

Crystallography News

British Crystallographic Association



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IUCr Meeting - Florence p6-10



BCA Spring Meeting 2006 - Lancaster p12-19

Science and Mankind p20-21

Reports p22-26

Books p28-30



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Items may include technical articles, news
about people (e.g. awards, honours,
retirements etc.), reports on past meetings
of interest to crystallographers, notices of
future meetings, historical reminiscences,
letters to the editor, book, hardware or
software reviews.

Please ensure that items for inclusion in
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BCA News December 2005

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This month's cover: Florence!
...and what a meeting it was!
*The inset is a view of Lancaster
University campus.*

From the President



ONE of our main purposes on BCA Council is to contribute to the good and continuing health of the organisation, and I am acutely aware of this as I prepare to hand over to a new President.

This includes the vital task of forward financial planning; as you may have noticed we have effectively been running a small deficit for several years now, and clearly this is not sustainable in the long term. Along with Treasurer, **Sheila Gould**, and the rest of Council, we have been reviewing the situation, which was discussed in detail at the Autumn Council meeting. It is important that as well as building and maintaining our ability to run from day to day and year to year, in an efficient and appropriate manner, we are also able to support our necessary charitable expenditure, for example to support education initiatives (both centrally and those organised by the groups), the Young Crystallographers group, and other relevant activities. Feedback on Council discussions will be given as they evolve.

Returning from the Florence IUCr congress, I had seriously mixed feelings. It was a superb meeting, with around 2900 delegates (just outdoing in terms of numbers Glasgow 1999 which you may recall attracted around 2700). The science was excellent, plenty of colleagues to meet and talk with, and as expected lots to do both scientifically and with various organisational things. Moreover, it is a pleasure to record that **Chris Gilmore** was elected to the IUCr Executive, for a six-year term. In addition, many of our nominations to the IUCr commissions were successful; together with existing commission members this ensures that UK representation on these bodies has returned to a more healthy level. I would like to thank all those who agreed to be nominated for Commissions, whether elected or not; to maintain our influence and input into the work of the Union, it is important that people are prepared to stand up and be counted in this way. Following the General Assembly in Florence, the Union is now led as President by **Professor Ohashi**, who was elected after a keenly fought contest. However, on the down side of Florence, I have to say I was disappointed that we failed to secure the European Crystallographic Meeting for Edinburgh in 2009. We put together what I believe to have been a very strong, well-argued and detailed bid, considerably aided by **Gill Moore** at Northern Networking Events and by the team at the Edinburgh International Conference Centre.

However, in spite of effective lobbying in Florence by the team (particularly by Edinburgh locals **Bob & Sheila Gould** and **Georgina Rosair**), we lost out to Istanbul, which was awarded the 2009 ECM. Having led the bid I felt keenly that we were not able to bring ECM to the UK, and was particularly disappointed considering the effort put in by many others in putting us in the frame. With ECM in 2010 allocated to Darmstadt and 2011 being an IUCr year (Madrid), we will therefore not be in a position to have ECM in the UK till at least 2012.



The British delegation to the IUCr General Assembly: left to right: John Evans, Sheila Gould, Chick Wilson, Elspeth Garman and Bob Gould.

On a much happier note, you will see in this issue the rapidly forming programme for the Annual Spring Meeting in Lancaster in April next year. I hope you agree that we have the usual high quality programme, put together by **Paul Raithby** and his programme committee who are thanked for all their hard work. It is a pleasure to confirm the participation of the British Association of Crystal Growth in the 2006 meeting, which has the central theme of Crystallisation - interpreted appropriately imaginatively in forming the programme. Plans for 2007 are also forming, with the venue likely to be in the South of England and possible participation by Non-Crystalline Diffraction & CCP-13 colleagues, along with a likely renewal of our XRF strand.

A final note - you will be aware that the position of BCA President is up for election at the Lancaster meeting; I hope we have a strong field and a competitive election for this senior position within the organisation. BCA Secretary Christine Cardin will be delighted to receive nominations (secretary@crystallography.org.uk). We also have vacancies for three Ordinary Members of Council for which nominations are also strongly encouraged.

Chick Wilson

Council Members

2005-06

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From the Editor



THE meeting of the IUCr in Florence was a remarkable experience, and, as usual, the British delegation was well in evidence.

The city is a certainly a great treat to be in, and, yes, we had A Room with a View, which you will see on the front cover! You will find graphic accounts of how it appealed to some

of our bursars in this issue. I did make an attempt to try to summarise more of the meeting by combining the reports of different people, but it proved too complex a task, and I have chosen three reports that caught much of the flavour of the experience at the largest crystallographic meeting ever.

Our bursars have been at many other meetings too, and you will find some reports of them here. We are very grateful to all those who write interesting accounts of the meetings they have attended, and the standard has been rising.

One of the greater spectacles at Florence was the Oxford Diffraction T-shirt campaign, to which you will see many references. The effect is not so good in monochrome photographs, in which the name of a quite different firm, who donated the badges, becomes more prominent! Although we were unsuccessful in our attempt to bring an ECM to Edinburgh, the take up of the mini-loch-ness-monsters supplied by the City of Edinburgh was nearly as great as that of the T-shirts, and we hope that it will encourage visits here, even if not ECMs.

Looking to the future, you will find much information about next spring's BCA in Lancaster. Many thanks to **Paul Raithby** and his committee for getting this together. It certainly looks as if it will be a very good meeting.

I am delighted that the Tony North's cursor suggestions have been taken so far - see the latest in colour on page 37 and find out how to get them. Thanks to **David Watkin** and **Dave Taylor** for their perseverance.

A real find has been the article which **Sir Lawrence Bragg** wrote at the time of the first atomic bomb in 1945. We reprint here the copy of the text which **Make Glazer** came across in a drawer in the Clarendon Laboratory.

A welcome back to our persistent correspondent **Professor Dolding Beetle** who seems to have undergone something of a Damascus Road experience, and is now supporting nano-technology. Will wonders never cease! I hasten to say that despite rumours, this person is not a pseudonym of mine. I write quite enough in my own name, and your letters and articles of all sorts are always welcome. Please keep them coming, and do try to send pictures with them.

Bob Gould



BCA Council

Front Row: Christine Cardin, John Finney, Chick Wilson and Sheila Gould. Back row: Bob Gould, John Helliwell, Sandy Blake, Jeremy Cockcroft, Sheila Gover, Elspeth Garman, Georgina Rosair, John Evans and Peter Moody.

Puzzle Corner

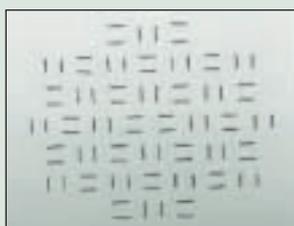
AND this month, we have a little more culture for a change!

One of the most fascinating talks at the ACA last summer was one by Bart Kahr of the University of Washington. Although the talk was entitled *Dyeing Crystals*, it featured much more (see the last issue). In particular, he emphasised the work of the German crystallographer, philosopher and educator F.W.A. Froebel (1782-1852), the inventor of the kindergarten. [see *Crystal growth in the Kindergarten*, Bart Kahr, *Crystal Growth and Design* **4**, 3-8 (2003) and also *Intimate Triangle: Architecture of Crystals*, Frank Lloyd Wright and the Froebel Kindergarten, by Jeanne Spielman Rubin, which was reviewed by Moreton Moore in *Crystallography News* **85**, June, 2003.]

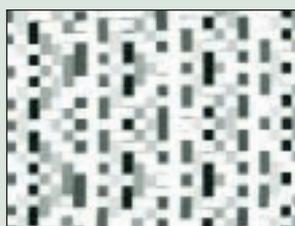
One of the results of Froebel's crystallographic background was a concern for symmetry and spatial concepts in general, which can be seen in the quality of the work of children in a Froebel kindergarten. Reproduced below are four pairs of artwork, taken from Norman Brosterman, *Inventing Kindergarten*, Harry N. Adams, New York 2002. In each case, one is by a kindergarten child and the other by Josef Albers, Paul Klee, Bart van der Leck or Piet Mondrian. Please identify the artist in each pair and which is his and which the child's. Be brave and have a go - I'd be interested in your reasoning too, which will contribute to your prizeworthiness! *Ed.*



Froebel on an East German stamp



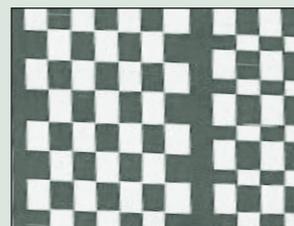
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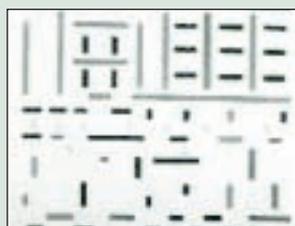
3a



4a



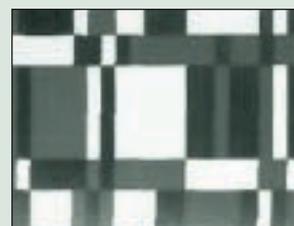
1b



2b



3b



4b

The solution to last month's "pseudo-Sudoku" was:

1. galactose
2. amorphous
3. merohedry
4. hexagonal
5. reflexion
6. dimorphic
7. insoluble
8. polymorph
9. aspartate

with the final hidden word being diaphragm. Some solvers questioned whether "diaphragm" really qualifies as a term connected with "structural science". However, as it can be a part of a camera, I feel that it does, and the Editor is never wrong in such matters! Congratulations to the winner who is Charlie Bond.

IUCR Meeting - Florence

XX Congress and General Assembly of the International Union of Crystallography

Florence, 22-31 August 2005

Our Bursars give their views:

Gary Nichol - University of Newcastle

FLORENCE. City of beautiful art, beautiful food, beautiful people and, for the last two weeks in August 2005, a home for some 2900 crystallographers from around the world who had converged on the Tuscan capital for the 20th IUCr Congress.

The eight-day long conference promised to be a worthy mix of talks, software demonstrations, competitions, social evenings and some commercial hard-sell, interspersed with the occasional bit of tourism and all the while keeping up-to-date with the latest developments in the Ashes Test match at Trent Bridge. The conference centre was the Fortezza da Basso, a converted fort which retains many original features including the omnipresent armed policemen and fire protection officers who were wandering throughout the conference. I have no idea what crimes they thought a collection of crystallographers would commit; by leaping out from behind a yucca plant armed with his digital camera, keen editors can stir high emotions, but no one would go *that* far, would they?...

So after registering (hands up all of those who went to the wrong counter!) and receiving our eye-catching, fragrant Bruker-sponsored backpacks we sat down to enjoy the opening ceremony. After the 'short' introductory speeches we were treated to a musical interlude performed by a brass quintet. As a horn player myself I was rather impressed by the performance, especially in such a large hall which I thought would have poor acoustics, however I would have liked to see more theatrical spit-emptying! Following this was the first lecture of the conference, the Ewald prize lecture presented by **Philip Coppens** who must have been wondering if he could fit all he had to say into the allotted time before the Welcome Cocktail Party. Our Italian hosts did a good job of providing enough food for the participants but perhaps reckoned without the

ability of the BCA members to see off the bottles of wine and by 10pm there was not a drop left.

Each day of the conference featured morning and early evening keynote sessions, a morning and afternoon of seven parallel sessions, lunchtime open meetings and computer workshops together with a daily poster session and an ongoing commercial exhibition. It was thus possible to spend a quite diverse day listening to presentations on very diverse areas and applications of crystallography and the close proximity of the various lecture rooms made moving between the sessions quite simple. One of my favourite sessions of the whole conference was on the first day. The Crystallography and Forensic Science session provided a rare opportunity to see X-ray diffraction applied to a vital area of everyday life. Examples were given of how powder diffraction has been used not just to identify 'white powders' (a rather obvious use) but, quite amazingly, how a sample of soil found on a shovel in the boot of a car in southern Australia could be traced, via its powder diffraction pattern, to a specific area of a quarry near Adelaide and subsequently the location of two murder victims was identified. Other examples included the analysis of tarmac residue on a policeman's gun to prove that a suspect was shot in the back by accident and not deliberately during a chase through a German town. This fascinating session was well attended and certainly opened my eyes to the wider uses of crystallography in the outside world.

That lunchtime the Open Commission on Journals provided those who attended the opportunity to hear about the progress made by the various IUCr journals over the last three years, and their plans for the future. In a time when the ubiquitous 'impact factor' of journals in which we publish is becoming increasingly important for obtaining research funding it was nice to learn that the impact factor of *Section B* has increased to 5.4 following the most recent review.

Many of the parallel sessions of interest to me as a chemist fell under the very broad theme of "crystal engineering"; thus there were sessions on non-bonded and non-covalent interactions, supramolecular chemistry, packing of organic molecular compounds and inorganic frameworks. One of the most thought-provoking talks was on the Thursday of the conference and was given by **Frank Allen**. His discussion of carbonyl-carbonyl interactions in structural chemistry almost makes me want to reanalyse three years of work! Also on Thursday was a second lunchtime session on the IUCr journals and we were updated on the latest developments made at the Chester office. The soon-to-be-released *pubCIF* will be an essential tool for the occasional writer of papers for *Sections C* and *E*, and maybe even for those of us who have taught ourselves to speak fluent CIF. Advice was also given on style and content of submitted

papers although the presenters commented that perhaps those attending were already fully aware of what to do. Thursday was also the day of my poster presentation and I had to juggle the poster session with my attendance at the lunchtime journals session, coupled with indulging in the generous buffet lunch provided daily. I did, however, manage to speak to all those who wished to see me (I think!).

Friday was Oxford Diffraction Orange T-shirt Day, wearing their T-shirt being a condition of the raffle by Oxford Diffraction to win an iPod or a laptop. However the eagle-eyed amongst the crowd noticed that the Russian winner of the iPod (**Sergei Stepanov**) was not wearing any Oxford Diffraction gear but that the laptop was collected by the suitably clad BCA member **John Gallagher** of Dublin City University! A nice coup for Oxford Diffraction who certainly generated a lot of new interest in the company. The day finished with a keynote given by **Guy Orpen** on synthetic crystallography, which is not simply concerned with pure synthesis but also crystal analysis, crystal shape and morphology. Talking about crystal synthesis with metal complexes (as opposed to pure organic materials) Guy showed how different architectures and structures can be obtained from relatively simple complexes by systematic variation of the ligands and counterions.

An excellent presentation by **Len Barbour** on porosity in crystals started the Packing of Organic Molecular compounds session on Saturday morning. Len described

how there are many examples of reported porosity in the literature which vanishes when a space-fill diagram of the structure is used. He also talked about some interesting systems exhibiting 'porosity without pores' whereby compounds can absorb material despite having no obvious pores in the structure. The other real significant event of Saturday took place at Trent Bridge, where for the first time in 191 Tests, Australia were invited to follow-on.

On Saturday evening an almost capacity crowd took their seats at the Teatro Verdi to hear a polished performance of music for string quartet and piano quintet. It is often said that string quartets are among the most difficult works in the repertoire since neither composer nor performer has any room for fault, nowhere to hide. It was uniquely refreshing then to hear some of the delicate *pianissimo* passages of Webern's *Langsamer Satz* augmented by the soft rumbles of the two gentlemen seated to my left snoring contentedly. Those of you sitting near the back of the balcony would probably have noticed myself and those around shaking with muffled laughter.

By Monday, conference fatigue was beginning to set in and the WinGX computer session led by **Louis Farrugia** was quite a relaxing way to wind down and learn something new at the same time. I'm told it was the best-attended computer session and well worth it too. The latest (as yet unavailable) version of WinGX contains many new features and future plans include developing an interface to the Bruker Apex software, something that will be worth the wait.



By the closing ceremony on Tuesday, England had beaten Australia to take a 2-1 series lead and the conference had witnessed some 36 keynote talks, 98 microsymbiosia, countless posters, computer sessions and the acquisition of lots of conference freebies from the exhibitors. It was only through looking at my notes to write this report that I realised just how much I'd done in that week. With any luck the next IUCr congress in Osaka will be just as balanced, informative and enjoyable. Just please make sure that a TV is provided so that we can watch England beat South Africa!

I thank the IUCr for providing funding to cover the conference fee and the BCA for an Arnold Beevers bursary.

Pauline Gavan - University of Bradford

SUCH an amazing conference!

We arrived at Pisa on Monday evening after a short flight from Manchester. Without even pausing to visit the tower, we were straight on a train, bound for 10 glorious days in Florence. We checked in to our hotel and after admiring the magnificent view overlooking the Duomo, quickly unpacked and hit the streets for dinner. Luckily I'd brought the original conference booklet, and as we perused the timetable over the first of many pasta suppers, I realised that I would in fact be spending the next day attending the Small Molecule Crystallisation Workshop from 9 till 5, rather than enjoying finding my bearings and exploring the area.

Registration began at 8.30am, and there was just enough time to collect a bright red conference rucksack (spot the crystallographer, and wonder what the strange smell following you was - it turned out to be the bag!) before the day began in earnest. The workshop was probably the most useful scientific aspect of the conference for me and I have come away with many ideas to pursue in my final experimental work and pass onto fellow colleagues. We were taken through some general techniques and applications, including Co-crystallisation (**Ram Jetti**), Basics of Crystallisation (**Ulrich Griesser**) and the revelation of interplanetary distances, *In-Situ* Cryo-Crystallisation Techniques (**Roland Boese**) including Ultrasonic seeding techniques by the use of an old TV remote control to induce crystal growth. After a quick break and a shot of Italian espresso to perk us up it was back to work and the use of Crystallisation In Gels (**Juan Garcia-Ruiz**) particularly as a method to grow better crystals by removing convection effects - every crystallographer's dream! Crystal Growth From Aqueous Solutions (**Eiken Haussühl**) illustrated thermostatically controlled growth over ~12 weeks to produce magnificent looking crystals over 2 cm in diameter! Characterisation and Thermodynamics of Solvates (**Luigi Nassimbeni**), focused on host-guest exchange and how to induce new polymorphs by guest solvent exchange.



We were more than ready for lunch by now and a chance to stretch out in the sun before returning to High Pressure and its applications in forming new polymorphs (**Colin Pulham & Francesca Fabbriani**) and the recovery of new polymorphs to ambient conditions that could then be used for seeding. An interesting analogy was the young long haired **Chick Wilson** transforming under pressure (including time, beer and organising IUCr sessions) to produce the structurally identical older Chick having more wrinkles and less hair! The role of Kinetic Factors in Polymorphism was discussed (**Elena Boldyreva**) along with the frustration experienced in obtaining irreproducible results. Nucleation from supercooled melts to produce crystals 1-2cm in diameter (**Helmut Klapper**) was interesting as was *In-Situ* Electrocrystallography, with mounting of the electrochemical cell in the diffractometer being a difficult enough task (presented on behalf of **Andy Parkin** by Chick Wilson). The session was concluded with the Crystallisation and Polymorphism of (almost) Insoluble Compounds (**Martin Schmidt**) and the difficulties of organic pigment structure determination. When faced with solubilities at ambient conditions of < 10 μ /litre, single crystal XRD is highly unlikely and structure determination from powder diffraction is the best option.

The opening ceremony later that evening brought home the scale of the conference, I've never seen so many crystallographers in one room (and likely never will again) and we were told over 2000 people were attending. The Ewald Prize Lecture was awarded to Professor **Philip Coppens** for his contributions to developing the fields of electron density determination and the crystallography of molecular excited states. Then the celebrations began with the welcome cocktail party; food aplenty, wine, ice cream and cantucci (hard almond biscuits) to dip into Vinsanto wine, what more could a girl ask for?

The next day heralded another early start as I had to have my poster, Investigating Weak Interactions in Pharmaceutical Co-crystal Systems, up on display by 8.30am and looking around the hall there were a few people suffering from the night before. The conference was

arranged into Keynote lectures at 8.30am and 5.30pm and we were honoured to have the Nobel Laureates: **Roald Hoffman**, **Harry Kroto** and **Ahmed Zewail** delivering three of them, and six parallel Microsymposia in the morning and afternoon sessions. There were a huge variety of subjects being covered and often there was more than one talk that I wanted to attend at the same time. To describe them all here would be a massive task, so I'll tell you the highlights of the conference for me personally.

Possibly the strangest talk I attended was the Application of X-Ray Diffraction in The Forensic Science Laboratory of Stuttgart (**W. Kugler**), seeing a TShirt, hammer and even a panel from a car mounted on a diffractometer was a sight to behold! Then it was a quick break before bouncing over to the Polymorphism Microsymposia to show support to fellow colleague **F. Leusen** (not that he needed it) followed by **M. Zaworotko** describing Polymorphism in Co-Crystals and Pharmaceutical Co-Crystals, their success by solvent mediated grinding and slurry preparation methods and the possible application of drug-drug co-crystals. It was great to finally put a face to a name that has been influential in my research and I came away with some new ideas for my own work.

After a quick lunch it was time for me to present my poster on the co-crystallisation and glycosylation of Sulfathiazole with sugars. It was an amazing opportunity to discuss my research of with those who are leading the field around the world. Not only did I get some useful advice and comments, but I was able to share some of my own experiences such as unexpected reactions, although dreaded intellectual property issues kept much of everyone's work shrouded in secrecy! I ended up staying at my poster well into the afternoon session, before having a quick look at the other posters that I was interested in. The day ended with **Sam Chong** of the University of Birmingham discussing 'Pushing the Boundaries' of Differential Evolution in SDPD and how the DE optimisation can be improved by updating the boundaries of the structure solution calculation and restricting the search to regions of low R factor that have previously been found within the initial search.

Other highlights of the conference included Elucidating the Structures of Nanoporous Microcrystals (**L. McCusker**), as I've had my own problems with structure determination of a microcrystalline product, and numerous structure determination from powder diffraction talks. A whole symposium was dedicated to Non-Covalent Interactions in Crystals of Small Molecules and included a talk from **F. Allen** on Carbonyl...Carbonyl Interactions and the use of the CSD in studying these systems. Another symposium of Controlled Building of Crystals From Non-Covalent Interactions included Understanding and Using Solution Chemistry in Direct Crystal Nucleation by **R. Davey**, where the role of solvent mediated assembly to produce different polymorphs from solution was discussed. Packing of Organic Molecular Compounds, in particular Crystal Structure Analysis and Solid Form Selection in

the Pharmaceutical Industry (**A. Gillon**) was of interest and described the difficulties in selecting the optimum solid dosage form of an active pharmaceutical ingredient (typically the most thermodynamically stable polymorph) via high throughput and manual analytical techniques.

As the conference drew to an end, the number of participants began to dwindle, but I was one of the die hards to stay to the bitter end if only to cheer on **Colin Seaton** from my office as he discussed Powders, Prediction and Epitaxy: Applications of Differential Evolution, where he described the applications of the DE algorithm in predicting crystal structures and epitaxial interfaces of organic crystals. The closing ceremony was rather an anti-climax, however the poster prizes were announced to eager anticipation and we were introduced to the new IUCr president and invited to Tokyo in three years time to do it all again!

It would be wrong not to tell you about the social side of the conference, all work and no play..., particularly the Marresearch company Traditional Party. This was held in a magnificent villa in the hills of Fiesole. It was amazing! The villa took your breath away, the views across the hills were spectacular and it was a fabulous party. When we went out for dinner the next night, the waitress in the restaurant had already heard about the infamous Marresearch party.

I also attended a chamber music Concert performed by the "Quartetto di Torini" and the pianist **Tiziano Mealli** (the Scientific Chairperson **Carlo Mealli**'s cousin!) organised by the IUCr at the Teatro Verdi. The theatre was wonderful and it was lovely to sit quietly and enjoy the music after so much rushing about. The Social Banquet in the "Meridiana" courtyard of Palazzo Pitti was a great end to the conference, and the fizzy red wine helped make it even better.

Having discovered the IUCr conference over two years ago and also that the venue was Florence, I had been looking forward to it ever since. I wasn't disappointed and it has definitely been the best conference that I have attended. I only wish it had been last year so that I would have more time to try all the new ideas that I have come back with to my own research.

I thank the BCA for their generous support in enabling me to attend such a memorable event.

Sophie H. Dale - University of Newcastle upon Tyne

MY choice of the most interesting and useful lectures I attended!

Mike Zaworotko (South Florida) presented on the synthesis of co-crystals, highlighting the recent debate by a number of leading researchers concerning the definition of a co-crystal. Mike discussed the application

of co-crystallisation to the pharmaceutical industry, where drug polymorphism is a phenomenon requiring extensive investigation before the drug can reach the market. Polymorphic co-crystals are very rare, and so the act of co-crystallising an active drug with another compound should reduce the chance of polymorphism occurring. A potentially useful application here is the co-crystallisation of two active drugs together, thus allowing the prescription of one combined tablet to the patient, rather than one tablet of each of the two separate drugs.

Lynne McCusker (Zürich) gave a very nice plenary lecture on zeolites and the use of powder diffraction in their characterisation. Lynne aimed this talk at a good level, targeting those in the audience (myself included) who, while having some appreciation of both zeolites and powder diffraction, were not experts in the field. Lynne discussed the uses of zeolites, ranging from everyday uses such as water softeners to more specific applications such as petrochemical catalysts and radioactive waste confinement.

Frank Allen (CCDC) presented on the presence of carbonyl-carbonyl interactions in structures held in the CSD, highlighting the fact that these are common and can represent quite strong interactions. One example is the antiparallel motif present in the acetone dimer, which has a strength approximating to that of a medium strength hydrogen bond. This talk has been useful in helping me to appreciate another important interaction to look for when analysing the interactions between molecules, particularly those without strong hydrogen bond donor and acceptor groups.

Jerry Atwood (Missouri-Columbia) gave a talk on the synthesis of large, molecular capsules. Jerry showed that by using phenolic compounds, hydrogen bonded capsules can be created, and that by adding metal ions, the phenolic groups are deprotonated to give phenoxide complexes, which assemble to give very similar structures to those of the hydrogen bonded aggregates.

Alan Williams (Geneva) presented on the use of functionality on the exterior of complexes to create supramolecular arrays through the coordination of additional metal ions and through intermolecular hydrogen bonding. Alan described the synthesis of chiral, polynuclear complexes through the use of polydentate ligands.

Jon Steed (Durham) reported on the results of an investigation into the synthesis of ureidopyridyl ligands and their use in the binding of anions through hydrogen bonding and in the coordination of cations. Jon discussed the use of NMR titration techniques to investigate the binding of anions to the ureidopyridyl ligands and also the use of the program PACHA to aid determination of the strength of hydrogen bonds using accurate coordinates, for example from neutron diffraction experiments.

Vincenzo Balzani (Bologna) gave an excellent talk on the design of molecular-level devices and machines, with

many captivating animations showing the devices he discussed. Molecular-level machines are a type of device requiring an external stimulus in order to give changes in the positions of the component parts of the machine. Vincenzo described a compound in which parts of the assembly moved depending on whether the assembly was protonated or not, hence the machine was operated through pH dependence. This talk really did catch my attention, for the uniqueness of the work, and for the way it was delivered to the audience using such carefully created animations.

Maciej Kubicki (Poznań) discussed the compromise required in the organisation of molecules to create the crystal structure, noting the need for a balance between such effects as intermolecular interactions, close packing and symmetry requirements. Maciej noted that $Z' > 1$ is more frequent in low symmetry and chiral space groups, with the geometry in symmetry-independent molecules being quite similar, leading to pseudosymmetry. Maciej provided a number of references during his talk, which have been very useful in my work.

Leonard MacGillivray (Iowa) gave a talk on the solid state [2+2] cycloaddition of molecules bearing C=C bonds. This photodimerisation will only occur if the C=C bonds in adjacent molecules are within 4.2 Å of each other. Where this distance is too large for photodimerisation to occur, hence the compound being photostable, Leonard described the use of a co-crystallisation strategy to direct the molecules, through the formation of hydrogen bonds, to lie within the prescribed distance range and thus allow the cycloaddition to occur.

Fabrizia Grepioni (Bologna) discussed the use of mechanochemical reactions (essentially grinding reactions) to give powders which were proven to have an identical structure to the material grown from solutions of the same starting materials; thus indicating that the reactions can be carried out in a solvent-free environment. Fabrizia highlighted the (perhaps often unnoticed) reactions that can occur between compounds and KBr or CsCl under the pressure required to create pellets for use in FT-infrared experiments. This is perhaps something for us all to be aware of; the spectrum recorded may not actually be that of the pure compound.

Gordon Barr (Glasgow) presented on the computer program *dSNAP*, and its applications to structural data mined from the Cambridge Structural Database. Gordon showed that the program can be used to group similar structures from the CSD using cluster analysis, thus reducing the time required to analyse a large hit-list compared to manual browsing in Conquest. Gordon's lecture was followed later by a very useful hands-on session in which the use of *dSNAP* was demonstrated with real examples.

Letters to Ed.

From Professor W. Clegg

Off to a flying start

Dear Bob

It was interesting to see that a number of the prizes awarded at the final ceremony of the IUCr Congress in Florence were donated by British enterprises. It was also a British firm that produced one of the most effective advertising stunts; it seems people (and I was among

them) will wear anything for a chance to win a laptop. In view of the bright orange colour of their promotional T-shirts and their currently marketed **Cryojet** and **Helijet** cooling devices, I wonder if Oxford Diffraction are planning a new and fully automatic push-button low-temperature apparatus called **Easijet**. It could come complete with humorous safety instructions like those given by the airline stewardesses.

Yours sincerely
Bill Clegg

From Professor P. Dolding-Beetle

Rescuing Crystallography using Nanotechnology: Replacing Diamond with Diamondoid

Dear Sir,

In a previous edition of this newsletter, I was inappropriately critical of the hype surrounding nanotechnology and its capability of destroying both integrity in science, and the public trust in science. That was before I realised, as others have done, that putting the word "nano" in grant applications makes it far easier to receive large amounts of funding. Thus I wish to reverse my position with the following modest proposal.

With the recent large investments in neutron facilities, such as the second target station at ISIS; and synchrotron facilities, such as Diamond, it is important to determine whether these investments are a wise use of tax-payers' money, when more reliable nanotechnological solutions can be developed.

Is building massive proton and electron synchrotron rings the right way to go? Instead of building larger and larger facilities to find out information about atomic-sized structures, should we not be building sensors that operate on the nano and subnano scale? Nanobots are now a well-established area of research. Self-assembly means that they promise to be a very cheap method of building complex scientific instrumentation. All the difficulties appear to be in actually constructing them, as they tend to be quite small.

Here I propose a new method of nanobot production which overcomes the problem of smallness. String and brane-theory tells us there are at least 10 spatial dimensions. Visionaries such as myself realise that one can use the other 7 spatial dimensions. The nanobots could then actually be quite large in these other folded dimensions, and only have a very small projection in our familiar 3 spatial dimensions. This makes construction of nanobots very much simpler; once trivialities such as how to access these other

dimensions have been determined. Crystallographers could be leaders in this field rather than restricting themselves to an archaic three physical dimensions as they have usually done in the past. After all, periodic resort to dimensions greater than three is hardly incommensurate with the experience of crystallographers. Crystallographers also have the most to gain from such instrumentation.

Nanobots could be programmed to sit on crystal surfaces. Unlike other methods that are restricted to surfaces, super-string nano-sensors are extended down into the crystal, again with very fine projections of objects that are quite large in the wasted hyperdimensions. By analysing the average as well as the variance of their positions as a function of time the complete elastic and inelastic spectrum can be determined.

I thus call on the BCA to demand that the UK Govt stop this massive investment in short-sighted neutron and X-ray sources, and instead divert the funding into more reliable, and simpler hyperdimensional nanobot research. When one considers that a) programs are already being called upon to replace our DNA with a more reliable nanotechnological equivalent (1), b) nanotechnology based phones have already been envisioned that respond to mental commands (2), and c) nanotechnology-enabled "smart yoghurt" is envisioned, where you might soon be able to have "conversation with your strawberry yogurt" (3); the above is all very reasonable and well considered.

Prof P Dolding-Beetle
Innovation Center for Nanotechnological Nano-nonsense and the Applications of String Theory, BSU.

- (1) Kurzweil proposes research programs to replace DNA, block bioterror viruses: http://www.kurzweilai.net/news/frame.html?main=news_single.html?id%3D3267
- (2) Bell Labs president projects long-term nanotech: <http://www.foresight.org/nanodot/?p=2033>
- (3) 2050 - and immortality is within our grasp: http://observer.guardian.co.uk/uk_news/story/0,6903,1489635,00.html

BCA 2006 Spring Meeting

Spring Meeting 4 - 6 April 2006 Lancaster University

The BCA meeting starts at 10.45am on Tuesday 4 April 2006, and concludes with tea at approximately 3pm on Thursday 6 April. There will be the customary Commercial Exhibition running from the Tuesday to Thursday along with a buffet poster session. This year, the exhibition and posters will take place across 4 rooms within the Conference Centre. There will be refreshments in each room along with email facilities which will facilitate interaction between exhibitors, poster presenters and fellow delegates.

Lancaster University offers superb conference facilities for both our delegates and exhibitors. Registration, Exhibition and Poster sessions will take place in the Conference Centre and all Scientific Sessions will occur within the Faraday Complex. This year there will be three Satellite meetings on Monday 3rd and five workshops scheduled from Tuesday 4 April - Friday 7 April. On Monday there will be two workshops; Young Crystallographers and Time Resolved Workshop, with one afternoon meeting - SR Users & Diamond SIG meeting. On Tuesday morning there will be two workshops prior to Registration; Young Crystallographers and Powder Diffraction Workshop with Synchrotron Chemical Crystallography for all taking place after registration. On Wednesday there is the Topology workshop and then on Thursday we have the TOPAS workshop. On Thursday afternoon there is the Hursthouse Event which concludes on Friday. More details of these and the main Scientific programme can be found overleaf.

For more information on the Exhibition and Sponsorship opportunities, or for any other enquiries about registration or accommodation, please contact Elaine Fulton at the BCA Administrative Office, 01355 244966 or email bca@glasconf.demon.co.uk



Registration

Early Registration Costs (before 6 March 2006)

Full Registration:	£135.00
Student/ Unemployed/ Retired:	£70.00
Non-Member Surcharge:	£25.00
One-Day Registration (no concessions):	£70.00

Late Registration Costs (after 6th March 2006)

Full Registration:	£190.00
Student/ Unemployed/ Retired:	£70.00
Non-Member Surcharge:	£25.00
One-Day Registration (no concessions):	£95.00

Accommodation

Two types of accommodation are available at Lancaster University:

Standard B&B	£35.00 per night
En-suite B&B	£42.00 per night

Accommodation is located within the John Creed, George Fox and Pendle buildings within the University campus. Breakfast and dinner will be served in Langdales restaurant.

Check in time is 14.00 - Reception is open from 08.00-23.00 after which time keys can be collected from the main security.

Catering

Morning coffee and afternoon tea will be served in each exhibition area within the Conference Centre.

Breakfast and dinner (including the Conference dinner) will be served in the Langdales restaurant.

Lunch and dinner must be booked in advance and will be ticketed.

Packed lunch	£6.00
Dinner on campus	£12.00

Social Events

On Tuesday 6 April, the Poster / Exhibitors reception will be held in the early evening. Wine and a buffet meal will be served. Delegates will have the opportunity to meet with the exhibitors and poster presenters in a relaxed and informal setting. There will be no additional charge for the wine or buffet reception, but sponsorship is welcome.

The Conference dinner will be held on Wednesday 7 April in the Langdales restaurant at a cost of £30.00/£15.00 for students.

Car Parking

Permits for parking will be issued to delegates with confirmation of registration; parking is concentrated mainly on the perimeter road surrounding Lancaster University grounds. Please book this permit on the registration form.

E-mail Facilities

Access to e-mail and internet facilities on designated terminals will be available within the exhibition rooms and library. Login passwords will be available from the registration desk.

Abstract Submission

Submission of Abstracts will be electronic only. For instructions or any other queries, please contact Chick Wilson on chick@chem.gla.ac.uk. The Abstracts web-site will be: www.chem.glas.ac.uk/BCA2006

Abstract Deadlines

Friday 13 January 2006 (Abstracts for consideration as contributed talks).

Friday 10 February 2006 (Poster abstracts and Bursary applications).

BCA Bursaries for BCA Spring Meeting

A limited number of Bursaries are available from the Arnold Beevers Bursary Fund to cover the cost of two nights accommodation, meals (including the Conference dinner) and registration. The bursary will not cover travel expenses and recipients will be expected to present a poster and produce a report on some part of the meeting.

Council is again seeking commercial sponsors of Spring Meeting Bursaries at £175.00 per student and it is hoped that some Named Bursaries will be awarded at this meeting.

Individual BCA members may also wish to give a living legacy by sponsoring their own named student bursary. All sponsors will receive a certificate of appreciation and be acknowledged in the annual bursary report.

The closing date for all applications is Friday 10 February 2006. Only on-line applications via the BCA website: www.crystallography.org.uk will be accepted.



BCA 2006 Spring Meeting - Scientific Programme

THE overall theme for the meeting in April 2006 is "Crystals and Crystallisation" and sessions on this general topic run throughout the meeting.

In this context, we are particularly pleased to welcome the British Association of Crystal Growth who will be joining us for the entire programme and who are contributing through joint and individual sessions. We hope that this will encourage interactions between the communities and make for a highly stimulating meeting.

Those of you who are regulars at the BCA Spring Meetings will find that there are a few changes to the schedule this year, and some old favourites are back. This year the plenary session at the beginning of the meeting has been replaced by four Keynote lectures, of general interest, associated with particular sessions, and spaced through the meeting. The topics covered range from "Crystallisations in Space" to "Topology and its Uses". By popular request the "Young Crystallographers" satellite meeting is back, allowing research students in the field to present their results in a relaxed and invigorating environment. There is also the possibility for young crystallographers to make contributions in the main programme. These contributions will be particularly welcome. After the success of the Exhibitors' Forum, which ran for the first time last year, this event is being repeated, and will allow the Exhibitors to make short presentations on their latest developments. The ever popular Powder Diffraction Workshop also runs again this year and will be of interest to academics and industrialists alike.

Scientific Sessions

There is something for everyone in the twelve main scientific themes spread over two and a half days together. In addition, there are a series of workshops and satellite sessions covering many aspects of modern crystallography. This year there is one BCA named lecture, the Lonsdale Lecture, and the CCG and PCG Prize lectures. As part of the main programme there will be TOPAS and topology workshops, and satellite workshops on time resolved diffraction and on synchrotron-based chemical crystallography. In addition, on the Monday afternoon, there is a joint SR Users Group and Diamond SIG Meeting and, after the formal end of the Meeting, there is a special event to honour Mike Hursthouse to recognise the contribution that he has made to chemical crystallography throughout his career. Everyone is welcome to stay for this event. If you wish to attend any of the satellite sessions please tick the relevant box on the main meeting registration form.

Thanks to the efforts of the programme committee and the session chairs the detailed scientific programme is progressing nicely, and on the following pages the planned

sessions and agreed speakers are outlined. It is particularly pleasing to see that the invited lecturers include a glittering array of scientists from overseas so that the Meeting is truly international. Further details of the programme can be found on the BCA Website at www.crystallography.co.uk as they become available.

Submit your abstracts for posters and talks on www.chem.glas.ac.uk/BCA2006. Deadlines are 13 January 2006 if you want to bid for a talk slot, and 10 February 2006 for posters.

Call for Abstracts and Bids for Talks

As for every BCA Meeting, much of the discussion of new science takes place around the posters. Please plan on showing a poster on your recent work, and encourage others in your group to do the same - remember: posters mean prizes!

Please submit your abstracts on line at www.chem.glas.ac.uk/bca2006.

The deadline is Friday 10 February 2006.

This year, there are slots in the oral sessions for contributed papers from crystallographers, young and old. We look forward to receiving bids for these slots - check out the sessions and see which one your talk will fit into best! The bidding procedure could not be easier: when you submit your abstract on the web just tick the box! The deadline for these bids is Friday 13 January, 2006.



Keynote Lectures

Keynote 1

Chair: Richard Pauptit (AstraZeneca)

Lecturer: **Larry De Lucas** (Birmingham, Alabama)

Keynote 2

Chair: Simon Parsons (University of Edinburgh)

Lecturer: **Mark Spackman** (University of Western Australia)

Visualizing and exploring intermolecular interactions in molecular crystals: A new toolkit for crystal engineering

Keynote 3 - Alun Bowen Lecture

Chair: Jeremy Cockcroft (UCL)

Lecturer: **Ulrich Griesser** (University of Innsbruck)

Keynote 4 - Teaching Plenary

Chair: Richard Pauptit (AstraZeneca)

Lecturer: various

Protein Crystallography for Non-experts

Named Lectures

The Lonsdale Lecture

Chair: Chick Wilson (University of Glasgow)

Lecturer: **Mike Glazer** (University of Oxford)

Parallel Sessions

High Pressures, Liquids and Surfaces

Chair: Dr David Allan (Edinburgh)

Lecturers:

Colin Pulham (University of Edinburgh)

Exploring crystallisation processes at high pressures

Dominic Fortes (UCL)

Crystallisation of ammonia hydrates under high pressure

Topology

Chair: Jacqui Cole (Cambridge)

Lecturers:

Simon Parsons (University of Edinburgh)

The Effect of High Pressure on the Topologies of Molecular Crystals

Elna Pidcock (CCDC)

The Box Model of Crystal Packing

Thomas Gelbrich (University of Southampton)

Title tba

German Sastre (University of Valencia)

Ring Topology and Strain in Zeolites

Caroll Johnson (ORNL)

Orbifolded thermal motion critical net topology

Neutron and Synchrotron Opportunities for Industrial Users

Chair: Jeremy Cockcroft (UCL)

Lecturers:

Alan Hewat (ILL)

Title tba

Crystallisation and Polymorphism of Pharmaceuticals

Chair and co-chair: Roy Copley (GSK) and Anne Kavanagh (AstraZeneca)

Lecturers:

Roger Davey (University of Manchester)

Controlling nucleation of enantiomers from solutions - the chiral enrichment of mandelic acid

Sally Price (UCL)

Progress and problems in computational prediction of crystallisation and polymorphism

Charge Density

Chair: Dr Mary Mahon (University of Bath)

Lecturers:

Piero Macchi (University of Milan)

The XD software package for charge density analysis

Louis Farrugia (University of Glasgow)

Experimental aspects of charge density studies

Paul Popelier (University of Manchester)

Quantum chemical topology

Crystal Structure and Growth at the Nano-Scale (joint BACG/IG Session)

Chair and co-chair: Kevin Roberts (University of Leeds), Richard Morris (Morris Analytical X-ray Ltd)

Lecturers:

Peter Langer (University of Graz)

How crystals are born: novel insight from small-angle X-ray scattering

Kevin Roberts (University of Leeds)

Solution phase nucleation: cluster size & shape and its correlation with crystallisation kinetics and polymorph selection

Powder Diffraction in Industry

Chair and co-chair: Judith Shackleton (Manchester) and David Beveridge (Ilford)

A diverse selection of industrial applications - details to be announced.

Crystal Engineering (BACG Session)

Chair and co-chair: Nick Blagden (University of Bradford), Kevin Roberts (University of Leeds)

Lecturers:

Dario Braga (University of Bologna)

Making Crystals by Reacting and Transforming Crystals

Christer Aakeroy (Kansas State University)

Constructing Co-crystals with Molecular Sense and Supramolecular Sensibility

Jonathan Steed (University of Durham)

Anion Binding Venus' Flytraps and Tweezers

Workshops

To avoid disappointment please ensure that you confirm your preferred workshops on the registration form.

A full day XRPD workshop on phase identification

Organisers: **John Faber** (ICDD), **David Rendle** (consultant) and **Dave Taylor** (consultant)

This is a modular workshop based on 4 distinct sessions which build to give a complete understanding of phase identification and its progression into quantitative analysis, culminating in a flexible hands-on computer session to gain practical experience with real examples. The modular structure will allow delegates, on the basis of their experience, to dip in and out of sessions through the day giving the package something to offer everyone with an interest in phase identification.

Module 1: 09:00 - 10:30 History & Structure of the Powder Diffraction File (PDF)

This module will cover important background information on the Powder Diffraction File with the emphasis on gaining an understanding of the various databases and how to interpret the data from an individual entry and select the best entry to use from multiple entries of the same compound.

Module 2: 11:30 - 12:00 Phase Identification

This module will cover collecting data for phase identification (PID). An understanding of the various manual search methods, alphabetical, Hanawalt, Fink and long 8 will underpin the knowledge required for automated search match techniques. It will cover selecting the database to use and subfile selection for particular applications.

Module 3: 13:00 - 15:00 Advanced Phase Identification and Quantitative Analysis

Here we will cover data mining, total pattern analysis and the methods of quantifying the phases detected, covering reference intensity ratio, spiking and Rietveld analysis.

Module 4: 15:30 - 17:15 Hands-on computer session

This module will allow you to put into practice the techniques covered in the workshop by using practical examples of both qualitative and quantitative problems for you to solve in a dedicated computer suite.

TOPAS Workshop

Organiser: Dr John Evans (University of Durham)

The PCG and CCG will be running a Topas-Academic workshop on the final afternoon of the BCA spring meeting 2006 at Lancaster University. Topas-Academic is a powerful software suite written by Alan Coelho which allows the analysis of both powder diffraction and single crystal diffraction data. Data from most laboratory/central facility diffractometers can be analysed. More features of the software are detailed below. Like some other software suites used by the academic community, it is available for academic use for a nominal fee (in this case 500 Euros) which helps the developer cover distribution and program support costs.

The workshop will be run along similar lines to the successful ones previously organised on packages like Jana and Crystals. A very brief overview of the software and how to operate it will be given. Attendees will then be encouraged to work through examples in their own specific areas of interest. Expert tutors will be on hand to assist with any difficulties. We will endeavour to prepare tutorials of relevance to molecular/extended systems and of interest to biologists/chemists/physicists. You can also bring your own data along to play with.

In order to attend this workshop, it is essential that you tick the relevant box on the registration form. Following this, you will be sent a form by email to complete to help us assess the background of attendees and prepare suitable tutorials.

Spring Meeting Exhibitors Forum

Following the success of the forum at the Spring Meeting last year the event will be repeated this year.

The forum will provide each exhibitor with the opportunity to present their latest developments and encourage participants along to their stands in the Commercial Exhibition. It is serious, but entertaining and enlightening, and we encourage participants to provide a good audience for this valuable session, to be held on the opening day of the main meeting.

To register your interest in presenting, please contact Elaine Fulton at the BCA Administrative Office, 01355 244966 or email: bca@glasconf.demon.co.uk

Satellite Meetings

Young Crystallographers Meeting

Organiser: **Andrew Parkin** (University of Glasgow)

Following the great success of the Young Crystallographers Meeting that took place at the BCA Spring Meeting two years ago, the event is being repeated. It provides a showcase for Ph. D. students and post doctoral workers to present their latest results in a relaxed and enlivening atmosphere.

Workshop: Ultrafast time resolved studies using X-rays

Organiser: **Mina Golshan** (SRS Daresbury Laboratory)

A range of topics involving dynamic and time resolved studies of the structure of matter using synchrotron radiation will be described.

Synchrotron chemical crystallography for all

Organiser: **Bill Clegg** (University of Newcastle and SRSR Daresbury Laboratory)

Single-crystal "small molecule" diffraction facilities were established at Daresbury SRS about ten years ago, and a Diamond beamline is planned for 2008. Access at the SRS is for specific research projects and also, since 2001, more widely as part of the EPSRC National Crystallography Service. Users and service providers will present some results and discuss past experience and future prospects. Come and see what's in it for you.

The Hursthouse Event

Organisers: **Paul Raithby** (University of Bath) and **Alan Welch** (Heriot Watt University)

A symposium and dinner in honour of **Mike Hursthouse** to recognise the outstanding contribution that he has made to Chemical Crystallography throughout his career.

Lecturers at the symposium include: **Martin Schröder** (Nottingham), **Simon Coles** (Southampton), **Alan Welch** (Heriot Watt), **Bill Clegg** (Newcastle) and **Paul Raithby** (Bath).

All are most welcome.

Central Facility User Meeting

Organiser: **Mina Golshan** (SRS Daresbury Laboratory)

A combined meeting for the SRS XRD User Community and the Diamond SIG will take place on Monday, 3rd April.

Insight into Lancaster

Lancaster is dominated by its medieval castle and the River Lune that runs through the city. The narrow, Georgian streets surrounding the castle contain a wealth of attractions, shops and restaurants - a hidden treasure that is definitely worth exploring.

The historic city of Lancaster is just minutes by public transport from the University. It is a friendly, bustling city which has all the amenities of a large city without having lost its charm and character.

Threading through the city is the canal with its waterside inns where you can watch the procession of boats glide by. There are punts for hire and a choice of craft offering cruises and restaurant facilities.

Most of the city centre is pedestrianised and in addition to the usual high street retailers, there is a shopping arcade and a large indoor market which contains a fish market selling fresh local catches from Morecambe Bay. Why not take the time to stroll around the city - you will be amazed at the numerous cafes and curiosity shops just waiting to be discovered.

Directions



By Road

Leave the M6 motorway at Junction 33 and take the A6 North towards Lancaster. After about one and a half miles, having passed through Galgate village you will reach a set of traffic lights at which you should turn right into the University drive.



By Rail

There are direct rail links between Lancaster and London, Birmingham, Leeds, Manchester, Oxford and major cities in Scotland. It is possible to make the return journey between Lancaster and London within the day (the single journey usually takes about three and a half hours).



By Air

From Manchester International Airport take the M56 motorway at Junction 5 and join the M6 motorway at Junction 20a (north). Follow the directions in the section headed 'By Road'. A rail link runs between the airport and Lancaster.

BCA 2006 Spring Meeting -

	Monday, 3rd April		Tuesday, 4th April					
	SATELLITE MEETING							
9.00 h			Young Crystallographers		Powder Diffraction Workshop			
9.45 h								
10.00 h								
10.30 h			Coffee and Registration					
11.00 h	Young Crystallographers	Time Resolved workshop	Registration	Synchrotron Chemical Crystallography for all	Powder Diffraction Workshop	Neutron & Synchrotron Opportunities		
12.00 h					Lunch & Exhibition 12.00 - 13.00			Lunch
			Young Crystallographers & User Meeting Lunch		Welcome and Keynote 1			Keynote
13.30 h	Young Crystallographers	Time Resolved workshop	High pressure, liquid & surfaces	Hot topics Crystallisation	Powder Diffraction Workshop	Crystallisation & Polymorphism		
15.00 h			Tea & Coffee		Tea & Exhibition			
15.30 h			Tea & Exhibition		CCG Prize Lecture	Crystallisation Methods Hot Topics	Powder Diffraction Workshop	Crystallisation & Polymorphism
16.00 h	Young Crystallographers	Time Resolved Workshop						
16.30 h			PCG Prize Lecture					
17.00 h		SR Users & Diamond SIG Meeting	Exhibitors' Forum					
17.30 h								
18.00 h								
18.30 h	Dinner for Young Crystallographers and User Group Members 18.30 - 19.30		Posters & Exhibition 18.30 - 22.00 Buffet & Wine Reception 19.00					
20.00 h								

Timetable

Wednesday, 5th April		Thursday, 6th April			Friday, 7th April
					SATELLITE MEETING
Keynote 2		Keynote 4 - Teaching Plenary			Hursthouse Event
Exhibition	Topology	Coffee & Exhibition			
Customised Crystallisation	Coffee	Charge Density	Crystal Structure and Growth at the Nanoscale	Getting the most out of your crystal	
	Topology				
Tea & Exhibition 12.00 - 13.00		Lunch & Exhibition 12.30 - 13.30			
Keynote 3 - Alun Bowen Lecture		Powder Diffraction in Industry	Crystal engineering	TOPAS Workshop	
Customised Crystallisations	Topology				
Tea & Exhibition		Tea - Closing Ceremony 16.00 - 16.15			
Customised Crystallisation	Topology Workshop	Hursthouse Event			
CA AGM 16.35 - 17.20		Hursthouse Dinner 19.30			
Macle Lecture 17.30 - 18.30					
Conference Dinner 19.30					

Science and Mankind



Sir Lawrence Bragg about the time this article was written

BY Sir Lawrence Bragg, F.R.S., Cavendish Professor of Experimental Physics in the University of Cambridge, and broadcast on Sunday 6th August 1945 on the BBC Home Service: (from Bristol).

(The manuscript of the following article was "discovered" by Mike Glazer while clearing out a laboratory at the Clarendon. We

thought that it greatly deserved reappearing 60 years after it was written, and I am delighted to say that Sir Lawrence's daughter and literary executor, Mrs Patience Thomson, thought so too. We are also grateful to Professor Frank James, keeper of the Bragg archive, for his encouragement. - Ed.)

I was asked last year to give a Sunday evening postscript on 'The Spirit of Science'. At that time, the progress that was being made toward using atomic energy was a closely-guarded secret. Now the world knows that another tremendous new power over nature has been added to those which science has already given us. Where are we heading, and what is the significance of the vast changes in the world which the progress of science is binging about?

I will not try to forecast what atomic energy will do in the near future, for instance what changes it may bring about in power or transport. It is probably all too recent for anyone as yet to see clearly what may be possible, and at any rate, it is for the experts who have done the work to make such predictions. It is clear that a terrific power for good or evil has been created by this awe-inspiring success, but I will not try to guess its immediate political or economic implications. I want to attempt a long-range view and show its relation to past events in human history and its portent of things to come.

The use of the energy locked up in the nucleus of the atom has been compared to man's discovery that he could use fire. The old legend, that Prometheus brought down fire from heaven was based on a truth. The sun warmed man by day, but when it set he was left to face the cold and dark of night. By discovering fire, he found a way of bringing back at will the sun's warmth and light stored up as energy in the fuel he burnt. Much later, in very recent times, he found another use for the stored

energy by making it develop power. The energy which the sun poured down long ago on the tropical forests of the coal measures appears again as light and power in our homes. But the latest atomic fire which has been stolen from heaven comes from a far more distant past and more awe-inspiring source than the sun's heat. It was imprisoned in the nucleus in some great cauldron when the stars were made, in regions packed with energy to an almost unimaginable extent. There, prodigious forces wound up the springs which the atomic explosion releases. It has been called cosmic force, it is of a different order altogether to the gentle changes in the outer envelope of the atom, where energy is stored up by the sun's mild rays and can be released again when we burn our fuel. There is one question which many must be asking. If these vast stores of energy are present in the atmosphere all around us, is there not a danger that further success in exploiting them may touch off the whole world like some vast magazine? Sometimes a star blazes into brief glory in the heavens and wanes again to insignificance. It was often jestingly said that a new star like that was a world where the experiments in atomic disintegration of another Rutherford had been only too successful.

Well, that joke may not appear so wildly improbable now, but I think we can be reassured... For if the whole world had been of this explosive kind, some accident would have fired it off long ago without our intervention.

The actual production of the atomic bomb has staggered everyone's imagination as an example of what the application of scientific discovery can bring about, but I think it is worthwhile once more to underline the distinction between science and the uses to which it can be put. Here is a contrast which I would like to present to you. We have all seen pictures in the papers of the vast plants assembled in America to produce the bomb, and have been told of the hundreds of millions of pounds that were spent on it. Now, in the Cavendish Laboratory at Cambridge we have a little museum in which are displayed some of the pieces of apparatus with which historical experiments have been made. There are two such examples, simply constructed little gadgets one can hold in the hand. One of them is the vessel in which Rutherford observed the scintillations which told him that nuclei were being broken up by the rays from radium; the other is the device with which Chadwick made experiments which led to the discovery of the neutron. Those experiments were made in search for pure knowledge, Rutherford's just after the last war, and Chadwick's in 1932 and at the time must have seemed as utterly remote from any possible practical application as any scientific discovery could well be. But it's such experiments as these and similar ones made in other countries, Germany, Italy, and Austria as well

as Britain and America which represent the scientists' contribution to the atomic bomb. People are apt to talk of the scientists turning their energies to inventing terrible engines of destruction, the internal combustion engine, the V weapons, and now the atomic bomb; but it does not happen in that way. Scientists accumulate a store of knowledge which can be used for any purpose, good or evil. In the stress of war, as the President of the Royal Society puts it, science, as an unwilling conscript, has become the direct agent of indiscriminating devastation. The scientist explains what he knows to the statesmen who guide policy and the engineers who plan production on a vast scale. How could he possibly withhold his help when his country is at war? It is war which is wrong, not science which knows no national boundaries and enjoys a world-wide co-operation in the disinterested pursuit of knowledge.

The far-reaching result of some simple initial experiment is a familiar story; electricity provides many examples. But there are two aspects of this latest achievement which are portents of things to come. The vast technical effort in America needed to produce the bomb was an act of faith different in scale to anything which has happened before. The scientific knowledge had been gained with the most minute quantities of material, which could not be detected except by refined experiments. The huge enterprise was based not on experience of anything which had gone before, but on a pure idea, on deductions made by a small band of scientific experts whom the statesmen were willing to trust. And again, the enterprise is an example of the collaboration of experts on a scale such as the world has never seen before. No other single undertaking has ever drawn together such a galaxy of talent from many countries. It is tragic that the end in view was the production of a destructive weapon, but as an example of what can be done, it is the greatest interaction of brain effort in history and really does mark the beginning of a new era.

For what is the main lesson to be learned from the atomic bomb? It is surely that which has been emphasised in many of the letters and articles which have appeared since the news of its achievement was announced. The whole world is becoming far more closely knitted together than it ever was before. Ships, trains, aeroplanes, telegraph, telephone, and radio have supplied it with blood vessels and nerves which link all countries together in an organic unity, and what happens in one part of the world may intimately concern the opposite ends of the earth. The general tendency of increased ease of communication and interdependence has been to bring about larger political groups. Paradoxically, increasing complexity and deadliness of weapons has on the whole been an effective way of bringing people together, teaching them better manners, and making life safer. With the war just over fresh in our minds you may think this a rash statement, but is it not true? When a stout right arm and a stick or knife were all-powerful, men had to go about their business even in time of peace armed for their own protection.

A child could now kill a grown man with a tiny automatic - but we walk abroad without fear of attack and any one who disturbs the peace is hounded down by society as a criminal. Confronted by this danger, society produces a cure. To pass from individuals to nations. When rifles and a few guns were all that was needed for a campaign, a number of small private wars were always going on while the rest of the world looked on as spectators. We are now so interdependent, and preparation for war is so complex an undertaking, that once the conflagration starts it spreads over the globe which divides itself into two hostile camps. Now, may we not take comfort from the fact that the only number less than two is one? For I join with the optimists who think that the inevitable end of our scientific and technical achievements is a world welded into one unit just as Great Britain, once a collection of little warring kingdoms, is now united. I even dare to hope that the last great achievement, atomic energy, may mark the final turning point and that we have seen the last great war - (unless some hothead in the future leads our descendants into the adventure of a campaign against Mars).

The discovery of how to release atomic energy is one more example, the most striking as yet, that something very big is happening just now. We are living at the beginning of one of those epochs when the whole structure of human society undergoes a vast change and reorganisation. These epochs come at long intervals, measured in tens of hundreds of thousands of years.

The command over nature given by science is a discovery of the same magnitude as the first use of fire, or of domestic animals, or of agriculture and it is bringing about, as they did, a general transformation of the kind of life it is possible for human beings to live.

We can best understand what the effect of science is going to be by recalling the effects of those other great discoveries. They must have brought many difficulties and disturbances in their train, but each meant in the end one more step away from the animal-like life of the primitive savage.

Power to control nature is not in itself civilization, but it is the foundation on which civilization is built. Each time that this power has been increased in the past, it has made possible a richer life, with higher forms of art, ethics, and religion - the standards by which we measure civilization.

What has happened in the past will happen again.

Lawrence Bragg, August 1945

Reports

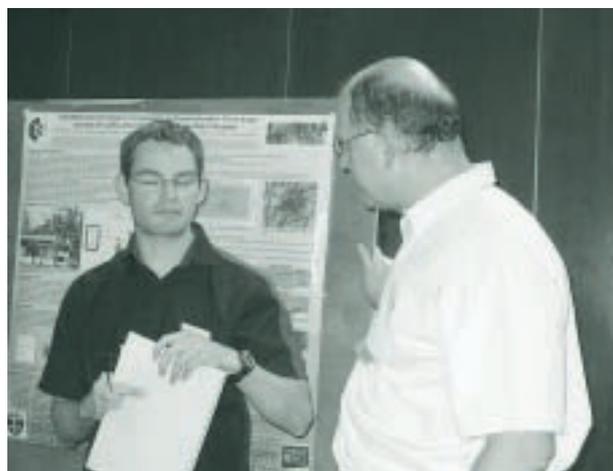
Summer School on New Advances in Crystal Growth and Nucleation

THE Il Ciocco conference centre in the beautiful surroundings of Barga, Italy, played host to this school, organised by **Nora de Leeuw** (University College London).

Over 59 people attended the event from 14 different countries. More than half of the people attending were students, who gave both oral and poster presentations. As well as the conference, a day trip to nearby Lucca was organised in which people had the opportunity to gift shop and to sample the local food and wine.

All aspects of crystal growth and nucleation were discussed in the first session, with both experimental and modelling aspects considered. The summer school started with an opening from **Kevin Roberts** (University of Leeds), which integrated both experimental and molecular modelling techniques, or, as was mentioned, three of the four M's, Modelling, Measurement and Manipulation. This presentation gave an introduction to the basic fundamental principles and associated experimental measurements underpinning nucleation and growth via crystallisation processes. Morphological modelling at the nano scale size was also discussed, making the link between theoretical and experimental work. **Roger Davey** (University of Manchester) then went on to discuss nucleation and crystal growth in further detail on the experimental laboratory scale with specific case examples making the link between rate kinetics, thermodynamics and crystal structure. **Sharon Cooper** (University of Durham) gave a presentation on exploiting phase inversions of w/o emulsions to o/w emulsions (glycine from decane with Tween20 and Span20 as stabilising surfactants) upon cooling to achieve highly anomalous crystallisation behaviour using surfactants that induce nucleation. Nucleation can be inhibited at this phase inversion, allowing systems held at or near this temperature to undergo crystallisation on either heating or cooling.

Richard Catlow (Royal Institute, London) gave an introduction and overview to computer modelling techniques. Modelling can be used for crystal building, crystal defects, inaccessible systems (e.g. extreme conditions) and prediction of various systems. The length and timescales of various types of modelling were introduced including high level Quantum mechanics (10^{-10} m, 10^{-12} s), Empirical and Semi Empirical, and Density Functional Techniques (10^{-9} m, 10^{-10} s). Various models and



Noel Hamill and Kevin Roberts in deep discussion about industrial applications at the poster presentation session

minimisation techniques were discussed as well as the pros and cons of these methods, such as local minima problems. The programs which employ these techniques and methods were discussed such as GULP, PARAPOCS, CRYSTAL and DL_POLY.

Bill Smith (Daresbury) gave a talk about the use of Molecular Dynamics in the crystal growth and nucleation field, explaining how the equations of motion can be applied by different algorithms to simulate the time evolution of various systems. The main needs for the use of Molecular Dynamics are computational speed, accuracy, stability, time reversibility and symplecticness, *i.e.* the long term stability of the system. The various algorithms and how they are applied to the systems of interest were explained in detail. It was explained that the main limiting factor is the timescale within MD work, for instance diffusion processes often have large timescales at low temperatures which is difficult to model using MD. Bill also talked about modelling on the mesoscale using a program, DL_MESO, which addresses longer time and length scales than atomistic simulation. This is relevant to both the chemical and engineering industries for use on polymers, colloids, rheology, mixing etc. **Antonio Tilocca** (University College London) then talked about the use of *ab-initio* methods for Molecular Dynamics. Although *ab-initio* methods cannot handle the timescales and amounts of particles used in classical MD, the interatomic potentials for the systems do not need to be known and are calculated from the instantaneous ground state of the framework of the DFT. The method can be used to model the dynamics of processes involving large re-arrangements of the electron density, such as bonds breaking or forming.

Stefano Piana (Curtin University of Technology, Australia) gave a fantastic presentation on the simulation of growth



A well earned coffee break in Il Ciocco

of molecular crystals of urea from both methanol and water using kinetic Monte Carlo methods in which surface sites were evolved according to the probability determined by some pre-computed reaction rate, which is often approximated. The full three-dimensional growth of a material was simulated at the microscopic level, offering insight into the roles of the solvent, the degree of supersaturation and the contribution of defects on the rate of crystal growth.

Nora de Leeuw gave an insight into the modelling of surfaces and interfaces, the methods and applications available. Both classical atomistic simulations and electronic structure calculations were used to model the structures and energetics of solid surfaces and interfaces to be used as a complementary tool with experimental results. The effects of water and adsorbates on surfaces of aragonite were examined with respect to crystal morphologies, surface growth and dissolution. The methodology for analysing both 2-d layers and 3-d slabs was also discussed.

Marilena Stimpfl (University of Arizona) gave a presentation on the origins of the earth's water and the possibility that hydrated material was incorporated into the accreting earth. Simulations of adsorption of water on interplanetary grains were carried out to examine a possibility of their having brought water to earth. MC simulations of adsorption at nebular conditions were carried out proving this is a possibility, although the role of porosity has not yet been rigorously examined. Olivine and water were used to simulate the systems.

Helen Baker (University of Manchester) looked at the possibility of generating more than one amorphous form for indomethacin with amorphous forms often offering enhanced pharmaceutical properties over their crystalline counterparts, for instance increased solubility

and bioavailability, leading to reduced side effects. NMR had been used to characterise the amorphous forms, as the lack of long range order precludes the use of X-ray diffraction. The two amorphous forms of indomethacin were used to utilise phase characteristics, structural properties and differences in re-crystallisation behaviour.

Simon Black (Astra Zeneca) gave talks on an industrial perspective of crystallisation: how thermodynamic data was consistent on scale-up from laboratory experiments but the time scales were unknown. Various temperature cycling procedures were found to change the morphology of the compounds and therefore can be optimised for scale-up. The compounds involved had large metastable zone widths in which seeds could be introduced to produce nucleation.

My poster presentation looked at the implementation of modelling potential parameters to a variety of nitrate compounds and then looked at the defect calculations therein. Several methods (Mott-Littleton, Supercell Method and Mean Field Approximations) were used to assess both interstitial and substitutional defects within the crystal lattice. Various properties for the defect lattices could then be calculated, including new volumes, solution energies, actual defect energies, lattice constants and elastic constants.

Poster presentations were given by the majority of students who attended the event. The summer school was a fantastic opportunity to learn more about the field of crystal growth and nucleation, to take part in debates struck up by various presentations and to gain valuable contacts in the field. Both experimental and modelling studies were discussed at the conference, giving people in either field the chance to look at the current work offered by the other.

Mike Orley, University of Leeds

16th International Symposium on Industrial Crystallisation

THE ISIC conference in Dresden, from 11-14 September was made up of five, half-day sessions on topics in the area of industrial crystallisation ranging from fundamentals to industrial problems.

The meeting was organised by Professor **Joachim Ulrich** from the University of Halle-Wittenberg, Germany and was held at Dresden's International Congress Centre.

After a welcome by the conference organisers the Monday morning session entitled the Thermodynamic Prediction of Physical Properties began with an interesting lecture by Professor **Gerard Coquerel** from the University of Rouen, France. The presentation described how phase diagrams may be drawn to show the effects of the presence of solid solutions when determining the relative stability of polymorphs. This was followed by talks about crystallisation in the presence of strong acids, the successful use of crystallisation as a purification method and the prediction of nucleation kinetics.

Over 100 posters were presented at the conference and the many poster sessions provided opportunities to meet people, discuss their work and find out more about other crystallisation research groups from around the world. The posters covered a broad range of topics from the design of new crystallisation vessels and processes to the latest computer modelling of solutions and crystallisation. I presented a poster entitled Crystallisation of Organic Salts from Aqueous Solutions: Controlling Physical Form through Solution pH in the section Crystallisation Problems in the Pharmaceutical and Food Industry.

The second session began with a presentation on Product Design and Characterisation by Professor **Hounslow** from University of Sheffield illustrating the problems still to be solved in crystallisation of products such as prediction of polymorphism and growth of crystals with specific size and morphology.

Next on the programme was a panel discussion led by Professor **Peukert** from the University of Erlangen and **Axel Eble** from Bayer Technology Services with the title *From Visions to Products in Industrial Crystallisation*. This discussion focussed on the materials chosen for study by crystallisation researchers and whether a greater diversity of substances should be studied, or there is value in continuing to study examples such as sodium chloride and calcium carbonate which are generally thought to be well understood.

Tuesday morning's session, Crystallisation Problems in the Pharmaceutical and Food Industry, began with a presentation by **Robert Docherty** from Pfizer on the



The restored Frauenkirche in Dresden

problems currently faced by the pharmaceutical industry. This was followed by talks on the growth mechanism of a pharmaceutical compound, additives for use in salt crystallisation, crystallisation of molecular salts and use of controlled crystallisation for the refining of lactose. This session was of particular interest to me as it focussed on crystallisation of organic compounds and salts. It was followed in the afternoon by a session on Conceptual Process Design. **Günter Hofmann** from Messo-Chemietechnik gave a presentation of the types of processes and design of crystallisation vessels used in industry over the last 40 years. The conference dinner on Tuesday evening was combined with a cruise on the River Elbe. This gave the opportunity to see some of the castles on the banks of the Elbe and to meet people from the conference in a more relaxed atmosphere.

Wednesday morning started with a second panel discussion led by Professors **Davey, Garside** and **Rousseau** on the future of crystallisation and the ways in which it could be used to tackle the major problems facing the world. Following this Professor Davey gave a presentation on the contributions of Professor Garside to crystallisation research and congratulated him on his retirement. The final session discussed Control of Batch Crystallisers with a presentation by Professor **Matsuoka** from Tokyo University.

Helen Jones, University of Manchester

14th International Conference on Internal Friction and Mechanical Spectroscopy (ICIFMS-14)

THIS triennial, international conference was held in Kyoto from 5-9 September, and was a unique opportunity to see the broad range of internal friction measurements being made and the variety of different applications of this method of experimentation, including insights into crystal defects, oxygen vacancy motion and grain boundary sliding mechanisms.

Attending talks and discussing work with fellow academics provided an invaluable experience and the first opportunity to present my work at an international conference.

The conference schedule was arranged to allow time in the evening and on several afternoons to explore some of the many temples, for which Kyoto is famous. A banquet on the last night allowed us to experience traditional Japanese food and drink, including sushi, sake and samurai sword lessons!

Overall it was an interesting week with a varied programme, with sessions on grain boundary sliding, high damping materials, ceramics and interfaces, in which I presented a talk entitled: 'Domain wall mobility and mechanical properties of LaGaO_3 perovskite over a first-order phase transition'. This research focuses on the effect of transformation twinning and twin domain motion on the internal friction measurements over a first-order phase transition and in the orthorhombic and rhombohedral phase, in the hope of learning more about the processes causing seismic attenuation in the lower mantle. A comparison of single crystal and polycrystalline samples enables a greater determination of whether grain boundary sliding or transformation twinning mechanisms are affecting the internal friction behaviour, and in turn the seismic attenuation in a possible mantle perovskite to post-perovskite phase transition.

Several highlights of the week include a talk by **M. Weller** from the Max Planck Institut für Metallforschung on high temperature damping in a variety of alloys, important for their possible use in high temperature environments, such as for parts in aeroplanes. **Professor Ian Jackson** (ANU, Canberra) gave an interesting talk on the behaviour of olivine, and the processes controlling the elastic, anelastic and viscoelastic response of samples of varying grain size and melt fraction. To conclude the week a series of talks on novel techniques was scheduled for the Friday morning, including a fascinating talk by **O. B. Wright** (Hokkaido University, Sapporo, Japan) on internal friction measurements at GHz frequencies using an acoustic sonar technique, enabling measurements of much higher accuracy than conventional methods.



The Golden Temple in Kyoto



The author with her apparatus!

Thank you to the British Crystallographic Association for the bursary which helped to enable my attendance at the ICIFMS-14, this year located in the beautiful city of Kyoto, Japan. I have returned to Cambridge after a week at the conference with a plethora of new ideas to explore.

Claire Jakeways, University of Cambridge

29th Symposium on the Scientific Basis of Nuclear Waste Management

THIS year's Symposium on the Scientific Basis of Nuclear Waste Management was held in the picturesque city centre of Ghent in East Flanders from 12-17 September, 2005.

The city is steeped in history from the 11th century onwards and 'Het Pand', the venue chosen for the conference, is just one of the many well preserved buildings to be found upon arrival. Once a Dominican monastery and now beautifully restored, the venue's surroundings, from the ornamental hedges and water-features, to the medieval cloisters where the poster sessions were held proved ideal for an informative and convivial meeting.

Historically, these meetings aim to draw together researchers involved in all aspects of a multi-barrier approach towards the long-term geological disposal of nuclear waste, in order to review recent progress and discuss future strategy. The excellent quality of the facilities and entertainment (including fire breathers and jesters at the conference dinner!) provided by the local organising committee were equally matched by the standard of science presented over the four days of poster and oral sessions.

For me, the opening session on International and National Overviews served to highlight the bigger picture of nuclear waste management, (sometimes forgotten when preoccupied with the minutiae of a PhD). The contrasting approaches of countries such as Finland, Japan and Belgium presented in key-note presentations by **Juhani Vira** (Posiva Oy), **Hiroyuki Umeki** (JNC) and **Johan Bel** (Ondraf/Niras) respectively, which included reports on recent developments in technology, licensing and repository excavation were highly insightful. Poster and Oral sessions focussing on bioceramics were more specifically relevant

to my studies and discussions with other delegates have suggested additional paths of research and potential collaborations. I also particularly enjoyed the oral session on Analogs, where talks by **Stephanie Gin** (CEA) and **Neil Chapman** highlighted links between waste management and areas of archaeology which I had not previously considered.

The final day was devoted to a technical visit to the Belgian nuclear facilities at Mol. We were shown around the low level radioactive waste (LLW) conditioning facilities operated by Belgoprocess and saw one of several interim storage warehouses, where the treated waste is placed before a final disposal site is selected. The sheer volumes of material being stored are incredible - over 7000 80-litre drums of LLW in just one warehouse! Such is the level of safety control, that in the treatment plant, the radiation level is lower than the natural background in the outside environment!

In the afternoon we donned hard hats and, feeling a little like miners, descended the 225m shaft into the BOOM clay stratigraphy, the chosen location for final disposal of Belgian high level radioactive waste (HLW). Somewhat giddy from the rapid vertical trip, we were shown around the Underground Research Laboratory 'HADES', where a variety of *in situ* experiments extensively characterise the long term retention of radionuclides in such an environment, as well as monitoring the integrity of the current excavations and their resistance to seismic activity.

Perhaps the most useful aspect of attending this conference was the co-operative atmosphere. This provided ample opportunities to meet researchers in the field, particularly during the discussion of my poster presentation, on the "Composition driven structural phase transitions in the $(Y_{1-x}La_x)_2Ti_2O_7$ system". The timing of this conference and its relevance to the conclusion of my studies and the choice of future career paths were highly beneficial.

Elizabeth Harvey, University of Cambridge

Conference delegates at the symposium. From L to R: Arther Day, Liz Harvey, Chris Griffith and Neil Hyatt



Fankuchen and Trueblood Awards

NOMINATIONS are solicited for the 2007 Fankuchen Memorial Award and the 2007 Kenneth N. Trueblood Award.

Both awards will be presented at the annual ACA meeting in Salt Lake City in July, 2007. The recipients will give their lectures at the special Fankuchen and Trueblood Award Symposia organized to honor them. Each award is given every three years and each consists of an honorarium plus travel expenses to accept the award. There are no geographic or age restrictions. The Fankuchen Award carries the additional responsibility that the Award Lecture should also be presented at an academic institution of the recipient's choice. Please submit nominations to the ACA office in Buffalo (see page 1 for address) no later than May 1, 2006. A nominating letter clearly indicating the accomplishments of the individual is required; an additional supporting letter and a c.v. for the nominee may be provided, but are not required. A nomination form is available on the ACA web site, <http://www.hwi.buffalo.edu/aca/>

The Fankuchen Award was established in 1971 in memory of Isidor Fankuchen, Professor of Physics at the Polytechnic Institute of Brooklyn from 1942 to 1964. It is given to recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography. Previous winners were: 2004: Alexander McPherson; 2001: James Stewart; 1998: E. Dodson; 1995: Jenny Glusker and Kenneth Trueblood; 1992: L. D. Casper; 1989: David Sayre; 1986: Michael G. Rossmann; 1983: Lyle H. Jensen; 1980: David Harker; 1977: Dorothy Hodgkin; 1974: A. Guinier; 1971: Martin J. Buerger.

The Kenneth N. Trueblood Award was given for the first time in 2004, to Richard E. Marsh. It was created to recognize exceptional achievement in computational or chemical crystallography. The award was established in 2001 in memory of Kenneth N. Trueblood, UCLA, who was a major force in the early use of computers and the development of crystallographic computer programs. He applied these programs to the examination of chemical and molecular details of many structures at the frontiers of research. His contribution to the famous work on vitamin B12 is one example. Ken Trueblood was a leader in the development of techniques for analysis of anisotropic motion and was also a superb teacher and a lucid author. The award is given every three years and consists of an honorarium plus travel expenses to accept the award.

The award selection committees are:

Fankuchen: Thomas F. Koetzle (Argonne), Chair; Bob Sweet (Brookhaven); Katherine Kantardjieff (Cal State U., Fullerton); Lachlan Cranswick (Chalk River, Canada).

Trueblood: Philip Coppens (SUNY Buffalo), Chair; Larry Dahl (Wisconsin); Doug Rees (Caltech); Jim Richardson (Argonne).

Glazebrook Medal and Prize

ANDREW Taylor, ISIS Director, has been awarded the 2006 Glazebrook Medal and Prize from the Institute of Physics for his contributions to neutron scattering physics through his leadership as director of ISIS and the realisation of the second target station project.

"It is a tremendous honour to join the ranks of men like Godfrey Stafford, Geoff Manning, and Paul Williams, all previous recipients of the Glazebrook Medal, who played such a strong part in shaping RAL in its early days," said a surprised, but happy Taylor.

"This award reflects as well the world-wide success that everyone at ISIS has achieved over the past 20 years. This is a good day for ISIS and we can look forward to a bright future for ISIS with the Second Target Station Project."

The Glazebrook Medal is one of the three premier awards from the Institute of Physics and is awarded annually for outstanding contributions to the organization, use or application of physics in an industrial, commercial, educational or National Laboratory environment. The medallist receives a silver medal and £1000 prize money and may be invited to give a lecture at an appropriate conference in the year in which the award is made.

Leadership in the revival of accelerator science in the UK was also recognised with Ken Peach, outgoing director of Particle Physics Department, receiving the Rutherford Medal and Prize. The prize was awarded for Peach's contributions to high-energy physics as leader of key experiments at CERN investigating CP violation and as director of particle physics at CCLRC's Rutherford Appleton Laboratory.

Martyn Bull - ISIS



Andrew Taylor



Ken Peach

IUCr Booklets no 21: Crystal Packing

by **Angelo Gavezzotti and Howard Flack**
International Union of Crystallography, 20 pages.

Electronic edition, free to download and copy for research and educational purposes.

THE IUCr's useful set of monographs has now reached maturity, being 21 in number! This one is a good member of the series, and those who have heard the authors lecture will be able to hear their voices coming through the explanations.

Thus, the coverage is a little idiosyncratic in parts, but this does not detract from the fact that the book provides a good introduction to the subject, and if readers are left with questions at the end, so much the better! No one could give a comprehensive coverage of this subject in 21 pages, and there is a substantial set of references and suggestions for further reading at the end, although a few more elementary texts might well have been mentioned.

The introduction, followed by a section on thermodynamics and kinetics is basically a clear and simple introduction to what a molecule is, and what differentiates a solid from a liquid. I would suggest, however, that SO_4^{2-} is not a good example of a species stable in the gas phase! Also, the sentence "...melting occurs because the entropy gain in your system by spatial randomisation of the molecules has overcome the enthalpy loss due to the breaking of crystal packing forces" should read "enthalpy gain", and in the equation that follows, this is correctly stated.

The treatment of ionic, polar and dispersion forces is good, but it should be noted that high polarisability is also important in raising the melting point (e.g. naphthalene, C_{10}H_8 , and nonane C_9H_{20}). Crystal symmetry is then treated, with a strong emphasis on the fact that small molecules do not like symmetry operations, other than the inversion centre, not involving translation. The space group frequency table is striking, although it probably does oversimplify the situation - all space groups now have at least one entry in the Cambridge database. A comparison is given with the ICSD to show how different

the symmetries on non-molecular structures are from those of molecular.

Probably the weakest feature of the monograph are the diagrams, which are well conceived, but done by hand, and so are not immediately obvious. In distinguishing a screw axis from a glide plane, groups of small men catching rugby balls (?) are used, and it takes a bit of effort to tell which way they are facing, which is crucial to the difference being shown! Hopefully this can be improved in a second edition.

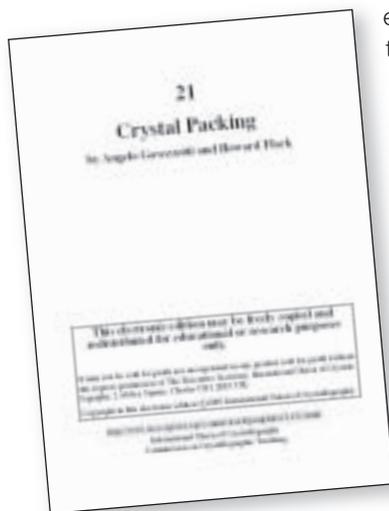
A valuable table shows how the symmetry of certain space groups leads to their symmetry elements tending to be involved in the formation of clusters, rows, layers and networks of molecules. The point is made that the "crystal structure descriptors" of density, packing coefficient and melting point should always be given with crystal structures. This would be very good, but there should be a proviso that the melting point should be stated to be unknown if that is the case, since spurious values would probably be invented by those who considered them to be unimportant - as was indeed done with "measured" densities when these were required!

There is a very good and outspoken section on chirality - as one would expect from these authors! In order to be complete, even the possibility of an achiral crystal formed from chiral molecules is considered: "in fact [the failure of this to happen] is due to the individuality of the molecules rather than to any underlying theorem of symmetry groups". Indeed - if one allows the molecules not to retain their individuality, anything may happen!

The pamphlet concludes with a concise introduction to polymorphism and some observations on experiments, including a plea that more notice should be taken by chemists of how their compounds do crystallize, since a huge amount of untapped information is lost daily by failure to note and publish this in some way.

This is a stimulating booklet, and is available free. It deserves a wide readership and even its few flaws contribute to its readability! Why not start a reading group and discuss it?

Bob Gould

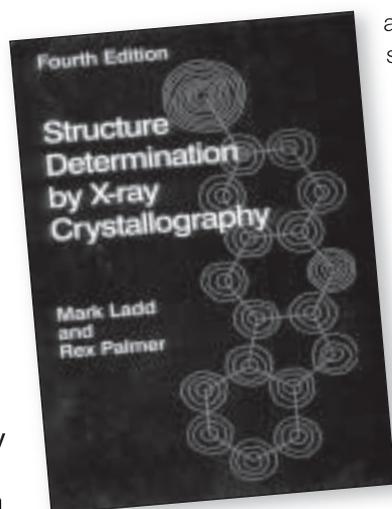


Structure Determination by X-Ray Crystallography, 4th Edition

**Mark Ladd and
Rex Palmer**

Kluwer/Plenum 2003 xliii +
819 pages plus CD
Price: £41 (paperback)
ISBN 0306474549

THE fourth edition of this classic text has been extensively revised and expanded: it is over 200 pages longer than the 3rd edition with three completely new chapters on "X-ray Structure Determination with Powders", "Proteins and Macromolecular X-ray Analysis", and "Computer-Aided Crystallography".



It must be emphasised from the outset that the 4th edition is not just the 3rd edition with new chapters: the original eight chapters have been extensively revised and sensibly re-organised with much new material being added and it is obvious that the authors have put a huge amount of work into creating this new edition. For example, chapter 3 now starts more logically (in my opinion) with the generation and properties of X-rays including those generated from a synchrotron source (this subject being relegated to an appendix in the earlier edition) before a discussion of how X-rays interact with crystals.

Starting at the beginning, the opening two chapters of the book begin with the timeless topic of crystal morphology and symmetry, a subject that is essential for a good understanding of crystallography. Chapter 3 then moves on to the subject of X-rays and how they interact with crystals. This leads on logically to the theme of the reciprocal lattice and how real-space symmetry is deduced from observations of the reciprocal lattice intensities. It would have been nice if the authors could have included lots of data sets on the CD-ROM for the new student to practice symmetry determination, but more on that subject later.

Continuing with chapter 4, I liked the fact that it still includes a section on the optical examination of crystals. This is a very practical subject required by all students who have to pick out a suitable crystal for their X-ray structure analysis. This chapter then continues with single-crystal X-ray instrumentation. Given the huge changes that have occurred in instrumentation during the last decade, mainly resulting from the introduction of the now ubiquitous CCD detector, this chapter on experimental methods has been greatly revised to include modern instrumentation. However, it still includes long sections on traditional film

methods and serial detector diffractometers: some aspects of the former may be relevant to modern single-crystal methods but much is of historical interest only as most high-throughput X-ray laboratories will now be equipped with CCD systems making a detailed discussion of, say, a CAD4 diffractometer somewhat irrelevant for the next student generation of X-ray crystallographers.

Chapters 5, 6, and 7 cover the classical subject areas related to X-ray structure solution, namely Fourier and Patterson maps plus direct methods. Although most of the underlying theory is now encoded in routinely-used black-box programs, e.g. those found in the SHELX software suite, these three chapters provide a useful "behind the scenes" view for the student who wants to know more about how structures are solved and refined by X-ray single crystal methods. These three chapters are then followed by chapter 8 that provides some practical examples. Although this chapter includes some pitfalls, personally, I feel it could be expanded further to include many more of the various problems that a new student to the field may encounter in their practical work, e.g. a discussion of how to cope with data from twinned crystals being an obvious one.

The new chapter 9 on structure determination from powders is a welcome addition to the book. In a single chapter, the authors can only provide the student with a useful overview as the subject could be expanded into a textbook by itself. While the subject is generally well-covered, a new student to the field may get the wrong impression as the chapter starts with a discussion of the now historical Guinier camera and completely misses out ultra high-resolution powder diffractometers at synchrotron sources, e.g. ID31 at the ESRF. However, the examples are very up-to-date and they cover all the various methods currently being used for structure determination by powder diffraction. The authors even include some of the latest work on polycrystalline protein samples, a highly-challenging area for powder diffraction analysis! It would be nice if some statistics had been given for structures solved by powder versus single-crystal: this would provide a new student to the field with some idea of the difficulties involved in this aspect of crystallography.

The second new chapter on macromolecular crystallography is aimed more at the student on the interface between chemistry and structural biology. As with the previous chapter, it can only provide an overview of a subject for which whole textbooks already exist. However, for students starting in small-molecule or materials crystallography and wishing to change field, this chapter provides a useful introduction to the subject.

The inclusion of the final chapter on computer-aided crystallography is certainly brave given how quickly this subject's dates. The chapter provides a good overview of some of the typical software packages available for both single-crystal and powder diffraction that should be useful

to the novice student. This chapter is accompanied by the CD-ROM containing a small number of DOS-based programs and a few data sets to illustrate particular teaching points made in the chapter. Personally, I feel the authors missed a real opportunity here: while software dates rapidly (especially with PC-based operating systems changing every few years as hardware changes), good-quality crystallographic data should last for an eternity. Thus a CD-ROM packed to the brim with example data sets (and corresponding solutions) collected by the authors during a lifetime's experience in the field would have been a real bonus for the new PhD student trying to get to grips with unfamiliar software.

Overall the book contains quite a large amount of mathematics: this may be slightly off-putting for the current generation of synthetic chemist who may want to use crystallography as yet another analytical technique in the same way as they use, say, NMR. Also, given that

colour printing has reduced dramatically in cost during the last decade or so, it is disappointing that academic publishers do not encourage it as some sections of the book could benefit from colour illustrations. For example, colour photographs of the optical examination of crystals showing good and bad crystals for X-ray analysis (plus a few corresponding colour frames from a CCD detector too) would benefit new students. Other positive points to note in this textbook are the excellent index and the problems with worked tutorial solutions at the end of the book.

Finally, it is very pleasing to see that the book has appeared from the outset as a paperback edition aimed at students (in marked contrast to many IUCr textbooks) rather than the usual hardback intended mainly for libraries, though the price may still deter purchase by the students to whom the book is clearly aimed.

Jeremy Karl Cockcroft

Blessed Nicolai Steno - a Crystallographic Saint in the Making?



STENO was a Dane, born in 1638, who may be regarded as the father of modern crystallography.

The idea that crystals are formed from repeating unit cells grew from his principle of the constancy of the angle. That is, the angle between pairs of corresponding faces is the same for any crystal

of a particular substance, regardless of the way it has grown or what shape it has. He was a fascinating and complex character, and, as **Carlo Mielli** mentioned in the IUCr Newsletter, his remains now lie in the Church of San Lorenzo in Florence. We paid a visit during this year's IUCr meeting, fortunately after getting a useful tip from **Rudolf Allmann** that it was pointless paying and looking in the main body of the church, where the tombs of the Medici are. His memorial is in the part reserved for private prayer – and is consequently free of charge!

But first a word about him. He was a true Renaissance man, and it instructive to see how many web-sites mention him. One, in fact, hails him as a “creation scientist” - rather normal, one would have thought, in the seventeenth century! He was trained in medicine, both in Denmark and the Netherlands, and rose to be Royal Anatomist in Copenhagen in 1667. Among other things, he gave his

name to the excretory duct of the parotid gland (*ductus stenorhianus*). On the side, he was a geologist, and it was his observation of quartz crystals that led to his famous principle. Perhaps as part of observing and tiring of the conflict in doctrine between Lutheran Denmark and Calvinist Holland, he gave up both, converted to Roman Catholicism, and moved to Italy. He became a priest, and in 1677 the titular Bishop of “Titiopolis”. For most of the rest of his life, he was an apostolic delegate in northern Germany, and seems to have stopped writing either medicine or science, but producing philosophical works of a very eirenic nature for their time.

After his death in 1686, he was buried in San Lorenzo, and now we return to our visit. We were greeted sternly at the door with the question, “Missa? [Mass?]” and we said yes and were let in. In fact, we got quite a bargain - not only a mass, but two divine offices as well! At the end of this, everyone else went out, and we were able to visit the side chapel. Above the main altar is the portrait of Steno I have tried to reproduce here. To the right of that is the tomb with a bas-relief and a text, emphasising his conversion from heterodoxy to orthodoxy. Most interesting, however, was the altar to the left, which was covered with a pile of small pieces of paper. Steno was beatified by Pope John Paul II in 1988, and part of the path to sainthood consists of evidence of assistance from beyond the grave, attested by these “votes”. We decided that we had done enough voting at the IUCr, and could abstain in this election. We slipped quietly away, but felt better for having got to know a saintly crystallographer better!

Bob Gould

Groups

Two meetings next year of particular interest to BSG Members:



The 2006 Gordon Research Conference on Diffraction Methods in Structural Biology, will be held July 16-21, 2006 at Bates College, Lewiston, Maine, USA. Chair: Paul Adams, Co-chair: Elspeth Garman.

The 13th BCA Summer School in Protein Crystallography will be held at the Biochemistry Department of Oxford University from 3rd Sep (Sunday afternoon) 2006 until 8th September (Friday afternoon) 2006.

Further details and a WWW based application form will be posted in the spring. Organisers: Elspeth Garman and Martin Noble.

BCA Industrial Group AGM



The Annual General Meeting of the BCA Industrial Group will be held at Lancaster University during the Spring Meeting, April 2006, exact date and time to be advised.

The following posts on the IG Committee will become vacant and are open for nominations:

Vice Chair
Secretary/Treasurer
3 Committee Members

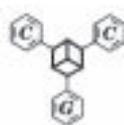
Please send all nominations to:

Judith Shackleton
Materials Science Centre
The University of Manchester
Grosvenor Street
MANCHESTER,
M1 7HX

Tel. 0161 306 3581
Fax. 0161 306 3586

Email Judith.Shackleton@manchester.ac.uk

Young Scientist Award 2006



The BCA-CCG Young Scientist Award 2006 is sponsored by the Cambridge Crystallographic Data Centre (CCDC). The award is made

on the basis of published research within the scientific field of interest of the CCDC and BCA-CCG, defined as:

"Original research in the field of chemical crystallography or the application of crystallographic information to structural chemistry. This definition shall include advances in instrumental, experimental, theoretical or computational techniques that contribute to this field."

Scientists nominated for the Prize shall be not more than 35 years of age on 1st January 2006, except that up to five additional years may be allowed if there has been a significant career break during which the nominee was unable to carry out research.

Please take some time to nominate someone you know who is eligible. There were many fine entries last year. Last year's winner was Dr Anders Markvardsen of ISIS who delivered his lecture on "Probability, Powders and Pathways"

The prize will be announced and the prize lecture presented at the 2006 BCA Spring Meeting in Lancaster.

Nominations must be received by me by 13 January 2006, and a nomination form may be found on the group website

Georgina Rosair, Secretary CCG
g.m.rosair@hw.ac.uk

Workshop on Patents in Crystallography



THE Industrial Group held a two day meeting in London on October 18-19 aimed both at crystallographers who need to know something about patents and at those with a legal background who need to know something about diffraction experiments.

The morning session of the first day was opened by **Samantha Towlson** (Pilkington plc), who introduced patents to crystallographers and explained that patents are a form of property that can be sold, mortgaged, or treated pretty much as physical property, and give the right to a 20-year monopoly on the process described therein. This must make at least one *claim* to be novel, and give a *description* which explains all that needs to be done to carry out the process. They are expensive both to obtain and to maintain and must, in Europe, give a technical solution to a technical problem, although wider definitions are acceptable in the USA. Crystallography is mainly involved by the use of powder diffraction to identify



Sam Towlson, Jeremy Cockcroft and Gareth Lewis



Martin Vickers and Mike Glazer

a material in the patent and to establish that the patent has been infringed. This talk was followed by **Jeremy Cockcroft** (UCL/Birkbeck) who gave a corresponding introduction to X-ray powder diffraction for patent people! Starting from the powder diffraction pattern as a fingerprint, he emphasised that an unindexed pattern gives no proof of the purity of a sample. He then went through the stages from precise data collection to three dimensional structure determination for suitable powder samples. He made a good case for his statement that XRPD is the primary characterization technique for all solids.

After lunch, **Gareth Lewis** (AstraZeneca) spoke on the particular case of XRPD and pharmaceuticals. In this case, many crystalline properties, particularly solubility, have a great importance in the usefulness of the material. In particular, the difference in solubility between a crystalline (less soluble) and an amorphous (more soluble) phase can vary enormously - it is 1:5 for caffeine and 1:270 for morphine. Getting an appropriate phase can be very complex, and large matrices of samples with varying solvents and counterions are normally prepared for possible crystallization and characterization. **Martin Vickers** (UCL/Birkbeck) followed this with a practical session in which we real patent specification to examine and to try to interpret. It was entitled "The Manufacture of Venlafaxine Hydrochloride and Crystalline Polymorphs thereof", and he illustrated very well the complexity of the problems involved, in particular whether it had been established that some pairs of samples were identical and others different.

After tea, **Jeremy Cockcroft** returned to present a "Quantitative PXRD Case Study", concerning two livestock disinfectants. The plaintiffs in this case were Antec International, producers of "Virkon", who claimed that "Virucidal Extra", made by Agricultural and Veterinary Supplies Ltd was essentially the same material and infringed their patent. The case was complex and was eventually won by the defendants, although they later failed to be able to patent their own product, as it was deemed to be "not novel"! The afternoon finished with **Mike Glazer** (Oxford) who told of his experiences in American Courts, including the dramatic presentation which he and **Steve Tarling** wrote some years ago, but which is still well worth hearing! Mike finished with his account of the cross-examination of the other side's "expert" witness, who soon showed that he was not all that expert. One question that undermined much of his credibility was, "Are you a member of the American Crystallographic Association?" To which he had to answer that he was not. So be warned! We do, of course, have in this country a much less expensive and equally prestigious organization which we might recommend to our friends.

(to be continued!)

Bob Gould

Electron Density Determination: The Sagamore Conference



THE fifteenth triennial "Sagamore" conference, so-named after the location of the first meeting (1964)

in Upper New York State, USA, will be held in the UK for the first time ever, on the 13th -18th August 2006 at Bosworth Hall Hotel, Warwickshire.

The Sagamore meetings, which usually attract 100-plus participants, ranging from PhD students to leading experts, are run under the auspices of the IUCr's Commission on Charge, Spin and Momentum Densities and cover the wide range of studies of charge density and electronic structure from simple elements to macromolecules. The meetings are traditionally held in countryside retreats, which have ranged from the Canadian National Parks to mountain tops in Japan and lakesides in Poland. There is strong emphasis on informal discussions, and poster

presentations, as well as formal lectures. Bosworth Hall, situated in a country park, provides an attractive out-of-the-way venue in the spirit of Sagamore.

Topics will include: Characterisation of Chemical Bonds, Photo-Crystallography; Density Functional Theory For Charge and Momentum Density; Electronic Density And Structure in Strongly Correlated Systems; Rare Earth and Actinide Magnetism; Charge Density in Macromolecules and New Directions.

The meeting follows on a couple of days after the European Crystallography Meeting in Leuven and the really committed and jet setters will be just in time to get to the International Meeting on Magnetism in Kyoto the following week. It is hoped that travel support and bursaries for early career scientists will be available. Details of registration and submission of abstracts etc will be mounted on the web site www.sagamore2006.com in January 2006.

Pam Thomas



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 December 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 **£600.00** per annum

To apply for Corporate Membership, or if you have any enquiries, please contact:

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BCA Administrative Office
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Oxford Diffraction Ltd
PANalytical
Rigaku MSC

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. The help of Dr Simon Parsons and the IUCr listing is gratefully acknowledged.

14 December 2005

PCG Winter Meeting,
Centre for Science at Extreme
Conditions, Edinburgh.
www.csec.ed.ac.uk/pcg.htm

9-13 January 2006

International Workshop on Crystal
Growth and Characterisation
of Advanced Materials, Anna
University, Chennai, India
(no website given)

25-27 January 2006

Protein Structure and Drug
Discovery, La Jolla, CA, USA.
www.molsoft.com

26-27 January 2006

PX Conference: Advances in
Protein Crystallography,
South San Francisco, CA, USA.
<http://otCrystConf.com>

27 January 2006

HASYLAB Users' Meeting
- Research with Synchrotron
Radiation and FELs,
Hamburg, Germany.
[http://www-hasylab.desy.de/
events/users_meeting.htm](http://www-hasylab.desy.de/events/users_meeting.htm)

14-16 February 2006

PPXRD-5, The 5th Pharmaceutical
Powder X-ray Diffraction
Symposium. Somerset, NJ, USA.
<http://www.icdd.com/ppxrd>

20-23 February 2006

RX 2006: 6th Colloquium on X-
Rays and Matter. Limoges, France.
<http://www.mtg.rx2006.pdf>

6-8 March 2006

Joint Meeting of German and
Polish Associations for Crystal
Growth, Berlin-Adlershof, Germany.
<http://jm2006.dgkk.de/>

6-8 March 2006

Basic and Advanced X-Ray
Powder Diffraction: Pharmaceutical
Applications, Part I Stamford,
CT, USA.
<http://www.assainternational.com>

9-10 March 2006

Basic and Advanced X-Ray
Powder Diffraction: Pharmaceutical
Applications, Part II, Stamford,
CT, USA.
<http://www.assainternational.com>

15-19 March 2006

3rd International Conference
on Structural Analysis of
Supramolecular Assemblies by
Hybrid Methods,
Lake Tahoe, CF, USA.
[http://www.burnham.org/
hybridmethods2006](http://www.burnham.org/hybridmethods2006)

3-6 April 2006

Jahrestagung der deutschen
Gesellschaft für Kristallographie
(DGK), Freiburg/Brsg, Germany.
<http://www.dgk-2006.de>

4-6 April 2006

BCA/BACG Spring Meeting,
University of Lancaster.
<http://www.crystallography.org.uk>

2-5 May 2006

Polymorph Screening: Techniques
and Applications, Mallorca, Spain.
<http://www.assainternational.com>

8-9 May 2006

International Workshop on
the Pharmaceutical Physical
Characterization of the Amorphous
State, Stamford, CT, USA.
<http://www.assainternational.com>

10 May 2006

X-Ray Fluorescence meeting of
general interest, British Geological
Survey, Keyworth, Nottingham.
www.crystallography.org.uk/ig

12 May 2006

Journé Scientifique "E.F.
BERTAUT", CNRS-Polygone,
Grenoble, France.
Contact: hodeau@grenoble.cnrs.fr

22-25 May, 2006

Polymorph Screening: Techniques
and Applications,
Stamford, CT, USA.
<http://www.assainternational.com>

28 May - 3 June 2006

Ninth International Conference
on Synchrotron Radiation
Instrumentation,
Daegu, Exco, Korea.
<http://sri2006.postech.ac.kr/>

9-18 June 2006

The Structure Biology of Large
Molecular Assemblies: the 38th
crystallographic course at the
Ettore Majorana Centre,
Erice, Italy.
crystallalice.org/futuremeet.htm

18-24 June 2006

Eighth International Workshop on
the Physical Characterization of
Pharmaceutical Solids,
Rhodes, Greece.
<http://www.assainternational.com>

9-13 July 2006

The XIII-th International
Conference on Small-Angle
Scattering, Kyoto, Japan.
[http://www2.scphys.kyoto-u.ac.
jp/sas2006/index.html](http://www2.scphys.kyoto-u.ac.jp/sas2006/index.html)

16-21 July 2006

2006 Gordon Research Conference
on Diffraction Methods in
Structural Biology, Bates College,
Lewiston ME, USA.
[http://www.grc.uri.edu/
06sched.htm](http://www.grc.uri.edu/06sched.htm)

10-13 July 2006

Colloque de l'Association Française de Cristallographie, Toulouse, France.
<http://www.afc2006-toulouse.org>

22-27 July 2006

ACA 2006 - The American Crystallographic Association Annual Meeting (2006). Honolulu, HI, USA.
<http://www.hwi.buffalo.edu/aca/>

23-28 July 2006

IMA 2006 - 19th General Meeting of the International Mineralogical Association. Kobe, Japan.
http://www.congre.co.jp/ima2006/index_e.html

30 July - 2 Aug 2006

ZMPC 2006 - International Symposium on Zeolites and Microporous Crystals, Yonago, Japan
<http://www.chem.tottori-u.ac.jp/~zmpc2006/main.html>

4-6 August 2006

ECM-23 Satellite Meeting on Mathematical and Theoretical Crystallography, Leuven, Belgium.
<http://www.lcm3b.uhp-nancy.fr/mathcryst/leuven2006.htm>

6-11 August 2006

ECM-23, European Crystallographic Meeting, Leuven, Belgium.
<http://www.ecm23.be>

13-18 August 2006

Sagamore XV: The fifteenth international conference on Electron Charge Spin and Momentum Densities, Bosworth Hall Hotel, Warwickshire.
<http://www.sagamore2006.com>

27-31 August 2006

1st European Chemistry Congress, Budapest, Hungary.
<http://www.euchems-budapest2006.hu>

1-4 September 2006

EPDIC 10, European Powder Diffraction Conference, Geneva.
<http://www.sgk-sscr.ch/EPDIC10/EPDIC10.html>

3-8 September 2006

13th BCA Summer School in Protein Crystallography, Biochemistry Department, Oxford University.
(website not yet available)

4-8 September 2006

44th European High Pressure Research Group meeting, Prague, Czech Republic.
<http://kfes-80.karlov.mff.cuni.cz/EHPRG/>

10-15 September 2006

Summer School - Ecole thematique: Analyse structurale par diffraction des rayons X, cristallographie sous perturbation, Nancy, France.
<http://www.lcm3b.uhp-nancy.fr/nancy2006/>

13-15 September 2006

ECRS 7 - The 7th European Conference on Residual Stresses, Berlin, Germany.
<http://www.ECRS7.de/>

25-28 September 2006

PNCMI 2006 - The sixth International Workshop on Polarised Neutrons in Condensed Matter Investigations, Berlin, Germany.
<http://www.hmi.de/bensc/pncmi2006/>

2-5 October 2006

Polymorph Screening: Techniques and Applications, Stamford, CT, US.
<http://www.assainternational.com>

16-19 October 2006

Polymorph Screening: Techniques and Applications, Ettlingen, Germany.
<http://www.assainternational.com>

23-26 October 2006

Polymorph Screening: Techniques and Applications, Mallorca, Spain.
<http://www.assainternational.com>

23-25 October 2006

Basic and Advanced X-Ray Powder Diffraction: Pharmaceutical Applications, Part I: Basic crystallography and its application in X-ray powder diffractometry; sample preparation and measurement strategies, Stamford, CT, US.
<http://www.assainternational.com>

26-27 October 2006

Basic and Advanced X-Ray Powder Diffraction: Pharmaceutical Applications, Part II: Basic and advanced structure-solving solutions from X-ray powder patterns. Stamford, CT, US.
<http://www.assainternational.com>

18-19 November 2006

Theoretical Crystallography and Materials Science - Satellite Conference of the AsCA'06 /CrSJ meeting, Tsukuba, Japan.
<http://www.lcm3b.uhp-nancy.fr/mathcryst/asca2006.htm>

14-19 January 2007

International School on Mathematical and Theoretical Crystallography, The University of Havana, Cuba.
<http://www.lcm3b.uhp-nancy.fr/mathcryst/havana2007.htm>

7-17 June 2007

Engineering of Crystalline Materials Properties: the 39th crystallographic course at the Ettore Majorana Centre, Erice, Italy.
<http://www.crystalerice.org/futuremeet.htm>

13-17 August 2007

BSR2007 - Ninth International Conference on Biology and Synchrotron Radiation, Manchester, UK.
<http://www.srs.ac.uk/bsr2007/>

22-27 August 2007

ECM-24, European Crystallographic Meeting, Marrakech, MA.
www.ucam.ac.ma/fssm/ecm24

dSNAP

The University of Glasgow (Theoretical Crystallography group) and Bruker AXS announce the release of dSNAP, a new software to help users automatically classify and visualise the results of database searches using the Cambridge Structural Database.

With the explosion in high quality structural determinations in the area of small molecule crystallography, the problem of efficient mining of the CSD is very relevant for structural chemists. The CSD represents an enormously powerful resource, but faced with more than 300,000 structures, the attempt to extract meaningful chemical information can be daunting. Many search algorithms and data mining

strategies already exist, but with dSNAP we present a method of extracting chemical information from such datasets using cluster analysis.

dSNAP is available free of charge, to receive your free copy please visit www.chem.gla.ac.uk/snap or www.bruker-axs.de. The software is copyrighted and copy-protected, and will initially function only seven days. A free unlock code is required and will be provided on registration.

**Arnt Kern,
BrukerAXS**

(Note - this version of dSNAP is genuinely free, although it is a subset of commercially available software - Ed.)

Good and bad news from the COD

(Of all the crystallographic on-line correspondence that comes my way, without doubt none is as exciting as that on rietveld_j@ill.fr! Some of it is very practical - the enquiries of beginners are sympathetically read and replied to. Some of it is very philosophical, and some is what the communists used to call "frank and comradely". The Committee for Open Data or COD is trying to make as much electronic data as possible freely available. Here is one of their recent communications, following the IUCr in Florence, reproduced by kind permission of the author. - Ed.)

Good:

1300 YES signatures to the "Petition for Open Data in Crystallography".

<http://www.crystallography.net/petition/>

See the poster presented at IUCr XX, Florence :

<http://sdpd.univ-lemans.fr/florence/>

Bad:

None of the monopolistic crystallography toll-databases seem to be ready to turn into the PDB, NCD or AMCSD open models, as was requested by those 1300 petitioners.

Good:

Consequently, the COD decided to keep on and sent a call to the petitioners for obtaining more help :

<http://www.crystallography.net/volunteers.html>

More than 30 positive answers were obtained.

Bad :

ACS, RSC, IUCr are still not giving official permission to download the CIFs available freely at their web sites. The next step will be to ask journals not only to recommend that their authors deposit CIFs with CCDC and Karlsruhe for CSD and ICSD, respectively, but also to recommend that they deposit CIFs with the COD (this would only be fair... don't you think so? The CCDC has already obtained more than 160.000 CIFs in that way, from 84 journals).

Good :

RSC, answering to a letter from the COD, says: "The RSC has a non-exclusive licence from authors to publish CIFs in RSC journals (print and online). The copyright for this material remains with the authors".

from: **Dr Jamie Humphrey**, BA MA CSci CChem FRSC, Editor, Dalton Transactions, Royal Society of Chemistry.

This should open the door to crystallographers afraid to send their CIFs to the COD, believing that they would violate some copyright law.

<http://www.crystallography.net/faq.html>

There is no risk; send us your CIFs at :

<http://www.crystallography.net/upload.html>

Good also :

The volunteers are furnishing a lot of CIFs so that the COD should grow much faster (20.000 entries attained in October). If the flux of data continues at the same rate, the COD should compose 40.000 entries by the end of 2006. This will be fewer than 10% of the entries needed for offering a complete database.

Anyway, let us keep on...

Best regards,

Armel le Bail

COD Advisory Board

<http://www.crystallography.net/>

(Needless to say, they do not have universal support. Several correspondents pointed out that someone has to pay someone to do some work, and one noted that you could get a lot of signatures for free beer on the internet too! But this is an issue of interest to us all, and one that will not go away. - Ed.)



Cursors! NOT Foiled again!

FOLLOWING the suggestions of **Tony North** (*Crystallography News 90, p 5 and 92 p. 4*) and **David Watkin** (*CN 94, p 14*), the Industrial Group has taken the plunge to support the large cursor as a means to get speakers to face audiences at all times!

The ones illustrated above can be looked at on the BCA IG website, (crystallography.org.uk/ig) where they are, of course, in glorious full-colour. David Watkin took some to the IUCr in Florence, where many had the chance to see them in action.

It is possible to download the cursors from the website, and full instructions are given there, including the reminder that ctrl-A in Powerpoint™ will keep the cursor on the screen even when it is inactive. Can you design a better BCA pointer? Send your design to the IG Web Editor. The best submissions will be added to the webpage.

The next task is to get Microsoft to include them automatically!

Dave Taylor (and others!)