waves, propagation vectors, representations, and basis functions, as these form the foundation of what magnetic structures are.

The international make-up of the participants affirms the interest and the importance of the subject. The tutors were **Juan Rodriguez-Carvajal** (ILL), **Paolo Radaelli** (ISIS), **Laurent Chapon** (ISIS), **Aziz Daoud-Aladine** (ISIS) and **Andrew S. Wills** (UCL). The workshop began with a summary of the different types of diffractometer available (PR), and the mathematics of the diffraction process (PR, ADA) before the first practical workshop on the indexing the magnetic reflections (JRC). Use of FullProf Studio (LC) allowed simple visualisation of different magnetic structures and an opportunity to become familiar with the Fourier summations that express their language.

The second day took representations from the world of molecular spectroscopy to crystals (LC and ADA) and then to magnetic structures (ASW). These symmetry calculations are daunting to most researchers, not because they are particularly complex, but because they can be long. As programs such as SARA*h* (ASW) and BasiReps (JRC) perform them in a matter of seconds, care was taken to introduce concepts that will become clear when the participants begin to study their own systems. Introductions to these programs and using them to aid refinements with GSAS and FullProf were also given.

The third day explored the use of Shubnikov space groups (PR). These symmetries are an extension of the space groups familiar to crystallographers and offer opportunities to visualise the interplays between the different symmetries in magnetic structures - *the reader is cautioned that they are a limited symmetry description, and representational theory is far more general: a statement that was repeated many times at the workshop (!), and exemplified by an example of a refinement using both GSAS and the results of representational theory (ASW).*

Participants and tutors at the 2008 PCG/ISIS Magnetic Structure Determination Workshop.

During the final day of the workshop, the PCG winter meeting, the participants heard a collection of talks that expanded on the concepts introduced in the workshop, showing some of the challenges faced by the modern researcher. Starting the day **Oleg Petrenko** (Warwick) gave a summary of recent work on the kagomé staircases $Ni_3V_2O_8$ and $Co_3V_2O_8$. As well as giving an excellent overview of the diffraction and specific heat studies required to build a picture of the complex magnetism in these materials, his talk served to introduce the subject of frustration that was continued by the following speaker **Tom Fennell** (UCL), this time detailing the fantastic intricacies of the spin ice pyrochlores.

A key take-home message for the meeting is that magnetic structures are subtle, and that thought and care needs to go into their study. This was beautifully shown in a presentation by **Jane Brown** (ILL) and was an outstanding introduction to Spherical Neutron Polarimetry, as realised by CRYOPAD. Her tour through its use showed well how even the simplest of systems can still hold questions that may only be answered by considered and careful experiment.

The meeting was closed by **Alessandro Bombardi** (Diamond) and a moment away from the dominance of neutron diffraction as a tool for the study of magnetic structures. Alessandro introduced the use of resonant and non-resonant X-ray scattering in V_2O_3 and $HoMn_2O_5$ showing how the orbital and spin contributions of the transition metal and rare earth can be probed through the different resonances. The final of many inspirational talks that were comfortably before the next set of proposal deadlines!

Andrew S. Wills

The 64th Annual General Meeting of the Physical Crystallography Group of the British Crystallographic Association and Structural Condensed Matter Group of the Institute of Physics:
1pm Wednesday 18th April 2007, Canterbury

There were 16 members present. Committee members present: Paolo Radaelli, Dave Allan, John Loveday, Matt Tucker, Ivana Evans

1. Formal apologies for absence were received from Andrew Wills.

2. Minutes of the 63rd AGM held at Lancaster were circulated and accepted as an accurate record of the meeting.

3. There were no matters arising from minutes

4. Chairman's report: Paolo Radaelli reported on another active year for the PCG/SCMP. Specific topics discussed were:

a) Training & Teaching
The **Rietveld Refinement Workshop** took place in Durham on Jan 7-10 2007. The workshop attracted 60 attendees, both UK and foreign, from academia and industry. It is intended that the Structural Rietveld and the Magnetic Rietveld Workshops will run in alternate years. The next **Magnetic Rietveld Workshop** will take place at Cosener's house in early January 2008.

b) Winter Meeting 2006
The **2006 Winter Meeting** was organised by John Loveday, and took place on Oct 25, 2006 at CSEC, University of Edinburgh. It featured "A cross section of Physical Crystallography in the UK", with talks on high-pressure structure studies of the elements (L.Lundegaard, University of Edinburgh), studies of alkali ammonia solutions, (C.J.Howard, University College London), dynamics from diffusion (A.Goodwin, University of Cambridge) and multiferroics (L. Chapon, ISIS Facility). It is envisaged the **Winter Meeting 2007** will take place in Cosener's House in conjunction with the MRW, with a theme related to that of the Workshop.

c) Communication with Members
In spring 2007, we published the first issue of the **PGC-SCMP newsletter**, edited by Ivana R. Evans. We also refurbished completely the **PCG web site**, which now takes the form of a "WIKI" (thanks to M. Tucker).

d) Future activities
PCG will sponsor the "**Protein crystal structure from powder diffraction**" workshop, to be held at ESRF on 22-23 June 2007.

e) Next BCA
Physical Crystallography will feature prominently at the **BCA Spring Meeting 2008**. John and Ivana Evans will be Program Chairs, with Matt Tucker as the PCG representative. The theme will be "Structure, Property, Function". It is proposed that the RSC Solid State group (and possibly the ISIS Crystallography User Group) hold their annual meeting in conjunction with the BCA Spring meeting.

f) Vacancies
Two **Committee vacancies** (Ordinary Members) are announced. The election will take place at this AGM.

g) Prizes
This year, the PCG awards two prizes - the PANalytical Thesis prize in Physical Crystallography and the PCG Poster prize. The winners will be announced at the Banquet.

5. Honorary Secretary/Treasurer's report:

a. The secretary/treasurer presented the annual activity report to the meeting and the financial summary appended.

b. The funding bid submitted to the new IOP funding model was described and detail are giving in the financial summary appended. The bid was very successful and resulted in a large increase of our annual budget.

6. Committee posts for ordinary members (retirement of Jon Wright and Andrew Wills at the end of a three year term; resignation of Mina Golshan) were available. Nominations for posts are detailed below. All were elected unopposed.

a. Ordinary Member: Andrew Wills (re-election). Proposed Paolo Radaelli; Seconded: Dave Allan.

b. Ordinary Member: Andrew Goodwin. Proposed Ivana Evans; Seconded: Matt Tucker.
c. Student representative: Helen Maynard was co-opted as the young crystallographers representative on the PCG committee.

7. As detailed in the Chair's report the PCG-SCMP now has a new website and email list.

8. Future meetings are detailed in the Chair's report above.

Matt Tucker, Secretary

Powder Diffraction and Rietveld Refinement School

On behalf of the Physical Crystallography Group of the British Crystallographic Association, I am pleased to announce the Powder Diffraction and Rietveld Refinement School at Durham University, 30th March-3rd April 2008. Lectures will be given by **Jeremy Cockcroft**, **Andy Fitch**, **John Evans** and **Ivana Evans**. There will also be small group tutorials and a large number of practical hands-on computer sessions.

Topics to be covered will include:

- Data collection strategies for X-ray and neutron diffraction
- Constant wavelength and time of flight diffraction
- Modelling peak shapes
- Indexing powder patterns
- Rietveld, Le Bail and Pawley fitting methods
- X-ray and neutron combined Rietveld refinement
- Extended solids and molecular systems
- Restrained refinements
- Rigid body refinements

Accommodation will be at a Durham College and lectures/ computer workshops will be held in the Chemistry Department.

We have managed to raise significant sponsorship from EPSRC, PCG and IUCr, and will be able to offer a significant number of bursaries to the UK students and a smaller number of bursaries to overseas participants.

The number of participants is limited and applications are accepted online, via the school website:

http://www.dur.ac.uk/john.evans/webpages/pcg_rietveld_school_2008.htm.

For more information please email

john.evans@durham.ac.uk or
ivana.radosavljevic@durham.ac.uk

Ivana Evans

Contributed talks and posters at YC2008

THE Young Crystallographers Group of the BCA will again be holding a satellite meeting at the BCA Spring Meeting in York. We will be following the familiar format of preceding the Spring meeting with a day of talks (4 sessions with invited plenary speakers) and an evening poster, buffet and wine session. I am also pleased to announce the establishment of the 'Durward Cruickshank Young Crystallographers' Prize', which will be presented to the Young Crystallographer making the 'best contribution' to this meeting. The meeting will be held from lunchtime on Monday 7th April and will run into the main BCA Spring meeting. Registration for YCG members is free of charge.

For further details see:

http://www.chem.gla.ac.uk/yc/

where you will have to register (a simple and rapid process) to login to the members area to submit.

YC2008 is deliberately not a themed meeting so that our members, who come from all areas of our field, can present their work in a relaxed environment. Short (0.5>1 page A4) abstracts had to be submitted through our website before the deadline of 11th January 2008. Those abstracts that did not get accepted for a talk will be invited to present their work as a poster or exceptional poster submissions may be asked to contribute a talk! We intend to make the poster session considerably more interactive this year and may be calling on submitters to contribute a little bit more than just a static poster!

Finally, we have a lot of difficulty in maintaining a membership list, so have developed a 'registration' system on our website. If you are eligible to be a Young Crystallographer, you will need to receive up to date information about our activities and therefore we urge you to register under the member section of our website.

Please forward this information on to your friends / colleagues / students / Post Docs as appropriate.

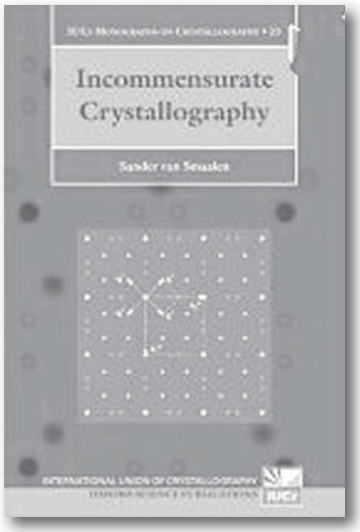
Many thanks and best wishes from the Young Crystallographers.

Simon Coles

Books

INCOMMENSURATE CRYSTALLOGRAPHY

Sander van Smaalen University of Bayreuth
Oxford University Press, 2007
Price: £65.00 (hardback)
ISBN 978-0-19-857082-0, xii+270 pages



THIS twenty-first title in the series of IUCr Monograph on Crystallography concerns the study of incommensurate crystal structures. The author's own research in this field spans almost 25 years.

A textbook on Incommensurate Crystallography, like this one, has been needed by researchers in that field for quite some time. Of course, several review articles exist, but the only other related textbook I am aware of is "Quasicrystals" by C. Janot from 1997. Although it has a general chapter on higher dimensional crystallography, it deals, as its name says, with quasicrystals only. Then finally, in 2007 two IUCr Monographs on Crystallography on the topic appeared: this one and "Aperiodic Crystals" by **T. Janssen**, **G. Chapuis**, and **M. de Boissieu**, reviewed in the December 2007 issue of Crystallography News.

Incommensurate crystallography is not a very easy topic to fully understand, and may require several readings of the introduction before a person becomes familiar with it. I do not know of many people who were able to grasp the concept immediately, as most beginners in this field initially required quite long periods of study, before becoming confident with the concept. However, I can recommend this text book to all who wish to (or have to!) study the subject on their own from a text without someone experienced around. Although the book contains a lot of mathematics, the principle of the higher dimensional approach is not treated in terms of mathematical definitions alone. Instead, the reader is led from 3D translational symmetry towards (3+1) dimensions and further to (3+n) dimensions in a step-by-step process. Always remember that it will take time for the reader to get used to more than 3 dimensions, and for the reader's logic to fully digest all the information, even when delivered in small portions. A newcomer to incommensurate crystallography will probably take a few days to read the concept, before they fully understand and memorize the basic definitions and the terms used for the phrasing processes described in the first 5 pages. But after that, the rest of the book will be relatively easy to understand. This can be an advantage, but also a drawback at the same time, because it is difficult to look up a topic in the index, and then read the respective pages without first reading the previous chapters beforehand. This effect is especially noticeable at the beginning of any such study. It is also most useful to the reader to look up the explanations in the glossary of symbols, which can be found in the appendix.

Chapter 1 introduces building principles of aperiodic crystals, and gives the reader an introduction to incommensurate crystallography. This includes such things as the mathematical notations and definitions, giving an account of the actual arrangement of atoms in a real 3D crystal by accurate wording and excellent graphics. In addition, an explanation of the basic types of incommensurate crystals, (1) crystals with modulated structures, (2) incommensurate composite crystals, and (3) quasicrystals is given. Based on this information, Chapter 2 introduces reciprocal and direct superspace, again with excellent graphics and explanations, which are very comprehensible, and a real improvement on the often too brief introduction in review articles. The concept of the phase shift of the modulation wave and t-plots is given and fully explained with the example of $Sr_2Nb_2O_7$. It is a general feature in this book to illustrate many newly introduced concepts with literature examples from the last 30 - 40 years of research. Chapter 3 illustrates the symmetry of modulated crystals, the centring of the superspace lattice, and the way the superspace approach describes symmetry of incommensurate modulated crystals. Superspace groups, and their symbols in different notations, are also given. Although there are numerical examples of symmetry operators in superspace, this chapter would particularly benefit from exercises regarding symmetry operators and superspace group symbols. In general, a reader may well feel that the whole book would greatly benefit from such exercises.

Having read and understood everything so far, the reader should then find Chapter 4, on incommensurate composite crystals, much easier to understand. Also, the reader will find that Chapter 5, on developing the relationship between incommensurate crystals and superstructures, will be seen as straightforward, at this stage.

The remainder of the book describes the methods used for the structural analysis of incommensurately modulated structures. Chapters 6 and 7 address the quantitative

presentation of diffracted intensities, the structure factor, the problems of such things as overlapping reflections and twinning. They also contain information on structure refinement from crystal powder data and give details on such topics as the refinement of modulation parameters, constraints, restraints and rigid bodies. Chapter 8 deepens the knowledge of incommensurately modulated structures in the field of electron density in superspace and introduces the maximum entropy method as a tool for the determination of the precise shape of the modulation function. Chapter 9 gives a theoretical approach as to how the determination of the superspace group may be carried out. As stated above, with reference to the lack of worked examples in Chapter 3, Chapter 9 is yet another case where worked examples and exercises are badly needed. In Chapter 10, the main methods of structure solution (1) Trial and error, (2) Patterson function methods, (3) Direct methods and, last but not least, (4) Charge Flipping, are briefly summarised for the reader. Finally, in chapter 11, the crystal chemistry of the most prevalent group of compounds with incommensurate crystal structures is outlined in terms of the superspace approach.

A very helpful list of all programs for the analysis of incommensurate crystals, together with an internet link for their availability, is clearly arranged in the appendix.

The intention and primary function of the book's Chapters 1 through 6, is "to help and assist the reader to fully understand the special structural features of aperiodic crystals", while the remaining 7 to 11 chapters aim to enable crystallographers to "determine the atomic structures of modulated and composite crystals from diffraction data", as the author states himself. However, it cannot be stressed enough, that the reader must have an understanding of incommensurate crystallography, which is obtained from the first 3 chapters, before continuing to study any of the later chapters. Without this basic understanding, the reader may find that it is not possible to fully understand the later chapters, and finally solve and refine the structure of a modulated crystal.

Clivia Heijny
University of Innsbruck

Meetings of interest

FURTHER information may be obtained from the website given. If you have news of any meetings to add to list please send them to the BCA Web Master cockcroft@img.cryst.bbk.ac.uk or to the Editor, gould@ed.ac.uk.

3-6 March 2008
16th Annual meeting of the German Society of Crystallography.
Erlangen, Germany
www.conventus.de

5-7 March 2008
ARC 2008: International Symposium on Pulsed Neutron and Muon Sciences, Mito, Japan.
www.ips08.com

9-13 March 2008
The Minerals, Metals and Materials Society (TMS) 2008 New Orleans LA USA
www.tms.org/Meetings/Annual-08/AnnMtg08Home.html

11-13 March 2008
Polymorphism & Crystallisation 2008 London
www.iqpc.com/uk/poly

11-14 March 2008
International School On Surface Analytical Techniques.
Potsdam-Golm, Germany
http://cost-d43.mpikg.mpg.de/

24-28 March 2008
Materials Research Society - 2008 Spring Meeting. San Francisco, CA USA
www.mrs.org/s_mrs/sec.asp?CID=6689&DID=174642

28-29 March 2008
II International Workshop - Layered Materials: Structure and Properties.
Vercelli, Italy
www.layeredmaterials.mfn.unipmn.it

30th March-3rd April 2008
PCG Rietveld School 2008.
Durham, UK
www.dur.ac.uk/john.evans/webpages/pcg_rietveld_school_2008.htm

6-11 April 2008
Rapid Data Collection and Structure Solving "RapiData 2008" - Brookhaven National Laboratory, Upton NY USA
www.px.nsls.bnl.gov/RapiData2008/

8-10 April 2008
BCA Spring Meeting, York
www.crystallography-meetings.org.uk

24 April–10 August 2008
Exhibition: From Atoms to Patterns - Crystal Structure Designs from the 1951 Festival of Britain. London
www.wellcomecollection.org.uk

27 April - 3 May 2008
Summer School on Mathematical and Theoretical Crystallography. Gargnano, Garda Lake, Italy
www.lcm3b.uhp-nancy.fr/mathcryst/gargnano2008.htm

2-5 May 2008
Workshop and International School on Protein Crystallization Cancun, Mexico
www.iccbm12.com.mx/

4-8 May 2008
2008 Beam Instrumentation Workshop.
Lake Tahoe, CA, USA
www-als.lbl.gov/biw08/

4-8 May 2008
3rd French school on Reflectivity SAXS, GISAXS and Diffraction from Surfaces.
Presqu'île de Giens, France
www.univ-lemans.fr/~gibaud/ecoledegiens

5-8 May 2008
Science of Solar System Ices (SciSSI) - Oxnard CA USA
www.lpi.usra.edu/meetings/scssi2008/

6-9 May 2008
ICCBM12 2008 International Conference on the Crystallisation of Biological Molecules. Cancun, Mexico
www.iquimica.unam.mx/ICCBM12/

11-15 May 2008
ACNS2008 - American Conference on Neutron Scattering. Santa Fe, New Mexico, USA
www.lansce.lanl.gov/acns2008/index.html

14-16 May 2008
Alberta Powder Diffraction Workshop. Alberta, Canada www.cins.ca/apdw/index.html"

18-23 May 2008
7th Symposium on High Temperature Corrosion and Protection of Materials. Les EMBIEZ, France
www.htcpm-2008.uhp-nancy.fr/

18-24 May 2008
Hercules Specialised Course: Synchrotron Radiation and Neutrons for High Pressure Studies, Grenoble, France
hwww.esrf.eu/events/conferences/HSC/HSC7

18-24 May 2008
Hercules Specialised Course: Synchrotron Radiation and Neutron Techniques in Environmental Sciences. Grenoble, France
www.esrf.eu/events/conferences/HSC/HSC8

18-25 May 2008
IWCGT-4 Fourth International Workshop on Crystal Growth Technology. Beatenberg, Switzerland
www.beatenberg.ch/IWCGT-4

21-23 May 2008
Surfaces and Interfaces in Soft Matter and Biology: the impact and future of neutron reflectivity, ILL, Grenoble, France
www.ill.fr/Events/rktsymposium/

25-30 May 2008
Advanced Beam Dynamics Workshop "NANOBEAM-2008" - Novosibirsk, Russia
http://ssrc.inp.nsk.su/NB08/

31 May - 3 June 2008
XVII International Synchrotron Radiation Conference "SR-2008" - Novosibirsk, Russia
http://ssrc.inp.nsk.su/SR2008/

31 May - 5 June 2008
ACA Annual Meeting - Knoxville, TN, USA
www.hwi.buffalo.edu/ACA/

6-11 June 2008
5th European Charge Density Meeting (ECDM5) - Gravedona, Italy
http://ecdm5.istm.cnr.it/

8-13 June 2008
IWPCPS-10: 10th International Workshop on Physical Characterization of Pharmaceutical Solids, Bamberg, Germany
www.assainternational.com/

15-20 June 2008
ISSRNS 2008 - 9th International School and Symposium on Synchrotron Radiation in Natural Science. Poland
www.synchrotron.org.pl/ISSRNS2008/index.html

18-22 June 2008
International Summer School - Structure Determination from Powder Diffraction Data. Paul Scherrer Institut, Villigen, Switzerland
http://user.web.psi.ch/powder08/

19-20 June 2008
Protein Crystallography Europe. Amsterdam, Netherlands
www.selectbiosciences.com/conferences/PCE2008/

22-27 June 2008
21st International Conference on X-ray and Inner-Shell Processes Paris, France
http://x08.spectro.jussieu.fr/

22 June - 5 July 2008
The Zurich School of Crystallography 2008. University of Zurich, Switzerland
www.oci.unizh.ch/diversa/xtal_school

6-11 July 2008
ICQ10 - 10th International Conference on Quasicrystals. Zurich, Switzerland
http://icq10.ethz.ch/

7-10 July 2008
Colloque de l'Association Française de Cristallographie - Rennes, France
www.afc2008.univ-rennes1.fr/

13-18 July 2008
Gordon Research Conference: Diffraction Methods in Structural Biology, Lewiston ME USA
www.grc.org/programs.aspx?year=2008&program=diffrac

20-23 July 2008
SRMS-6 - 6th International Conference on Synchrotron Radiation in Materials Science. Campinas, Brazil
www.srms-6.com.br/

21-26 July 2008
XRM2008 9th International Conference on X-ray Microscopy. ETH Zurich, Switzerland
http://xrm2008.web.psi.ch/

18-23 August 2008
2008 Kyoto Crystallographic Computing School. Kyoto, Japan
www.iucr.org/iucr-top/comm/ccom/kyoto2008school_announce.html

23 - 31 August 2008
21st Congress of the International Union of Crystallography 2008. Osaka, Japan
www.congre.co.jp/iucr2008/greeting.html

31 August – 4 September 2008
ECTP2008:18th European Conference on Thermophysical Properties. Pau, France
http://ectp.univ-pau.fr

1-5 September 2008
7th International Workshop on Polarised Neutrons in Condensed Matter Investigations - Tokai
www.neutron-eu.net/nmi3/jra4/

7-12 September 2008
BCA/CCP4 Summer School in Macromolecular Crystallography, Oxford
www.biop.ox.ac.uk/www/bcasummer2008.html

9-14 September 2008
WATOC-08 World Association of Theoretical and Computation Chemists. Sydney, Australia
www.ch.ic.ac.uk/watoc

15-17 September 2008
XTOP2008 - 9th Biennial Conference on High Resolution X-Ray Diffraction and Imaging. Linz, Austria
www.hlphys.jku.at/xtop2008/xtop2008.html

15-19 September 2008
2008 E-MRS Fall Meeting. Warsaw, Poland
www.e-mrs.org/meetings/fall2008/

18-22 September 2008
EPDIC-11 European Powder Diffraction Conference
Warsaw Poland
www.epdic-11.eu/

20-24 September 2008
ICSG 2008: International Conference on Structural Genomics. Oxford
www.spine2.eu/ISGO

9-14 November 2008
EMBO World Lecture Course - Recent Developments in Macromolecular Crystallography. Pune, India
http://cwp.embo.org/wpc08-02/index.html

17-20 November 2008
14th International Conference on Thin Films. Ghent, Belgium
www.ICTF14.UGent.be